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Preface

Dear Reader,

in this book you will find the Proceedings of the Summer School – Conference “Advanced Problems in Mechanics (APM) 2008”. The conference had been started in 1971. The first Summer School was organized by Prof. Ya.G. Panovko and his colleagues. In the early years the main focus of the School was on nonlinear oscillations of mechanical systems with a finite number of degrees of freedom. Since 1994 the Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences organizes the Summer School. The traditional name of “Summer School” has been kept, but the topics covered by the School have been much widened, and the School has been transformed into an international conference. Now it is held under the patronage of the Russian Academy of Sciences. The topics of the conference cover now almost all fields of mechanics, being concentrated around the following main scientific directions:

- aerospace mechanics.
- computational mechanics;
- dynamics of rigid bodies and multibody dynamics;
- fluid and gas;
- mechanical and civil engineering applications;
- mechanics of media with microstructure;
- mechanics of granular media;
- nanomechanics;
- nonlinear dynamics, chaos and vibration;
- molecular and particle dynamics;
- phase transitions;
- solids and structures;
- wave motion.

The Summer School – Conference has two main purposes: to gather specialists from different branches of mechanics to provide a platform for cross-fertilization of ideas, and to give the young scientists a possibility to learn from their colleagues and to present their work. Thus the Scientific Committee encouraged the participation of young researchers, and did its best to gather at the conference leading scientists belonging to various scientific schools of the world.

We believe that the significance of Mechanics as of fundamental and applied science should much increase in the eyes of the world scientific community, and we hope that APM conference makes its contribution into this process.

We are happy to express our sincere gratitude for a partial financial support to Russian Foundation for Basic Research (grants 08-01-06072-g, 08-01-06073-g), Russian government, Russian Academy of Sciences, and St. Petersburg Scientific Center. This support has helped substantially to organize the conference and to increase the participation of young researchers.

We hope that you will find the materials of the conference interesting, and we cordially invite you to participate in the coming APM conferences. A part of the papers published in this Volume is planned to be published in Materials Physics and Mechanics Journal by agreement between APM 2008 organizers and Editors of Materials Physics and Mechanics. You may find the information on the future “Advanced Problems in Mechanics” Schools – Conferences at our websites:

http://www.apm-conf.spb.ru/

With kind regards,

Co-Chairmen of APM 2008

Dmitri A. Indeitsev, Anton M. Krivtsov
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Charged dust particles system response on impulse loading

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Abstract

Peculiarities of dust particle systems behavior at external confinement field under different types of impulse loading are investigated. The interparticle interaction is described by the Yukawa isotropic pair potential. The characteristics of wave propagation generated by external loading are calculated. It is shown that three regimes of structural response of dust particle systems on impulse loading exist.

1 Introduction

Dusty (or complex) plasma has been the subject of intensive investigation for more than ten years[1, 2, 3]. Now it is well known that microparticles of matter in plasma of different origin can acquire high electric charges and exhibit properties of gas, fluid or a solid. Of particular interest was the discovery of so-called plasma crystals ordered structures of dust particles [4, 5, 6]. However, attempts to obtain homogeneous three-dimensional crystal modifications in gas-discharge devices usually used in laboratories ran into serious difficulties such as chainlike ordering of dust particles in the vertical direction and formation of a void in a dust cloud [7, 8, 9]. The difficulties were overcome in recent experiments[10, 11, 12], which allowed researchers to produce so-called Coulomb balls (CB), i.e. almost spherical systems of dust particles of one size. The rf discharge device employed in the experiment differed from an ordinary one by the presence of a heated electrode with a glass box mounted on it in which a CB was formed. The examination of the experimental device has revealed [11] that there are no strong ion fluxes in the glass box, and the gravitational force acting on a dust particle is compensated by the combination of the thermophoretic force produced by the heated cathode and electrostatic force.

More often researchers consider models where particles interacting by one or another law are confined in the harmonic potential $U_{ex}(r) \sim r^2$ whose origin is independent of direction. However, in experiments on the production of CB [10, 11, 12]
the situation is aggravated because the dust system is maintained by forces of different origin. Main purpose of conducted research was investigation of structural response of CB under mechanical loading of outer shell and under instant confinement field changing.

2 Model

We assume that in all considered cases the dust particle interaction has a purely Debye character. Such interaction is chosen because of a good agreement of the simulation results for the CB structure with experimental data [12]. With regard to the close values of interparticle distance $a$ and screening length $\lambda_d$, the choice is well corroborated by the results of a direct experimental study of dust particle interaction in similar cases [13]. Since the dust radius $R$ and length $\lambda_d$ meet the condition $R \ll \lambda_d$, we represent the potential of any dust particle as

$$\phi = \frac{Q}{4\pi \varepsilon_0 r} \left( -\frac{r}{\lambda_d} \right)$$

(1)

where $Q$ is the particle charge. The theoretical estimation of the dust particle charge as the particle size function was carried out within an analytical approach [14, 15], which is a generalization of the known charge theory in the orbit motion limited (OML) approximation 2 in case if ion scattering on neutral atoms is taken into account. Such process at buffer gas pressure 20-120 Pa(Ar) [11] causes a significant dust charge reduction as compared to the estimates obtained in the framework of the OML theory [15]. Besides, in the first approximation we considered for a decrease in the concentration of electrons in the plasma volume owing to their localization on the dust particle surface as well as for the quasineutrality condition[2]. The temperature of the dust systems is determined by the below-given values of the coupling parameter $\Gamma = \frac{Q^2}{4\pi \varepsilon_0 akT}$

3 Simulation results

CB mechanical loading scheme is presented in Fig.1. Loadings were performed by adding center oriented velocity to particles on the outer shell. These velocities varied in the interval from 0.1 sm/s till 10 sm/s, while CB contained from 500 till 5000 dust particles. Dust particles had characteristics of melamine-formaldehyde balls with $4.8\text{mkm}$ diameter and $\rho = 1514 \frac{\text{kg}}{\text{m}^3}$ mass density. Converging spherical waves occur in CB at impulse radial loading. Simulations showed that outer shell oscillations have beat form. The main reason of such response is close values of frequencies of outer shells. Beat amplitude almost decays after few dozen periods. That occurs since synchronization of outer shell oscillations (Fig 2.). As can be seen from Fig. 2, oscillation amplitude increases with loading intensity, while oscillation frequency remains the same. It should be pointed out, that shell oscillation frequency depends
Figure 1: CB with 5000 dust particles in cylindrical coordinates. Outer shell loading scheme.

Figure 2: Time dependence of distance from centre of CB for dust particles on outer shell(1) and shell after outer(2) under uniform loading.
Figure 3: Outer shell oscillation period for CB with different number of DP substantially on CB size. This dependence can be written as $T \approx 0.006 + 0.009 e^{-\frac{N}{1000}}$ (Fig. 3). As can be seen from this formula, limiting period is equal to 0.006 s.

According to intensity of radial loading three regimes of structure response can be formulated. Shell structure saves under small impulse loading (the first regime) (Fig. 4), while under some greater values of loading the shell structure starts destroying and CB melts (the second regime). CB explodes under considerable loading since some dust particles in the central region of CB obtain enough energy in order to leave CB boundaries (the third regime) (Fig. 5). Dust particles obtain that energy from spherical waves converging in the center of CB. It should be noted that under uniform loading of spherical rigid bodies the focusing of shock waves in the center of material

![Figure 4: CB with 2000 dust particles in cylindrical coordinates a) before loading ($\Gamma = 13000$), b) after $t = 2$ s under impulse loading with $V = 0.8 \text{ sm/s}$ ($\Gamma = 800$)]
Note that under uniform loading of a solid body of a spherical shape, the shock wave focusing in the centre of a sample can lead to the huge energy pumping into the central region of material. Here the staging of structural changes can be observed in the sample depending on shock wave intensity and its penetration depth. The structural peculiarities of the CB response at abrupt change of the external electric field are investigated. Under this action, not only amplitude, but also the oscillation frequency of CB shells depends on the value of the electric field jump (Fig.6). In contrast to the first method of loading, even the external force tripling, connected with corresponding value of the electric field jump, does not lead to the CB failure, since the oscillations of all the CB layers are synchronized from the moment of the external force change. Nevertheless, if the pumping energy leads to the sufficient kinetic energy, the shell structure of CB fails.

4 Conclusion

There are three modes of structural response under pulse mechanical radial compression of the external CB shell: a) at low loading rates the shell structure of CB is saved; b) under higher loading rates, the shell structure fails and CB passes into the liquid state; c) at further loading rate increase, the CB fails owing to the wave focusing in its central region and attainment of DP from the central region of kinetic energy sufficient for the emission of particles. The loading intervals, where one or another behavior mode is realized, depend on CB sizes of (quantity of DP). Under pulse radial compression of the external shell with low oscillation rates, CB is initially characterized by pulsations due to the difference in shell oscillation phases, but in a certain period, time of shell oscillation is synchronized. The oscillation frequency of CB shells is described by the exponential law depending on the number of DP. At abrupt change of the external electric confinement field f the shell, CB
oscillates synchronously. Nevertheless, the shell structure of CB will fail, if the acquired energy of DP will be sufficient for their failure. Frequencies and amplitudes of shell oscillations of CB increase when increasing the jump value of the external electric field.

References


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On the Application of Zhilin’s Theory of Simple Shells to Plates made of Functionally Graded Materials

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Abstract

Functionally Graded Materials (FGM) are useful in many modern applications like aircraft and automotive industries. They combine good mechanical properties with low weight, and by this way they show advantages in comparison to the classical materials which are used in the engineering practice. In addition, they have applications in the case of thermal protection coatings. A nitrided steel, for instance, could be also regarded as a FGM. Modern FGMs are constructed for complex requirements, such as the heat shield of a rocket or implants for humans. The gradual transition between the heat or corrosion resistant outer layer (often made of a ceramic material) and the tough metallic base material increases in most cases the life time of the component.

The analysis of plates made of FGMs can be performed on the base of classical theories like the Kirchhoff plate theory. It can be shown that such approach results in some application cases in wrong predictions of the static and dynamic global behavior. At the same time Zhilin’s approach to the theory of shells and plates added with the effective properties concept allows a more precise prediction. Here the case of statics and eigenvibrations of plates made of FGMs is discussed considering the elastic material behavior. This approach can be extended to viscoelastic behavior applying the correspondence principle.

The classical plate theory can be applied to thin plates made from materials like steel. The first theory allowing a satisfying analysis of such plates was elaborated by Kirchhoff [26]. But this approach was connected with various limitations (e.g., constant material properties in the thickness direction). In addition, some mathematical inconsistencies like the order of the governing equation and the number of boundary conditions were accepted. During the last century many suggestions for improvements of the classical plate theory were made [28, 32, 36, 37] among others. The engineering direction of improvements was ruled by applications (e.g., the use of
laminates or sandwiches as the plate material) and so new hypotheses for the derivation of the governing equations were introduced. In addition, some mathematical approaches like power series expansions [24] or asymptotic integration techniques were applied. A conceptional other direction is connected with the direct approach in the plate theory. The paper presents the extension of Zhilin’s direct approach in the shell theory [48] to plates made of functionally graded materials.

An example of a FGM is a porous material with a nonhomogeneous distribution of porosity. Engineering structures made of porous material, especially metal or polymer foams, have different applications in the last decades [11, 12, 13, 17, 19, 31]. A foam is a cellular structure consisting of a solid material (metal or polymer) containing a large volume fraction of gas-filled pores. Such structures are applied in the automotive or airspace industries since they combine low weight, high specific strength, and excellent possibilities to absorb energy. The technical realization is mostly performed as sandwich panels (plates or shells with hard and stiff face sheets and a core layer made of a foam). From the mechanical point of view, a foam is a very complex material which demonstrate many non-classical properties (for example, some foams have a negative Poisson ratio). The foam itself can be modeled as a functionally graded material with mechanical properties changing over the thickness direction. There are two types of metal or polymer foams. One is the closed-cell foam, while the second one is the open-cell foam. The defining characteristic of the foams is the very high porosity: typically well over 80%, 90% and even 98% of the volume consists of void spaces. Examples of closed-cell foams with different porosity are presented in Fig. 1, while the open-cell polymer foam is presented in Fig. 2. In addition, perspective material are composite materials synthesized by filling a metal, polymer or ceramic matrix with hollow particles called microballoons (see, e.g. [18, 21]). This type of foams is named syntactic foam.

![Figure 1: Polymer closed-cell foams with different density (photos by curtesy of Arnim Kraatz, German Institute for Polymers, Darmstadt [27])](image)

Another example of a FGM is a material with thermal coating. Such material obtained by processes in which melted or heated metallic or non-metallic materials are sprayed onto a surface. The thickness of the thermal coating ranges between approximately 20 micrometers and several millimetres depending on the process. The porosity is one of the important characteristics of thermal coating.

Here we present a new theory based on the direct approach in the plate theory
added by the effective properties concept. We consider plates made of foams with highly nonhomogeneous structure through the thickness (see Fig. 3) and apply the theory of plates and shells formulated earlier in [2, 5, 6, 47, 48]. Solving some problems of the global mechanical analysis it will be demonstrated that in some cases the results significantly differ from the results based on the classical Kirchhoff-type theory. The paper is an extension of results presented in [9, 10].

1 Introduction

The Kirchhoff’s plate theory suggested more than 150 years ago [26] was worked out for thin plates made from homogeneous isotropic materials and the case of bending. Introducing the deflection of the midplane the theory is limited by the assumption that each point of the midplane has one independent degree of freedom. Finally, the governing equation for the bending problem can be deduced as

\[ \Delta \Delta w = \frac{q}{D} \]  

(1)
with the deflection \( w \), the surface load \( q \), the Laplacian \( \Delta \) and the bending stiffness \( D \). In the background of this theory one can see very fruitful for engineering applications assumptions: instead of the stresses the stress resultants (averaged stresses in the thickness direction) are introduced – the forces and the moments – which have a clear mechanical interpretation, and the individual mechanical properties can be presented by another averaged property – the bending stiffness which is an effective property combining the Young’s modulus \( E \), the Poisson’s ration \( \nu \) and the plate thickness \( h \)

\[
D = \frac{Eh^3}{12(1-\nu^2)}
\]

On the other hand one observes very rough limitations which are not helpful in modern applications. Examples of such limitations are the thinness hypotheses, the isotropy assumption, the homogeneity assumption, the small deflection assumption and the assumption that the plate behavior (out-of-plane) and the plane stress behavior (in-plane) are decoupled (the last one is ignored in the Kirchhoff’s theory). Focussing the attention on the applications to modern materials (laminates, sandwiches, foams among others) various improvements of the classical theory are suggest. For example, considering sandwich structures with soft core Reissner worked out a theory which takes into account the transverse shear which was neglected by Kirchhoff [37, 38, 39]. Similar governing equations (only some effects were not included) were derived by Mindlin introducing additional degrees of freedom for the points of the midplane [32]. On the classical approaches and their improvements one can get more information, for example, from [3, 4, 6, 7, 24, 25].

Summarizing the monographs and reviews of the last 50 years (see [5, 16, 20, 29, 33, 40, 41, 48]) one can conclude that there are two different possibilities to deduce the plate equations:

- Starting with the three-dimensional equations of solid mechanics the two-dimensional equations are established with the help of some hypotheses or mathematical treatment.

- Introducing a two-dimensional deformable surface the two-dimensional continuum equations are derived by the direct approach.

The advantages/disadvantages are evidently. In the first case we get the constitutive equations by the same way like the other governing equations applying the hypotheses or the mathematical treatment of the, for example in the elastic case, Hooke’s law. The correctness and the approximation degree are often unknown. The direct approach is in this sense better - the two-dimensional equations are physically-based and so exact like the three-dimensional continuum mechanics equations. But the constitutive equations must be identified which is a non-trivial problem. It was shown in [2, 5, 47, 48] among others that the concept of effective properties can support the handling of the identification. The goal of this paper is to show how a two-dimensional theory deduced with the help of the direct approach can be applied to plates made of a FGM.

The discussion will be limited by the consideration of linear elastic and viscoelastic material behavior and the geometrically linear relations. In contrast to the
classical plate theory the deformations will be taken into account like in the theory of laminated plates with unsymmetrical cross-section properties that means the in-plane behavior and the out-of-plane behavior are coupled [8]. The introduced theory is not restricted by the assumption that the transverse shear strains are neglected.

2 Governing Equations

The direct approach is based on the Cosserat theory in continuum mechanics [34, 42]. In continuum mechanics any theory is based on the cutting principle, the assumption “actio = reactio” and some governing equations. Two different models can be introduced: the non-polar or the polar. In the first case only force actions are assumed. From this follows the symmetry of the stress tensor and only translations are considered. But in the basic course of Mechanics the following statements are given: the static equilibrium for forces and moments or the equation of motion as the balance of momentum and the balance of moment of momentum (both are independent relations in the general case, which was shown, for example, by C. Truesdell [46]). For the second model one has force and moment actions too. From this it follows that there are a symmetric and a nonsymmetric stress tensor and translations and rotations can be introduced independently. Now any continuum (three-, two- or one-dimensional) can be introduced by a natural way: geometrical relations (kinematics), material independent balances of mass, momentum, moment of momentum, energy, entropy and the material dependent equations (constitutive equations and evolution equations). Finally, one needs boundary and may be initial conditions.

2.1 Symbolic Presentation of the Equations

Since the direct approach is a natural way to describe the behavior of plates (the stress resultants which are used in most of plate theories can be interpreted as forces and moments) a two-dimensional plate theory which allows to model homogeneous and inhomogeneous plates can be presented as follows.

2.1.1 Linear Basic Equations

Let us introduce two basic assumptions:

**Assumption 1**: The plate (homogeneous or inhomogeneous in transverse direction) can be represented by a deformable surface.

**Assumption 2**: Each material point is an infinitesimal rigid body with 5 degrees of freedom (3 translations and 2 rotations).

The last assumption is introduced for the sake of simplicity.

In addition, the theory presented here is limited by small displacements and rotations and the quadratic strain energy. The basics are presented in [5, 6, 47]. The following governing equations can be introduced:
• First and second Euler’s law (balances of momentum and moment of momentum)

\[ \nabla \cdot T + q = \rho \ddot{u} + \rho \Theta_1 \cdot \ddot{\varphi}, \quad \nabla \cdot M + T_x + m = \rho \Theta_1^T \cdot \dot{u} + \rho \Theta_2 \cdot \dot{\varphi} \]  

Here \( T, M \) are the tensors of forces and moments, \( q, m \) are the surface vectors of loads (forces and moments), \( T_x \) is the vector invariant of the force tensor \([30]\), \( \nabla \) is the nabla (Hamilton) operator (pseudovector), \( u, \varphi \) are the vectors of displacements and the rotations, \( \Theta_1, \Theta_2 \) are the first and the second tensor of inertia, \( \rho \) is the density (effective property of the deformable surface), \((...)^T\) denotes the transposed tensor and \((...)\) the time derivative, respectively.

• Geometrical relations

\[ \mu = (\nabla u \cdot a)^{sym}, \quad \gamma = \nabla u \cdot n + c \cdot \varphi, \quad \kappa = \nabla \varphi \]  

\( a \) is the first metric tensor (plane tensor, that means two-dimensional!), \( n \) is the unit normal vector, \( c = -a \times n \) is the discriminant tensor \([48]\), \( \mu, \gamma \) and \( \kappa \) are the strain tensors (tensor of in-plane strains, vector of transverse shear strains and the tensor of the out-of-plane strains), \((...)^{sym}\) denotes symmetric part of the tensor.

• Boundary conditions

\[ \nu \cdot T = f, \quad \nu \cdot M = l, \quad (l \cdot n = 0) \quad \text{or} \quad u = u^0, \quad \varphi = \varphi^0 \quad \text{along } S \]  

Here \( f \) and \( l \) are external force and couple vectors acting along the boundary of the plate \( S \), while \( u^0 \) and \( \varphi^0 \) are given functions describing the displacements and rotation of the plate boundary, respectively. \( \nu \) is the unit normal vector to \( S \) \( (\nu \cdot n = 0) \). The relations (4) are the static and kinematic boundary conditions. Other types of boundary conditions are possible. For example, the boundary conditions corresponding to a hinge are given by

\[ \nu \cdot M \cdot \tau = 0, \quad u = 0, \quad \varphi \cdot \tau = 0 \]  

Here \( \tau \) is the unit tangent vector to \( S \) \( (\tau \cdot n = \tau \cdot \nu = 0) \).

2.1.2 Two-dimensional Constitutive Equations

Limiting our discussion by the elastic behavior and small strains (for example, rubber-like materials cannot be analyzed by these equations) the following statements for the constitutive modeling can be done. At first, the strain energy can be expanded in a Taylor series limited by quadratic terms. In addition, we assume that the eigenstresses can be neglected (the linear terms in the series are dropped out).

At second, the positive definiteness is guarantied.

• Strain energy of the deformable surface \( W \)

\[ W(\mu, \gamma, \kappa) = \frac{1}{2} \mu : A + \mu : B + \frac{1}{2} \kappa : C + \frac{1}{2} \gamma : \Gamma + \gamma : \gamma : [\Gamma_1 : \mu + \Gamma_2 : \kappa] \]  


A, B, C are 4th rank tensors, \( \Gamma_1, \Gamma_2 \) are 3rd rank tensors, \( \Gamma \) is a 2nd rank tensor of the effective stiffness properties. They depend on the material properties and the cross-section geometry. In the general case the tensors contain 36 different values - a reduction is possible assuming some symmetries.

- Constitutive equations

  - In-plane forces
    \[
    T \cdot a = \frac{\partial W}{\partial \mu} = A \cdot \mu + B \cdot \kappa + \gamma \cdot \Gamma_1
    \] (7)

  - Transverse forces
    \[
    T \cdot n = \frac{\partial W}{\partial \gamma} = \Gamma \cdot \gamma + \Gamma_1 \cdot \mu + \Gamma_2 \cdot \kappa
    \] (8)

  - Moments
    \[
    M^T = \frac{\partial W}{\partial \kappa} = \mu \cdot B + C \cdot \kappa + \gamma \cdot \Gamma_2
    \] (9)

2.2 Basic Equations in Cartesian Coordinates

Let us assume the Cartesian coordinate system \( x_1, x_2 \) (in-plane coordinates) and \( z \) (orthogonal to the midplane). Then the unit normal vectors are \( e_1, e_2 \) and \( n \). With respect to the introduced coordinate system the following representations are valid:

- Displacement and rotation vectors
  \[
  u = u_1 e_1 + u_2 e_2 + w n, \quad \varphi = -\varphi_2 e_1 + \varphi_1 e_2
  \] (10)

  \( u_\alpha (\alpha = 1, 2) \) are the in-plane displacements, \( w \) is the deflection and \( \varphi_\alpha \) are the rotations about the axes \( e_\alpha \), respectively.

- Force and moment tensors
  \[
  T = T_1 e_1 e_1 + T_1 (e_1 e_2 + e_2 e_1) + T_2 e_2 e_2 + T_{1n} e_1 n + T_{2n} e_2 n,
  M = M_1 e_1 e_2 - M_{12} (e_1 e_2 - e_2 e_1) - M_2 e_2 e_1
  \] (11)

  \( T_\alpha, T_{12} \) are the in-plane forces, \( T_{1n} \) are the transverse shear forces, \( M_\alpha \) are the bending moments and \( M_{12} \) is the torsion moment.

- Strain tensors
  \[
  \mu = \mu_1 e_1 e_1 + \mu_{12} (e_1 e_2 + e_2 e_1) + \mu_2 e_2 e_2,
  \gamma = \gamma_1 e_1 + \gamma_2 e_2,
  \kappa = \kappa_1 e_1 e_2 - \kappa_{12} e_1 e_1 + \kappa_{21} e_2 e_2 - \kappa_2 e_2 e_1
  \]

  \( \mu_k \) are the strains, \( \mu_{12} \) is the shear strain, \( \gamma_k \) are the transverse shear strains, \( \kappa_k \) are the bending deformations and \( \kappa_{12} \) is the torsion deformation.
• External loads

\[ q = q_1 e_1 + q_2 e_2 + q_n n, \quad m = -m_2 e_1 + m_1 e_2 \]  

(12)

\( q_k \) are the in-plane forces, \( q_n \) is the transverse force, \( m_k \) are the moments.

How the symmetries of the “microstructure” do affect the physical properties? The answer comes from the Curie-Neumann’s principle in the physics of crystals [35]:

**Curie-Neumann’s principle:** The symmetry group of the reason belongs to the symmetry group of the consequence.

The symmetry group of the “reasons” for the plate is the intersection of:

- Symmetry of the material (fibre-reinforced material, rolled sheets, . . . ),
- Symmetry of the surface shape (shell or plate)
- Symmetry of the internal structure of the plate (laminated plates – symmetry of the stacking sequence with respect to the mid-surface, . . . )

Let us consider orthotropic material behavior and a plane mid-surface. In this case instead of the general form of the effective stiffness tensors one gets [48]

\[
\begin{align*}
A &= A_{11} a_1 a_1 + A_{12} (a_1 a_2 + a_2 a_1) + A_{22} a_2 a_2 + A_{44} a_4 a_4, \\
B &= B_{11} a_1 a_3 + B_{12} a_1 a_4 + B_{22} a_2 a_3 + B_{24} a_2 a_4 + B_{42} a_4 a_2, \\
C &= C_{22} a_2 a_2 + C_{33} a_3 a_3 + C_{34} (a_3 a_4 + a_4 a_3) + C_{44} a_4 a_4, \\
\Gamma &= \Gamma_1 a_1 + \Gamma_2 a_2, \\
\Gamma_1 &= 0, \\
\Gamma_2 &= 0
\end{align*}
\]

with

\[
\begin{align*}
a_1 &= a = e_1 e_1 + e_2 e_2, \\
a_2 &= a = e_1 e_1 - e_2 e_2, \\
a_3 &= c = e_1 e_2 - e_2 e_1, \\
a_4 &= e_1 e_2 + e_2 e_1
\end{align*}
\]

\( e_1, e_2 \) are unit basic vectors. In addition, one obtains the orthogonality condition for \( a_i \) (\( i = 1, 2, 3, 4 \))

\[
\frac{1}{2} a_i \cdot a_j = \delta_{ij}, \quad \delta_{ij} = \begin{cases} 
1, & i = j, \\
0, & i \neq j
\end{cases}
\]

Now the first and the second Euler’s law, the geometrical relations and the constitutive equations take the form (static case):

• First and second Euler’s law

\[
\begin{align*}
T_{1,1} + T_{12,2} + q_1 &= 0, \\
T_{1n,1} + T_{2n,2} + q_n &= 0, \\
M_{1,1} + M_{12,2} - T_{1n} + m_1 &= 0, \\
M_{12,1} + M_{22,2} - T_{2n} + m_2 &= 0
\end{align*}
\]  

(13)
• Boundary conditions (for brevity, we present it when $S$ is a part of line $x_1 = \text{const}$ ($\nu = e_1, \tau = e_2$))

Static boundary conditions

$$T_1 = f_1, \quad T_{12} = f_2, \quad T_n = f_n, \quad M_1 = l_1, \quad M_{12} = l_2$$ (14)

Kinematic boundary conditions

$$u_1 = u_1^0, \quad u_2 = u_2^0, \quad w = w^0, \quad \varphi_1 = \varphi_1^0, \quad \varphi_2 = \varphi_2^0,$$ (15)

Boundary conditions for a hinge

$$M_1 = 0, \quad u_1 = u_2 = w = 0, \quad \varphi_2 = 0$$ (16)

• Geometrical relations

$$\mu_1 = u_{1,1}, \quad \mu_2 = u_{2,2}, \quad \mu_{12} = \frac{1}{2}(u_{1,2} + u_{2,1}),$$

$$\gamma_1 = w_{,1} + \varphi_1, \quad \gamma_2 = w_{,2} + \varphi_2,$$

$$\kappa_1 = \varphi_{1,1}, \quad \kappa_2 = \varphi_{2,2}, \quad \kappa_{12} = \varphi_{2,1}, \quad \kappa_{21} = \varphi_{1,2}$$ (17)

• Constitutive equations

$$T_1 = (A_{11} + 2A_{12} + A_{22})\mu_1 + (A_{11} - A_{22})\mu_2$$

$$- (B_{13} + B_{23} - B_{14} - B_{24})\kappa_1 - (B_{13} + B_{23} + B_{14} + B_{24})\kappa_2,$$

$$T_2 = (A_{11} - A_{22})\mu_1 + (A_{11} - 2A_{12} + A_{22})\mu_2$$

$$- (B_{13} - B_{23} + B_{14} + B_{24})\kappa_1 - (B_{13} - B_{23} + B_{14} - B_{24})\kappa_2,$$

$$T_{12} = 2\mu_{12}A_{44} + (\kappa_{12} + \kappa_{21})B_{42},$$

$$T_{1n} = (\Gamma_1 + \Gamma_2)\gamma_1, \quad T_{2n} = (\Gamma_1 - \Gamma_2)\gamma_2,$$

$$M_1 = (-B_{13} - B_{23} + B_{14} + B_{24})\mu_1 - (B_{13} - B_{23} - B_{14} + B_{24})\mu_2$$

$$+ (C_{33} - 2C_{34} + C_{44})\kappa_1 + (C_{33} - C_{44})\kappa_2,$$

$$M_2 = (-B_{13} + B_{23} + B_{14} + B_{24})\mu_1 - (B_{13} - B_{23} + B_{14} - B_{24})\mu_2$$

$$+ (C_{33} - C_{44})\kappa_1 + (C_{33} + 2C_{34} + C_{44})\kappa_2,$$

$$M_{12} = 2\mu_{12}B_{42} + C_{22}(\kappa_{12} + \kappa_{21})$$

From the last equations can be seen that the $A_{ij}$ are the effective in-plane stiffness tensor components, the $B_{ij}$ are the components of the coupling stiffness tensor, the $C_{ij}$ are the effective plate stiffness tensor components, and the $\Gamma_\alpha$ are the components of the transverse shear stiffness tensor.

2.3 Stiffness Identification – Orthotropic Material Behavior

The individuality of each class of plates in the framework of the direct approach is expressed by the effective properties (stiffness, density, inertia terms, etc.). Let us focus our attention on the stiffness expressions. The identification of the effective
stresses should be performed on the base of the properties of the real material. Let us assume the Hooke’s law as

\[
\begin{align*}
\varepsilon_1 &= \frac{1}{E_1} \sigma_1 - \frac{\nu_{21}}{E_2} \sigma_2 - \frac{\nu_{n1}}{E_n} \sigma_n, \\
\varepsilon_2 &= \frac{1}{E_2} \sigma_2 - \frac{\nu_{12}}{E_1} \sigma_1 - \frac{\nu_{n2}}{E_n} \sigma_n, \\
\varepsilon_n &= \frac{1}{E_n} \sigma_n - \frac{\nu_{1n}}{E_1} \sigma_1 - \frac{\nu_{2n}}{E_2} \sigma_2, \\
\gamma_{12} &= \frac{\tau_{12}}{G_{12}}, \\
\gamma_{n1} &= \frac{\tau_{n1}}{G_{n1}}, \\
\gamma_{2n} &= \frac{\tau_{2n}}{G_{2n}}
\end{align*}
\]  

(18)

with $\nu_{ij} E_j = \nu_{ji} E_i$. Equations (18) are valid in the following cases:

**Case 1:** Homogeneous plates – all properties are constant (no dependency from $z$).

**Case 2:** Inhomogeneous plates (sandwich, multilayered, functionally graded) – all properties are functions of $z$, e.g., $E_i = E_i(z)$.

The identification of the effective properties can be performed with the help of static boundary value problems (two-dimensional, three-dimensional) and the comparison of the forces and moments (in the sense of averaged stresses or stress resultants)

\[
\mathbf{T} = \langle \mathbf{a} \cdot \mathbf{\sigma} \rangle, \quad \mathbf{M} = \langle \mathbf{a} \cdot \mathbf{\sigma z} \cdot \mathbf{c} \rangle
\]

$\mathbf{\sigma}$ is the stress tensor, and $\langle \ldots \rangle$ denotes the integration over the plate thickness.

### 2.3.1 Classical Stiffness Values

**Problem 1: Tension and bending** The following two-dimensional kinematical field is given

\[
\mathbf{u} = D_1 x_1 \mathbf{e}_1 + D_2 x_2 \mathbf{e}_2 - \frac{1}{2} \left( \frac{x_1^2}{R_1} + \frac{x_2^2}{R_2} \right) \mathbf{n}, \quad \mathbf{\varphi} = -\frac{x_2}{R_2} \mathbf{e}_1 + \frac{x_1}{R_1} \mathbf{e}_2
\]

$D_1, D_2, R_1$ and $R_2$ are constants. The two-dimensional strain tensors can be calculated as follows

\[
\mathbf{\varepsilon} = D_1 \mathbf{e}_1 \mathbf{e}_1 + D_2 \mathbf{e}_2 \mathbf{e}_2, \quad \mathbf{\gamma} = 0, \quad \mathbf{\kappa} = \frac{1}{R_1} \mathbf{e}_1 \mathbf{e}_2 - \frac{1}{R_2} \mathbf{e}_2 \mathbf{e}_1
\]
and the two-dimensional constitutive equations can be calculated

\[
T_1 = D_1(A_{11} + 2A_{12} + A_{22}) + D_2(A_{11} - A_{22}) - \frac{1}{R_1}(B_{13} + B_{23} - B_{14} - B_{24}) \quad \text{and} \quad T_2 = D_1(A_{11} - A_{22}) + D_2(A_{11} - 2A_{12} + A_{22}) - \frac{1}{R_1}(B_{13} - B_{23} + B_{14} - B_{24}),
\]

\[
M_1 = \frac{1}{R_1}(C_{33} - 2C_{34} + C_{44}) + \frac{1}{R_2}(C_{33} - C_{44}) \quad \text{and} \quad M_2 = \frac{1}{R_1}(C_{33} - C_{44}) + \frac{1}{R_2}(C_{33} + 2C_{34} + C_{44})
\]

Now assuming the three-dimensional strain tensor components corresponding to the two-dimensional problem

\[
\varepsilon_1 = D_1 + \frac{z}{R_1}, \quad \varepsilon_2 = D_2 + \frac{z}{R_2},
\]

the stress tensor components undo assumptions of the plane stress state and the Hooke’s law (18) are

\[
\sigma_1 = \frac{E_1}{1 - \nu_1 \nu_2}(\varepsilon_1 + \nu_2 \varepsilon_2), \quad \sigma_2 = \frac{E_2}{1 - \nu_1 \nu_2}(\varepsilon_2 + \nu_1 \varepsilon_1)
\]

Finally, the stress resultants can be estimated

\[
T_1 = D_1(\frac{E_1}{1 - \nu_1 \nu_2}) + \frac{1}{R_1} \left( \frac{E_1 z}{1 - \nu_1 \nu_2} \right) + D_2 \left( \frac{\nu_2 E_1^2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_2} \left( \frac{\nu_2 E_1^2}{1 - \nu_1 \nu_2} \right),
\]

\[
T_2 = D_2 \left( \frac{E_2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_2} \left( \frac{E_2 z}{1 - \nu_1 \nu_2} \right) + D_1 \left( \frac{\nu_1 E_2^2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_1} \left( \frac{\nu_1 E_2^2}{1 - \nu_1 \nu_2} \right),
\]

\[
M_1 = D_1 \left( \frac{E_1 z}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_1} \left( \frac{E_1 z^2}{1 - \nu_1 \nu_2} \right) + D_2 \left( \frac{\nu_2 E_1 z^2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_2} \left( \frac{\nu_2 E_1 z^2}{1 - \nu_1 \nu_2} \right),
\]

\[
M_2 = D_2 \left( \frac{E_2 z^2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_2} \left( \frac{E_2 z^2}{1 - \nu_1 \nu_2} \right) + D_1 \left( \frac{\nu_1 E_2 z^2}{1 - \nu_1 \nu_2} \right) + \frac{1}{R_1} \left( \frac{\nu_1 E_2 z^2}{1 - \nu_1 \nu_2} \right)
\]
The comparison of the stress resultants (19) and (20) allows the calculation of the following stiffness tensor components

\begin{align*}
A_{11} &= \frac{1}{4} \left( \frac{E_1 + E_2 + 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right), \\
A_{12} &= \frac{1}{4} \left( \frac{E_1 - E_2}{1 - \nu_{12} \nu_{21}} \right), \\
A_{22} &= \frac{1}{4} \left( \frac{E_1 + E_2 - 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right), \\
B_{13} &= -\frac{1}{4} \left( \frac{E_1 + E_2 + 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right), \\
B_{24} &= \frac{1}{4} \left( \frac{E_1 + E_2 - 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right), \\
C_{33} &= \frac{1}{4} \left( \frac{E_1 + E_2 + 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right), \\
C_{34} &= -\frac{1}{4} \left( \frac{E_1 - E_2}{1 - \nu_{12} \nu_{21}} \right), \\
C_{44} &= \frac{1}{4} \left( \frac{E_1 + E_2 - 2E_1 \nu_{12}}{1 - \nu_{12} \nu_{21}} \right). 
\end{align*}

**Problem 2: Plane shear** Let us assume the two-dimensional kinematical field

\[ \mathbf{u} = S_1 x_2 \mathbf{e}_1 + S_1 x_1 \mathbf{e}_2 - S_2 x_1 x_2 \mathbf{n}, \quad \varphi = -S_2 (x_1 \mathbf{e}_1 - x_2 \mathbf{e}_2) \]

The corresponding three-dimensional strain tensor component is

\[ \gamma_{12} = u_{1,2}^* + u_{2,1}^* = S_1 + S_2 z \]

The comparison of the computed stress resultants yields in

\[ A_{44} = < G_{12} >, \quad B_{42} = - < G_{12} z >, \quad C_{22} = < G_{12} z^2 > \]  \hspace{1cm} (22)

### 2.3.2 Non-classical Stiffness Values

**Problem 3: Torsion** Let us introduce a deformable strip (\(|x_1| \leq l_1, |x_2| < \infty\)) under constant torsion moment at the boundaries \(x_1 = \pm l_1\). Then one gets the two-dimensional kinematical field

\[ \mathbf{u} = u_2(x_1) \mathbf{e}_2, \quad \varphi = -\varphi_1(x_1) \mathbf{e}_1 \]

and the force and moment tensors

\[ \mathbf{T} = (A_{44} u_{2,1} - B_{42} \varphi_{2,1}) \mathbf{a}_4 + (\Gamma_1 - \Gamma_2) \varphi_2 \mathbf{e}_2 \mathbf{n}, \quad \mathbf{M} = (B_{42} u_{2,1} - C_{22} \varphi_{2,1}) \mathbf{a}_2 \]

The dual three-dimensional problem (strip \(|x_1| \leq l_1, |x_2| < \infty, |z| \leq h/2\)) results to the displacements

\[ u_1^* = w^* = 0, \quad u_2^* = u_2^*(x_1, z), \]

the stress tensor

\[ \sigma = G_{12} \frac{\partial u_2^*}{\partial x_1} \mathbf{a}_4 + G_{2n} \frac{\partial u_2^*}{\partial z} (\mathbf{e}_2 \mathbf{n} + \mathbf{n} \mathbf{e}_2) \]
and the equilibrium equation
\[ G_{12} \frac{\partial^2 u_2^*}{\partial x_1^2} + \frac{\partial}{\partial z} \left( G_{2n} \frac{\partial u_2^*}{\partial z} \right) = 0 \]

The solution with respect to the boundary conditions \( \sigma_n = \tau_{1n} = \tau_{2n} = 0 \) at \( |z| = h/2 \) can be obtained by the following Fourier’s ansatz: \( u_2^*(x_1, z) = X(x_1)Z(z) \) which yields a Sturm-Liouville problem
\[ \frac{d}{dz} \left( G_{2n} \frac{dZ}{dz} \right) + \lambda_2^2 G_{12} Z = 0, \quad \frac{dZ}{dz} \bigg|_{z=\pm h/2} = 0 \]

and
\[ \frac{d^2 X}{dx_1^2} - \lambda_2^2 X = 0 \]

With the lowest non-trivial positive solution \( \lambda_* \) one obtains
\[ X(x_1) = B \frac{\sinh \lambda_* x_1}{\lambda_* \cosh \lambda_* l_1} \quad \text{and} \quad u_2^* = BZ(z) \frac{\sinh \lambda_* x_1}{\lambda_* \cosh \lambda_* l_1} \]

Finally, after comparison the two-dimensional and the three-dimensional solutions one gets
\[ \lambda = \lambda_* = \sqrt{\frac{(\Gamma_1 - \Gamma_2)A_{44}}{A_{44}C_{22} - B_{42}^2}} \]  \hspace{1cm} (23)

\( \Gamma_{12} \) and \( M_{12} \) obtained by the two-dimensional and the three-dimensional approaches are in a full agreement. For the kinematical fields one gets
\[ < G_{12}(u_2^* - u_2 - z\varphi_2)^2 > = \min(u_2, \varphi_2) \]

\[ u_2 = \frac{M_{12} < G_{12}z >}{< G_{12} > < G_{12}z^2 > - < G_{12}z^2 > \lambda_* \cosh \lambda_* l_1} \]
\[ \varphi_2 = \frac{-M_{12} < G_{12} > < G_{12}z^2 > - < G_{12}z^2 > \lambda_* \cosh \lambda_* l_1}{< G_{12} > < G_{12}z^2 > - < G_{12}z^2 > \lambda_* \cosh \lambda_* l_1} \]

In addition, one has to analyze the similar problem for the second direction in the two-dimensional case \( |x_1| < \infty, |x_2| \leq l_2 \) as in the three-dimensional case \( |x_1| < \infty, |x_2| \leq l_2, |z| \leq h/2 \) with the constant torsion moment at the boundaries \( |x_2| \leq l_2 \). Now one obtains
\[ \frac{d}{dz} \left( G_{1n} \frac{d\tilde{Z}}{dz} \right) + \eta^2 G_{12} \tilde{Z} = 0, \quad \frac{d\tilde{Z}}{dz} \bigg|_{z=\pm h/2} = 0, \quad \eta = \sqrt{\frac{(\Gamma_1 + \Gamma_2)A_{44}}{A_{44}C_{22} - B_{42}^2}} \]  \hspace{1cm} (24)

Considering Eq. (23) and the last of the Eqs (24) we get the following expressions for the transverse shear stiffness tensor components
\[ \Gamma_1 = \frac{1}{2}(\lambda^2 + \eta^2) \frac{A_{44}C_{22} - B_{42}^2}{A_{44}}, \quad \Gamma_2 = \frac{1}{2}(\eta^2 - \lambda^2) \frac{A_{44}C_{22} - B_{42}^2}{A_{44}} \]  \hspace{1cm} (25)
2.4 Special Case – Isotropic Behavior

In the case of isotropic material behavior one has to set in Eq. (18)

\[ E_1 = E_2 = E_n = E(z), \quad \nu_{ij} = \nu(z), \quad G_{12} = G_{n1} = G_{2n} = G(z) = \frac{E(z)}{2(1 + \nu(z))} \]

Instead of (21)–(25) the following non-zero components of the stiffness tensors are valid:

the in-plane stiffness tensor components

\[ A_{11} = \frac{1}{2} \langle E \rangle, \quad A_{22} = \frac{1}{2} \langle E \rangle = A_{44} = < G >, \]  
\[ (26) \]

the coupling stiffness tensor components

\[ B_{13} = -\frac{1}{2} \langle E \rangle, \quad B_{24} = \frac{1}{2} \langle E \rangle = -B_{42} = < Gz >, \]  
\[ (27) \]

the plate stiffness tensor components

\[ C_{33} = \frac{1}{2} \langle E \rangle, \quad C_{44} = \frac{1}{2} \langle E \rangle = C_{22} = < Gz >, \]  
\[ (28) \]

the transverse shear stiffness tensor components

\[ \Gamma_1 = \lambda^2 \frac{A_{44}C_{22} - B_{42}^2}{A_{44}} \]  
\[ (29) \]

with \( \lambda \) following from

\[ \frac{d}{dz} \left( G \frac{dz}{dz} \right) + \lambda^2 Gz = 0, \quad \frac{dz}{dz} \bigg|_{z=\frac{h}{2}} = 0 \]  
\[ (30) \]

3 Examples of Effective Stiffness Properties

3.1 Homogeneous Plate

The simplest test for the correctness of the estimated stiffness properties is the homogeneous isotropic plate. The basic geometrical property is the plate thickness \( h \), the plate is symmetrically with respect to the mid-plane which results in \( B \equiv 0 \).

Let us assume the following material data: the Young’s modulus and the shear modulus \( E, G = E/2(1 + \nu) \) and \( \nu \) – the Poisson’s ratio. All material properties are constant, that means they do not depend on the thickness coordinate \( z \). The non-zero components of the classical stiffness tensors are

\[ A_{11} = \frac{Eh}{2(1 - \nu)}, \quad A_{22} = \frac{Eh}{2(1 + \nu)} = A_{44} = Gh, \]
\[ C_{33} = \frac{Eh^3}{24(1 - \nu)}, \quad C_{44} = \frac{Eh^3}{24(1 + \nu)} = C_{22} = \frac{Gh^3}{12} \]
The classical plate (bending) stiffness follows as
\[ C_{33} + C_{44} = \frac{Eh^3}{12(1-\nu^2)} \]  
(31)

and can be found in the textbooks, e.g. [45]. The transverse shear stiffness follows from
\[ \Gamma = \lambda^2 C_{22} \]
with
\[ \frac{d^2 Z}{dz^2} + \lambda^2 Z = 0, \quad \frac{dZ}{dz} \bigg|_{z=\frac{h}{2}} = 0 \]

The solution \( \cos \lambda z = 0 \) yields to the smallest eigenvalue \( \lambda = \frac{\pi}{h} \) and finally one obtains
\[ \Gamma = \frac{\pi^2 G h^3}{h^2} = \frac{\pi^2 G h}{12} \]
\( \pi^2/12 \) is a factor which is similar to the shear correction factor which was first introduced by Timoshenko [44] in the theory of beams. Here this factor is a result of the non-classical establishments of the transverse shear stiffness. Comparing this value with the Mindlin’s estimate \( \pi^2/12 \) [32] and Reissner’s estimate \( 5/6 \) [37] one concludes that the direct approach yields in the same value like in the Mindlin’s theory (note that Mindlin’s shear correction is based on the solution of a dynamic problem, here was used the solution of a static problem). The Reissner’s value slightly differs.

The density and the rotatory inertia coefficient are
\[ \rho = \rho_0 h, \quad \Theta = \frac{\rho_0 h^3}{12}. \]  
(32)

### 3.2 Classical Sandwich Plate in Reissner’s Sense

Now we assume the following geometry: \( h_c \) is the core thickness and \( h_f \) the thickness of the face sheets \( (h_c \gg h_f) \). The material properties of the core and the face sheets are \( E_c, G_c, G_f \) with \( E_c \ll E_f, G_c \ll G_f \). We have again a symmetry with respect to the mid-plane that means \( B = 0 \). With the thickness \( h = h_c + h_f \) one gets

\[ A_{11} = \frac{1}{2} \left( \frac{E_f h_f}{1-\nu_f} + \frac{E_c h_c}{1-\nu_c} \right), \quad A_{22} = \frac{1}{2} \left( \frac{E_f h_f}{1+\nu_f} + \frac{E_c h_c}{1+\nu_c} \right) = A_{44}, \]
\[ C_{33} = \frac{1}{24} \left[ \frac{E_f (h^3 - h_c^3)}{1-\nu_f} + \frac{E_c h_c^3}{1-\nu_c} \right], \quad C_{44} = \frac{1}{24} \left[ \frac{E_f (h^3 - h_c^3)}{1+\nu_f} + \frac{E_c h_c^3}{1+\nu_c} \right] = C_{22} \]

The bending stiffness results to
\[ C_{33} + C_{44} = \frac{1}{12} \left[ \frac{E_f (h^3 - h_c^3)}{1-\nu_f^2} + \frac{E_c h_c^3}{1-\nu_c^2} \right] \]
The transverse shear stiffness can be computed by

\[ Z(z) = \begin{cases} 
A \cos \lambda \left( z - \frac{h}{2} \right) & \frac{h_c}{2} \leq z \leq \frac{h}{2}, \\
B \sin \lambda z & |z| \leq \frac{h_c}{2}, \\
-A \cos \lambda \left( z + \frac{h}{2} \right) & -\frac{h}{2} \leq z \leq -\frac{h_c}{2}.
\end{cases} \]

This yields in a transcendent equation

\[ \mu \cos \frac{\lambda h_f}{2} \cos \frac{h_c}{2} - \sin \frac{\lambda h_f}{2} \sin \frac{h_c}{2} = 0 \]

or

\[ \mu \cos \gamma (1 - \alpha) \cos \gamma \alpha - \sin \gamma (1 - \alpha) \sin \gamma \alpha = 0, \]

with

\[ \gamma = \lambda \frac{h}{2}, \quad \alpha = \frac{h_c}{h} \]

\( \mu \) and \( \alpha \) take the values \( 0 \leq \mu = G_c/G_f < \infty \) and \( 0 \leq \alpha \leq 1 \). A typical sandwich structure has a very weak core. Then the bending stiffness can be approximated by

\[ C_{33} + C_{44} = \frac{1}{4} E_f h^2 h_f, \quad (33) \]

the transverse shear stiffness by \( \Gamma = G_c h_f \). This solution was obtained first by Reissner [39].

The density and the rotatory inertia coefficient are

\[ \rho = \rho_c h_c + \rho_{f0} h_f, \quad \Theta = \frac{\rho_c h_c^3}{12} + \frac{\rho_{f0} (h^3 - h_c^3)}{12}. \quad (34) \]

### 3.3 Functionally Graded Material

Functionally graded materials are composite materials where the composition or the microstructure are locally varied so that a certain variation of the local material properties is achieved. In this paragraph we consider small deformations of a functionally graded plate made of a foam. For the panel made from a porous foams the distribution of the pores over the thickness can be inhomogeneous (see, for example, Fig. 3). Let us introduce \( h \) as the thickness of the panel, \( \rho_s \) as the density of the bulk material and \( \rho_p \) as the minimum value of the density of the foam. Examples of distribution functions of the porosity are shown in Fig. 4.

#### 3.3.1 Linear Symmetric Distribution

Let us introduce a FGM with changing mechanical properties. The material is assumed to be isotropic. The mechanical properties are changing linear and the changes are symmetrically with respect to the mid-plane. In addition, it will be
suggested that the changing properties are related to the Young’s and the shear modulus. To make the calculation as simple as possible the Poisson’s ratio is set to be approximately constant ($\nu \approx$ const). Then the distribution of the Young’s and the shear modulus can be given as

$$E(z) = E_o \left[ \frac{2}{h} |z| + \frac{E_m}{E_o} \left( 1 - \frac{2}{h} |z| \right) \right], \quad G(z) = G_o \left[ \frac{2}{h} |z| + \frac{G_m}{G_o} \left( 1 - \frac{2}{h} |z| \right) \right]$$  \hspace{1cm} (35)

Here the index o denotes the value on the outer surfaces ($z = \pm h/2$) and m at the mid-plane ($z = 0$). Due to the symmetry to the mid-plane $BBB \equiv 000$. The classical stiffness tensor components can be computed analytically

$$A_{11} = \frac{E_o h}{4(1-\nu)} \left( 1 + \frac{E_m}{E_o} \right), \quad A_{22} = \frac{E_o h}{4(1+\nu)} \left( 1 + \frac{E_m}{E_o} \right) = A_{44},$$

$$C_{33} = \frac{E_o h^3}{96(1-\nu)} \left( 3 + \frac{E_m}{E_o} \right), \quad C_{44} = \frac{E_o h^3}{96(1+\nu)} \left( 3 + \frac{E_m}{E_o} \right) = C_{22}$$  \hspace{1cm} (36)

The transverse shear stiffness tensor components results from

$$\Gamma_1 = \lambda^2 C_{22} = \lambda^2 G_o h^3 \frac{G_m}{48} \left( 3 + \frac{G_m}{G_o} \right)$$

with $\lambda$ following from

$$\frac{d}{dz} \left[ G(z) \frac{dZ}{dz} \right] + \lambda^2 G(z) Z = 0, \quad \frac{dZ}{dz} \bigg|_{|z|=\frac{h}{2}} = 0$$

Instead of $G(z)$ one has to take the second equation of (35). This spectral problem was solved numerically by using the shooting method [43]. Dependence normalized $\Gamma_1$ versus $g_m \equiv G_m/G_o$ is shown in Fig. 5 (a) (solid line), the Reissner’s solution is presented by the dashed line.

The Reissner’s solution gives understated values of the transverse stiffness when the difference between elastic moduli is significantly big. On the other hand, the Reissner’s solution gives overstated values when the elastic moduli are approximately the same. The Reissner’s formula gives us good coincidence with our results only when the $g_m \approx 0.6$. 

![Figure 4: Distribution of the porosity $V$: a) symmetric; b) non-symmetric](image-url)
The transverse shear stiffness can be estimated as

\[
\Gamma_1 = \lambda^2 \frac{A_{44} C_{22} - B_{42}^2}{A_{44}} = \frac{\lambda^2}{72} \frac{[3(G_u + G_l)^2 - (G_u - G_l)^2]h^3}{G_u + G_l}
\]

with \( \lambda \) following from

\[
\frac{d}{dz} \left[ G(z) \frac{dZ}{dz} \right] + \lambda^2 G(z) Z = 0, \quad \frac{dZ}{dz} \bigg|_{z = \frac{h}{2}} = 0
\]

Instead of \( G(z) \) one has to take the second equation of (37). The solution of this spectral problem may be written by using Kummer functions [1]. Dependence \( \Gamma_1 \) versus \( g_l \equiv G_l/G_u \) is shown in Fig. 5 (b). It is easy to prove that a good approximation of this curve is given by

\[
\frac{\Gamma_1}{G_u h^3} = \frac{\pi^2}{12} + 0.416(1 - g_l).
\]
3.3.3 Nonlinear Symmetric Distribution

In this section we consider the small deformations of functionally graded plate made of metallic or polymer foams. For the panel made from porous metallic foams the distribution of the pores over the thickness can be inhomogeneous. Let us introduce \( h \) as the thickness of the panel, \( \rho_s \) as the density of the bulk material and \( \rho_p \) as the minimum value of the density of the foam. For the description of the symmetric distribution of the porosity we assume the power law [9]

\[
V(z) = \alpha + (1 - \alpha) \left| \frac{2z}{h} \right|^n,
\]

(38)

where \( \alpha = \rho_p/\rho_s \), \( n \) is the power. \( n = 0 \) corresponds to the homogeneous plate, for \( n = 1 \) we have the linear distribution of the porosity through the thickness. The distribution can be established, for example, if the plate is made of two symmetric layers. If \( n > 1 \) one has a more complex distribution. If \( n \gg 1 \) the plate core has an approximately constant porosity, but the distribution of the density in the face layers is significant inhomogeneous. Examples of the distribution functions are shown in Fig. 4 (a) for \( n = 0, 1, 10, 50 \) with \( \alpha = 0.1 \).

The elastic properties of metallic foams highly depend on the porosity and the cell structure. The dependence of Young’s modulus and shear modulus on the porosity is given by the power law [11, 19]

\[
\frac{E_p}{E_s} \sim \alpha^m, \quad \frac{G_p}{G_s} \sim \alpha^m,
\]

(39)

where \( E_p \) and \( G_p \) are the Young modulus and the shear modulus of the foam, respectively, \( E_s \) and \( G_s \) are the Young’s modulus and the shear modulus of the material which is used to synthesize the foam. The value \( m \) depends on the structure of the foam. For the closed-cell foam \( m = 1 \), for the open-cell foam \( m \approx 2 \). For the isotropic case, the graphs of the normalized \( A_{11}, A_{44}, C_{33}, C_{22} \) are given in Fig. 6. Here are assumed \( m = 2, \alpha = 0.1, \nu = 0.3 \).

To obtain the dependence of transverse shear stiffness we have to solve Eq. (30). The solution of the spectral problem (30) was performed numerically by using the shooting method [43]. The values of normalized \( \Gamma_1 \) versus \( n \) are given in Fig. 7.

The density and the rotatory inertia coefficient are

\[
\frac{1}{\rho_s} = \alpha h + \frac{(1 - \alpha) h}{n + 1}, \quad \frac{1}{\rho_s} = \frac{1}{12} \alpha h^3 + \frac{1}{4} \frac{(1 - \alpha) h^3}{3 + n}
\]

(40)

From (40) one can see that for \( n \gg 1 \) \( \rho \approx \rho_p h \) and \( \Theta \approx \frac{1}{12} \rho_p h^3 \) which coincide with (34) if \( h_f \to 0 \).

3.3.4 Nonlinear Non-symmetric Distribution

For the description of the non-symmetric distribution of the porosity we assume again the power law

\[
V(z) = \alpha + (1 - \alpha) \left( \frac{x + h/2}{h} \right)^n
\]

(41)
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Examples of the distribution are shown in Fig. 4 (b) for $n = 0, 10, 50$ with $\alpha = 0.1$. For the isotropic case, the graphs of the normalized stiffness $A_{11}, A_{44}, C_{33}, C_{22}, B_{13}, B_{24}$ are given in Fig. 8. The values of normalized $\Gamma_1$ versus $n$ are given in Fig. 9.

Equations of a Symmetric Orthotropic Plate

Let us consider the equilibrium equations of a symmetric orthotropic plate. In this case Eqs (13) split into two parts: the in-plane problem for tangential displacements $u_1$ and $u_2$, and the bending problem for the $w, \varphi_1$ and $\varphi_2$, respectively.

The constitutive equations for a symmetric orthotropic plate can be given as
follows

\[
T_1 = (A_{11} + 2A_{12} + A_{22}) \mu_1 + (A_{11} - A_{22}) \mu_2,
\]

\[
T_2 = (A_{11} - A_{22}) \mu_1 + (A_{11} - 2A_{12} + A_{22}) \mu_2,
\]

\[
T_{12} = 2A_{44} \mu_{12},
\]

\[
T_{1n} = (\Gamma_1 + \Gamma_2) \gamma_1, \quad T_{2n} = (\Gamma_1 - \Gamma_2) \gamma_2,
\]

\[
M_1 = (C_{33} - 2C_{34} + C_{44}) \kappa_1 + (C_{33} - C_{44}) \kappa_2,
\]

\[
M_2 = (C_{33} - C_{44}) \kappa_1 + (C_{33} + 2C_{34} + C_{44}) \kappa_2,
\]

\[
M_{12} = C_{22}(\kappa_{12} + \kappa_{21})
\]

In Cartesian coordinates with the geometrical relations (17) the equations

\[
T_{1,1} + T_{12,2} + q_1 = 0, \quad T_{12,1} + T_{2,2} + q_2 = 0
\]

reduce to the form

\[
(A_{11} + 2A_{12} + A_{22})u_{1,11} + (A_{11} - A_{22})u_{2,21} + A_{44}(u_{1,21} + u_{2,11}) + q_1 = 0,
\]

\[
(A_{11} - A_{22})u_{1,12} + (A_{11} - 2A_{12} + A_{22})u_{2,22} + A_{44}(u_{1,22} + u_{2,12}) + q_2 = 0
\]

The equation

\[
T_{1n,1} + T_{2n,2} + q_n = 0,
\]

has the following form

\[
(\Gamma_1 + \Gamma_2)w_{1,11} + (\Gamma_1 - \Gamma_2)w_{2,21} + (\Gamma_1 + \Gamma_2)\varphi_{1,1} + (\Gamma_1 - \Gamma_2)\varphi_{2,2} + q_n = 0
\]

The equations

\[
M_{1,1} + M_{12,2} - T_{1n} + m_1 = 0, \quad M_{12,1} + M_{2,2} - T_{2n} + m_2 = 0
\]

result in

\[
(C_{33} - 2C_{34} + C_{44})\varphi_{1,11} + (C_{33} - C_{44})\varphi_{2,21} + C_{22}(\varphi_{1,22} + \varphi_{2,12}) - (\Gamma_1 + \Gamma_2)\varphi_1 - (\Gamma_1 + \Gamma_2)w_{1,1} + m_1 = 0,
\]

\[
(C_{33} + 2C_{34} + C_{44})\varphi_{2,22} + (C_{33} - C_{44})\varphi_{1,12} + C_{22}(\varphi_{1,21} + \varphi_{2,11}) - (\Gamma_1 - \Gamma_2)\varphi_2 - (\Gamma_1 - \Gamma_2)w_{2,2} + m_2 = 0
\]
4.1 One-dimensional Case

First, let us consider the bending of a rectangular plate when \( q_1 = 0, q_2 = 0, q_n = q(x), m_1 = m_1(x), m_2 = 0 \). Then we can assume that \( u_1 = u_2 = 0, w = w(x), \varphi_1 = \varphi(x), \varphi_2 = 0 \). Equation (46) reduces to

\[
(\Gamma_1 + \Gamma_2)w'' + (\Gamma_1 + \Gamma_2)\varphi' + q = 0,
\]

where \((\ldots)'\) denotes \((\ldots),_1\).

Equations (48) reduce to one equation

\[
(C_{33} - 2C_{34} + C_{44})\varphi'' - (\Gamma_1 + \Gamma_2)\varphi - (\Gamma_1 + \Gamma_2)w' + m_1 = 0
\]

Let us transform Eqs (49) and (50) to one equation with respect to \( w \). After some manipulations we obtain

\[
(C_{33} - 2C_{34} + C_{44})w''' = q - \frac{(C_{33} - 2C_{34} + C_{44})}{\Gamma_1 + \Gamma_2}q'' + m_1'
\]

If we consider the other one-dimensional case when \( q_1 = 0, q_2 = 0, q_n = q(y), m_1 = 0, m_2 = m_2(y) \), then we can assume that \( u_1 = u_2 = 0, w = w(y), \varphi_2 = \varphi(y), \varphi_1 = 0 \). Finally, Eqs (46) and (48) reduce to

\[
(\Gamma_1 - \Gamma_2)w'' + (\Gamma_1 - \Gamma_2)\varphi' + q_n = 0,
\]

\[
(C_{33} + 2C_{34} + C_{44})\varphi'' - (\Gamma_1 - \Gamma_2)\varphi - (\Gamma_1 - \Gamma_2)w' + m_2 = 0,
\]

where now \((\ldots)'\) denotes \((\ldots),_2\).

By using the same manipulations as in the previous case we obtain the equation with respect to \( w \)

\[
(C_{33} + 2C_{34} + C_{44})w''' = q - \frac{(C_{33} + 2C_{34} + C_{44})}{\Gamma_1 - \Gamma_2}q'' + m_2'
\]

Equations (51) or (54) differ from one-dimensional variant of Eq. (1). If \( m_1 = 0 \) or \( m_2 = 0 \) and \( \Gamma_1 + \Gamma_2 \rightarrow \infty \) or \( \Gamma_1 - \Gamma_2 \rightarrow \infty \) one gets the Kirchhoff’s plate equation with \( D = C_{33} - 2C_{34} + C_{44} \) or with \( D = C_{33} + 2C_{34} + C_{44} \).  

4.2 Two-dimensional Case

Let us eliminate the functions \( \varphi_1 \) and \( \varphi_2 \) from Eqs (46) and (48). For brevity, let us assume that \( m_1 = 0, m_2 = 0 \). By using operator notations, Eqs (48) may be rewritten in the form

\[
L_{11} \varphi_1 + L_{12} \varphi_2 = b_1 w, \quad L_{21} \varphi_1 + L_{22} \varphi_2 = b_2 w,
\]

where

\[
L_{11} = (C_{33} - 2C_{34} + C_{44})\partial_1^2 + C_{22}\partial_2^2 - \Gamma_1 - \Gamma_2, \\
L_{22} = (C_{33} + 2C_{34} + C_{44})\partial_1^2 + C_{22}\partial_2^2 - \Gamma_1 + \Gamma_2, \\
L_{21} = L_{12} = (C_{33} + C_{22} - C_{44})\partial_1\partial_2, \\
b_1 = (\Gamma_1 + \Gamma_2)\partial_1, \quad b_2 = (\Gamma_1 - \Gamma_2)\partial_2, \\
\partial_{\alpha}(\ldots) \equiv (\ldots),_\alpha, \quad \alpha = 1, 2
\]
From (55) we obtain the relations $L\phi_1 = L_1 w$, $L\phi_2 = L_2 w$, where

$$L = L_{11} L_{22} - L_{12} L_{21}, \quad L_1 = L_{22} b_1 - L_{12} b_2, \quad L_2 = L_{11} b_2 - L_{21} b_1$$

Using operator notations Eq. (46) can be rewritten as follows

$$L_w w + b_1 \phi_1 + b_2 \phi_2 + q_n = 0,$$

where $L_w = (\Gamma_1 + \Gamma_2) \partial_1^2 + (\Gamma_1 - \Gamma_2) \partial_2^2$.

Then we obtain one differential equation of 6th order with respect to $w$

$$L w \partial^2_1 + L_1 w \partial_1 + L_2 w \partial_2 + q_n = 0 \quad (56)$$

### 4.3 Two-dimensional Case of an Isotropic Plate

For the isotropic plate we have that $C_{22} = C_{44}$, $C_{34} = 0$, $\Gamma_2 = 0$. Then

$$L_{11} = (C_{33} + C_{44}) \partial_1^2 + C_{44} \partial_2^2 - \Gamma_1, \quad L_{22} = (C_{33} + C_{44}) \partial_2^2 + C_{44} \partial_1^2 - \Gamma_1,$$

$$L_{21} = L_{12} = C_{33} \partial_1 \partial_2,$$

$$b_1 = \Gamma_1 \partial_1, \quad b_2 = \Gamma_1 \partial_2,$$

and

$$L = [(C_{33} + C_{44}) \partial_1^2 + C_{44} \partial_2^2 - \Gamma_1] [(C_{33} + C_{44}) \partial_2^2 + C_{44} \partial_1^2 - \Gamma_1] - C_{33} \partial_1^2 \partial_2^2,$$

$$L_1 = \Gamma_1 [(C_{33} + C_{44}) \partial_1^2 + C_{44} \partial_2^2 - \Gamma_1] \partial_1 + \Gamma_1 C_{33} \partial_1 \partial_2^2,$$

$$L_2 = -\Gamma_1 C_{33} \partial_1^2 \partial_2 + \Gamma_1 [(C_{33} + C_{44}) \partial_2^2 + C_{44} \partial_1^2 - \Gamma_1] \partial_2$$

Finally, the bending equation (56) has the form

$$(C_{33} + C_{44}) \Delta \Delta w = \partial_1 m_1 + \partial_2 m_2 - \frac{C_{33} + C_{44}}{\Gamma_1} \Delta q_n + q_n \quad (57)$$

If $m_1 = m_2 = 0$ and $\Gamma_1 \to \infty$ one gets the Kirchhoff’s plate equation with the bending stiffness $D = C_{33} + C_{44}$.

### 5 Bending of a Plate made of FGM

In this case one gets a decoupling of the in-plane and the plate state. Let us assume the Kirchhoff’s plate bending. The governing equation (1) preserves the same form – only instead of the bending stiffness $D$ the effective bending stiffness with respect to (28) must be introduced as follows

$$D_{eff} = C_{33} + C_{44},$$

and the external load $q$ should be replaced by

$$\partial_1 m_1 + \partial_2 m_2 - \frac{D_{eff}}{\Gamma_1} \Delta q_n + q_n$$
31 On the Application of Zhilin’s Theory of Simple Shells

To analyze the influence of the transverse shear stiffness on the deflection of the plate let us consider a bending of a rectangular plate made of functionally graded material. For brevity, let us assume that \( m_1 = m_2 = 0, x_1 \in [0, a], x_2 \in [0, b] \), where \( a \) and \( b \) are the length and width of the plate. Using the assumption \([11, 19]\) that \( \nu = \text{const} \) and the Eqs (28), (29) are valid, we can rewrite Eq. (57) in the following form

\[
D_{\text{eff}} \Delta \Delta w = q_n - \frac{1}{1 - \nu} \frac{1}{\lambda^2 h^2} \Delta q_n \tag{59}
\]

Introducing dimensionless variables by formulas

\[
\ddot{w} = h^{-1} w, \quad \ddot{x}_1 = h^{-1} x_1, \quad \ddot{x}_2 = h^{-1} x_2, \quad \ddot{x}_1 \in \left[0, \frac{a}{h}\right], \quad \ddot{x}_2 \in \left[0, \frac{b}{h}\right], \quad q = \frac{q_n h^3}{D_{\text{eff}}},
\]

Equation (59) transforms to

\[
\Delta \Delta \ddot{w} = \ddot{q} - \frac{2}{1 - \nu} \frac{1}{\lambda^2 h^2} \Delta \ddot{q} \tag{60}
\]

Here \( \Delta = \frac{\partial^2}{\partial \ddot{x}_1^2} + \frac{\partial^2}{\partial \ddot{x}_2^2} \).

Let us consider a sinusoidal load \( \ddot{q} = Q \sin \frac{\pi h \ddot{x}_1}{a} \sin \frac{\pi h \ddot{x}_2}{b} \) (\( Q = \text{const} \)) and the boundary conditions of type (16). Then the solution of Eq. (60) is given by

\[
\ddot{w} = K \frac{\eta^2}{Q} \sin \frac{\pi h \ddot{x}_1}{a} \sin \frac{\pi h \ddot{x}_2}{b}, \quad \eta = 1 + \frac{2 \eta}{1 - \nu} \frac{1}{\lambda h^2}, \quad K = \left( \frac{\pi h}{a} \right)^2 + \left( \frac{\pi h}{b} \right)^2 \tag{61}
\]

For the Kirchhoff’s plate theory \( K = K_K \equiv 1 \), for the Mindlin’s plate theory \( K = K_M \equiv 1 + \frac{2 \eta}{1 - \nu} \frac{1}{\lambda^2} \), respectively. Let us consider the maximal deflection

\[ W = \frac{K}{\eta^2} Q. \]

Thus, for the Kirchhoff’s plate theory we obtain that \( W_K = \frac{1}{\eta^2} Q \), for the Mindlin’s plate theory we obtain that \( W_M = \frac{K_M}{\eta^2} Q \), and in the general case \( W_F = \frac{K}{\eta^2} Q \), respectively.

Let us use the following values \( \nu = 0.3, a = b, h = 0.05a \). Several normalized deflections are presented in the Table 1. It is easy to see that for the functionally graded plates the difference between the theories may be significant. Let us note that for the cases of other types of boundary conditions the influence of the structure of the plate on the deflection may be greater than for the simple support type boundary conditions.

6 Motion of a Symmetric Isotropic Plate

In this case Eqs (13) split into two parts: the in-plane problem for tangential displacements \( u_1 \) and \( u_2 \), and the bending problem for the \( w, \varphi_1 \) and \( \varphi_2 \), respectively.
In Cartesian coordinates with the geometrical relations (17) Eqs (13)₁,₂ reduce to the form

\[
\begin{align*}
(A_{11} + A_{22})u_{1,11} + (A_{11} - A_{22})u_{2,21} + A_{22}(u_{1,21} + u_{2,11}) + q_1 &= \rho \dddot{u}_1, \\
(A_{11} - A_{22})u_{1,12} + (A_{11} + A_{22})u_{2,22} + A_{22}(u_{1,22} + u_{2,12}) + q_2 &= \rho \dddot{u}_2
\end{align*}
\]

The Eq. (13)₃ has the following form

\[
\Gamma(w_{,11} + w_{,22}) + \Gamma(\varphi_{1,1} + \varphi_{2,2}) + q_n = \rho \dddot{w}
\]

The Eqs (13)₄,₅ result in

\[
\begin{align*}
(C_{33} + C_{22})\varphi_{1,11} + (C_{33} - C_{22})\varphi_{2,21} + C_{22}(\varphi_{1,22} + \varphi_{2,12}) - \Gamma\varphi_1 - \Gamma w_{,1} + m_1 &= \Theta \dddot{\varphi}_1, \\
(C_{33} + C_{22})\varphi_{2,22} + (C_{33} - C_{22})\varphi_{1,12} + C_{22}(\varphi_{1,21} + \varphi_{2,11}) - \Gamma\varphi_2 - \Gamma w_{,2} + m_2 &= \Theta \dddot{\varphi}_2
\end{align*}
\]

To eliminate the functions \(\varphi_1\) and \(\varphi_2\) from Eqs (63) and (64) let us differentiate the first equation of (64) with respect to \(x_1\), while the second one with respect to \(x_2\). Summing up these equations one gets

\[
[(C_{33} + C_{22})\Delta - \Gamma] (\varphi_{1,1} + \varphi_{2,2}) - \Gamma \Delta w + m_{1,1} + m_{2,2} = \Theta(\dddot{\varphi}_{1,1} + \dddot{\varphi}_{2,2})
\]
Here \( \Delta(\ldots) = (\ldots),_{11} + (\ldots),_{22} \).

Using (63) we can eliminate \( \phi_{1,1} + \phi_{2,2} \) from Eq. (65). Thus, we obtain considering the abbreviation (58) one equation with respect to \( w \) as follows

\[
\begin{align*}
D_{\text{eff}} \Delta \Delta w + \rho \ddot{w} + \frac{\rho \Theta}{\Gamma} w^{(4)} - \left( \Theta + \rho \frac{D_{\text{eff}}}{\Gamma} \right) \Delta \ddot{w} \\
= q_n + \frac{\Theta}{\Gamma} q_n - \frac{D_{\text{eff}}}{\Gamma} \Delta q_n + m_{1,1} + m_{2,2}.
\end{align*}
\]

(66)

Here \( w^{(4)} = \frac{\partial^4 w}{\partial t^4} \).

### 6.1 Dispersion Curves of a Rectangular Plate

To analyze the influence of the transverse shear stiffness and the rotatory inertia on the natural frequencies let us consider natural oscillations of a rectangular plate with simple support type boundary conditions. Let us assume that \( m_1 = m_2 = 0, q_n = 0 \), \( x_1 \in [0, a] \), \( x_2 \in [0, b] \), where \( a \) and \( b \) are the length and the width of the plate. Thus, we can rewrite Eq. (66) in the following form

\[
\begin{align*}
D_{\text{eff}} \Delta \Delta w + \rho \ddot{w} + \frac{\rho \Theta}{\Gamma} w^{(4)} - \left( \Theta + \rho \frac{D_{\text{eff}}}{\Gamma} \right) \Delta \ddot{w} = 0
\end{align*}
\]

(67)

Introducing dimensionless variables by formulas

\[
\begin{align*}
\bar{w} = \frac{w}{h}, \bar{x}_1 = \frac{x_1}{h}, \bar{x}_2 = \frac{x_2}{h}, \bar{x}_1 \in \left[0, \frac{a}{h}\right], \bar{x}_2 \in \left[0, \frac{b}{h}\right],
\bar{t} = \frac{t}{T}, T^2 = \frac{\rho h^4}{D_{\text{eff}}},
\end{align*}
\]

Eq. (67) transforms to

\[
\Delta \Delta \bar{w} + \ddot{\bar{w}} + \bar{\beta} \bar{w}^{(4)} - \bar{\zeta} \Delta \ddot{\bar{w}} = 0,
\Delta = \frac{\partial^2}{\partial \bar{x}_1^2} + \frac{\partial^2}{\partial \bar{x}_2^2}
\]

(68)

with the dimensionless parameters

\[
\bar{\beta} = \frac{\Theta D_{\text{eff}}}{\rho h^4}, \quad \bar{\zeta} = \frac{1}{h^2} \left( \frac{\Theta}{\rho} + \frac{D_{\text{eff}}}{\Gamma} \right)
\]

Let us note that if one formally considers the limit case \( \Gamma \to \infty \) and \( \Theta = 0 \) then \( \bar{\beta} = \bar{\zeta} = 0 \). Thus, from Eq. (68) follows immediately the equation of motion for the Kirchhoff’s plate

\[
\Delta \Delta \bar{w} + \ddot{\bar{w}} = 0
\]

(69)

It means that Eq. (68) contains two small parameters \( \bar{\beta} \) and \( \bar{\zeta} \) and can be considered as a singular perturbation of Eq. (69). While small parameters are the coefficients on derivative with respect to time of higher order then in Eq. (69) one can find the difference between solutions of Eqs (68) and (69) for highly oscillated modes. Equation (69) contains the term with a small parameter on mixed derivative with respect to time and space.
The solution of (68) is given by

\[ \tilde{w} = W_{mn} \exp(i\omega t) \sin \frac{\pi h m x_1}{a} \sin \frac{\pi h n x_2}{b}, \]

where \( m, n = 1, 2 \ldots \) are integer numbers, \( W_{mn} \) is the dimensionless magnitude of the oscillations. The solution (70) describes the natural oscillations of the plate, when \( \omega \) and \( \eta \) are connected by the dispersion relation

\[ \eta^4 - \omega^2 + \beta \omega^4 - \zeta \eta^2 \omega^2 = 0, \quad \eta^2 = \left( \frac{\pi h m}{a} \right)^2 + \left( \frac{\pi h n}{b} \right)^2 \]

(71)

All natural frequencies of the plate lay on the dispersion curves \( \omega = \omega(\eta) \), which are the solutions of Eq. (71).

Let us consider the solutions of (71) for different approaches to the plate theory. For the Kirchhoff’s plate theory we have \( \Gamma \to \infty, \Theta = 0 \). Then \( \beta = \zeta = 0 \) and one gets the standard dispersion relation

\[ \omega = \eta^2 \]

(72)

For the Mindlin’s plate theory without rotatory inertia \( (\Theta = 0) \) we can use Eqs (32), (31) and (85). Then we obtain that \( \beta = 0 \) and \( \zeta = 2/(1 - \nu) \). For example, for \( \nu = 1/3 \) one gets \( \zeta = 3 \). The dispersion relation is given by

\[ \omega = \frac{\eta^2}{\sqrt{1 + \zeta \eta^2}} \]

(73)

The dispersion curve presented by Eq. (73) coincides with dispersion curve for Kirchhoff’s plate when \( \eta \ll 1 \), but for \( \eta \gg 1 \) coincides with the asymptotic line \( \omega = \frac{1}{\sqrt{\zeta}} \eta \).

The dispersion curves are shown in Fig. 10. The solid curves marked by K and M correspond to Eqs (72) and (73), respectively. Here \( \nu = 1/3 \) was assumed.

For the Reissner’s sandwich plate theory we use Eqs (33) and assume that \( \Theta = 0 \). Then again \( \beta = 0 \). Let us consider the sandwich plate core made of metal foam while the faces made of a material used to synthesize the foam. Then one obtains notations \( E_f = E_s, G_c = G_p \), etc. Using Eqs (39) and considering \( \nu_c = \nu_f = \nu \) we get

\[ \zeta = \frac{h_f}{2h(1 - \nu)\alpha^m}. \]

(74)

For instance, if \( h_f = 0.1h, \alpha = 0.1, m = 2, \nu = 1/3 \) then \( \zeta = 7.5 \). For \( h_f = 0.05h, \alpha = 0.05, m = 2, \nu = 1/3 \) one observes \( \zeta = 15 \). The corresponding dispersion curves are shown in Fig. 10. They are marked by R1 and R2, respectively.

Let us investigate the influence of the rotatory inertia \( (\Theta \neq 0) \). For the Kirchhoff-type plate theory with \( \Gamma \to \infty \) using Eq. (32) we obtain that \( \beta = 0 \) while \( \zeta = 1/12 \). Thus, we have the dispersion relation (73) with a fixed value of \( \zeta \). The corresponding dispersion curve is marked by \( K_r \) in Fig. 10. One can see that if we neglect the transverse shear stiffness then the influence of the rotatory inertia is not significant.
For Mindlin-type plate theory we obtain that
\[ \beta = \frac{1}{6(1-\nu)}, \quad \zeta = \frac{1}{12} + \frac{2}{1-\nu} \]

Thus, in this case we have dispersion equations in the general form (71). For \( \nu = 1/3 \) the corresponding dispersion curve is marked by \( M_r \) in Fig. 10 (dotted line with box markers). One can see that for \( \beta \neq 0 \) the qualitative behavior of the dispersion curves is quite different. A new branch is appeared and started from the point \( \eta = 0, \omega = 1/\sqrt{\beta} \).

In the case \( \beta \neq 0 \) Eq. (71) has two solutions given by

\[ \omega_\pm = \left[ \frac{1 + \zeta \eta^2 \pm \sqrt{(1 + \zeta \eta^2)^2 - 4\beta \eta^4}}{2\beta} \right]^{1/2} \]  

(75)

One of the solutions (75) starts from the point \((0,0)\) while the second one starts from the point \( \left(0, \frac{1}{\sqrt{\beta}}\right) \). Both curves have linear asymptotics when \( \eta \to \infty \). They are given by

\[ \omega_\pm = \eta \left[ \frac{\zeta \pm \sqrt{\zeta^2 - 4\beta}}{2\beta} \right]^{1/2}, \quad \eta \gg 1 \]  

(76)
The solution $\omega_-$ describes the low-frequency bending oscillation modes or bending waves in the case of an infinite plate, while $\omega_+$ describes high-frequency oscillations.

For a sandwich plate with non-zero rotatory inertia we obtain that

$$\frac{\Theta}{h^2 \rho} = \frac{1}{12} \left[ 1 - \frac{h^3}{h^3 (1 - \alpha)} \right] \left[ 1 - \frac{h_e}{h} (1 - \alpha) \right]^{-1}, \quad D_{\text{eff}} \frac{h^2}{h^2 \Gamma} = \frac{h_t}{2 h (1 - \nu) \alpha^m} \quad (77)$$

The corresponding dispersion curves are shown in Fig. 10 for two sets of values $h_t = 0.1h$, $\alpha = 0.1$, $m = 2$, $\nu = 1/3$ and $h_t = 0.05h$, $\alpha = 0.05$, $m = 2$, $\nu = 1/3$. They are marked by $R_{r1}$ (dotted line with asterisk markers) and $R_{r2}$ (solid line), respectively.

Note that for the chosen values of the material and the geometrical parameters some of the curves are practically identical. Indeed, the low branch of the $M_r$-curve coincides with the $M$-curve, while the low branch of the $R_{r1}$-curve coincides with the $R_1$-curve.

Let us discuss the FGM plates more in detail. Using Eqs (40) and (29) we obtain that

$$\frac{\Theta}{h^2 \rho} = \frac{1}{4} \left[ 1 + \frac{1 - \alpha}{\alpha + \frac{1}{n} \frac{1 - \alpha}{n+1}} \right], \quad D_{\text{eff}} \frac{h^2}{h^2 \Gamma} = \frac{2}{1 - \nu} \frac{1}{h^2 \lambda^2}. \quad \text{(77)}$$

Note that $\lambda^2$ is the minimal eigen-value of the Sturm-Liouville problem (30) [3, 4].

For FGM plates the solution can be estimated using numerical methods, for example, the shooting method [43]. In Fig. 11 we present the dispersion curves for different values of $n$ and $\alpha$ with $m = 2$, $\nu = 0.3$. The dashed curves in Fig. 11 correspond to the Kirchhoff’s and the Reissner’s solutions, marked by K and R, respectively. On can see that the influence of $\alpha$ is significant in the case of high-oscillated branches of the dispersion curves. For low-oscillated branches the difference between the values $\alpha = 0.1$ and $\alpha = 0.05$ is not significant. For low dispersion curves, the Kirchhoff’s and the Reissner’s solutions can be used as a upper and lower bounds of the eigen-frequencies of the FGM plate. One can see that the Reissner’s sandwich plate approach demonstrates a good qualitative coincidence with our results on FGM plates as well as the Mindlin’s one. On the other hand, the classical plate models cannot describe the high-oscillated solutions corresponding to our dispersion curves described by $\omega_+$.

The normalized first eigen-frequencies of a quadratic plate are presented in Table 2. Here $a = b$, $h = 0.1a$, $\nu = 0.3$, $m = 2$, $\Omega = \omega/\omega_K$, and $\omega_K$ is the first eigen-frequency of the Kirchhoff’s plate given by (72). One can see for enough thick plates the structure of the various influences on the eigen-frequencies. The Kirchhoff’s theory gives us larger values of the eigen-frequency, while Reissner’s theory gives us smaller values of the eigen-frequency. So, they can be used as estimations for the modal analysis of FGM plates.

The considered example shows that the theory of sandwich plates may be not sufficient to describe the oscillations of FGM plates which are highly non-homogeneous in the thickness direction. The theory of laminated plates (see, e.g. [8]) may be more useful, but here the problem appears of determination the number of laminates and its properties appears.
7 Viscoelastic plates

Polymers near their glass transition temperature behave like viscoelastic materials. That means that the moduli of the polymers depend on the strain-rate or the time of loading. Thus, a foam made of such a polymer behaves viscoelastically too. Mechanics of viscoelastic plates made of polymer foams was developed in [10].

The two-dimensional constitutive equations of a viscoelastic plate were formulated in the general form in [2]. For brevity, let us consider a through-the-thickness symmetric structure of the plate under consideration and an isotropic material behavior. In this case it follows the constitutive equations for the stress resultants:

- In-plane forces

\[ \mathbf{T} \cdot \mathbf{a} = A\mathbf{\mu} \equiv \int_{-\infty}^{t} A(t - \tau) \cdot \dot{\mathbf{\mu}} d\tau, \]

- Transverse shear forces

\[ \mathbf{T} \cdot \mathbf{n} = G\mathbf{\gamma} \equiv \int_{-\infty}^{t} G(t - \tau) \cdot \dot{\mathbf{\gamma}} d\tau, \]
Table 2: Minimal normalized eigen-frequency of a quadratic plate and corresponding values of the normalized transverse shear stiffness and the rotatory inertia

<table>
<thead>
<tr>
<th>Model</th>
<th>$\Gamma/G, h$</th>
<th>$\Theta/\rho h^2$</th>
<th>$\Omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kirchhoff’s plate</td>
<td>$\infty$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Mindlin’s plate</td>
<td>$\pi^2/12$</td>
<td>0</td>
<td>0.8</td>
</tr>
<tr>
<td>Reissner’s sandwich plate $\alpha = 0.1, h_t = 0.1$</td>
<td>0.01</td>
<td>0</td>
<td>0.64</td>
</tr>
<tr>
<td>Reissner’s sandwich plate $\alpha = 0.05, h_t = 0.05$</td>
<td>0.025</td>
<td>0</td>
<td>0.51</td>
</tr>
<tr>
<td>Kirchhoff-type plate</td>
<td>$\infty$</td>
<td>1/12</td>
<td>0.99</td>
</tr>
<tr>
<td>Mindlin-type plate</td>
<td>$\pi^2/12$</td>
<td>1/12</td>
<td>0.8</td>
</tr>
<tr>
<td>Reissner-type sandwich plate $\alpha = 0.1, h_t = 0.1$</td>
<td>0.01</td>
<td>0.028</td>
<td>0.64</td>
</tr>
<tr>
<td>Reissner-type sandwich plate $\alpha = 0.05, h_t = 0.05$</td>
<td>0.025</td>
<td>0.015</td>
<td>0.51</td>
</tr>
<tr>
<td>FGM plate $\alpha = 0.1, n = 1$</td>
<td>0.061</td>
<td>0.12</td>
<td>0.81</td>
</tr>
<tr>
<td>FGM plate $\alpha = 0.1, n = 5$</td>
<td>0.015</td>
<td>0.15</td>
<td>0.73</td>
</tr>
<tr>
<td>FGM plate $\alpha = 0.1, n = 10$</td>
<td>0.012</td>
<td>0.14</td>
<td>0.78</td>
</tr>
</tbody>
</table>

7.1 Effective Properties

For elastic plates the identification of the components of the effective stiffness tensors was proved in [3, 4, 48]. By the same technique below the analogous viscoelastic stiffness tensor components are computed. Let us consider the three-dimensional viscoelastic constitutive equations [14, 22]

$$
\sigma = \int_{-\infty}^{t} 2\mu(t - \tau)\dot{\varepsilon}\,d\tau + \int_{-\infty}^{t} K(t - \tau)\varepsilon\,d\tau, \quad \varepsilon = \frac{1}{3} \text{tr} \varepsilon, \quad \sigma = \varepsilon - \varepsilon I
$$

or

$$
\varepsilon = \int_{-\infty}^{t} M(t - \tau)\dot{\sigma}\,d\tau + \int_{-\infty}^{t} J(t - \tau)\sigma\,d\tau, \quad \sigma = \frac{1}{3} \text{tr} \sigma, \quad \varepsilon = \sigma - \sigma I,
$$

where $\sigma$ and $\varepsilon$ are the tensors of stress and strain respectively, $I$ is the three-dimensional unit tensor. $\mu(t)$ and $K(t)$ are the shear and the bulk relaxation
functions, while $M(t)$ and $J(t)$ are the shear and the bulk creep functions. Alternative expressions (but not equivalent!) of the integral constitutive equations of a viscoelastic body are the differential constitutive equations [14]

$$P(\partial_t)\sigma = Q(\partial_t)\epsilon, \quad P_1(\partial_t)s = Q_1(\partial_t)e,$$  

(80)

where $\partial_t(\ldots)$ denotes the time derivative, $P(\partial_t)$, $P_1(\partial_t)$, $Q(\partial_t)$, $Q_1(\partial_t)$ are polynomials. In addition, there exist a third type of expressions based on the complex moduli representation.

A special case of (80) is the standard linear viscoelastic body [22]

$$\dot{\sigma} + \frac{\dot{K}}{\eta} \sigma = \frac{K_{\infty}}{\eta} \dot{\epsilon} + (K_{\infty} + \dot{K}) \epsilon, \quad \dot{s} + \frac{\dot{G}}{\eta_1} s = \frac{G_{\infty}}{\eta_1} e + (G_{\infty} + \dot{G}) \dot{e},$$

(81)

From (81) it yields that the following relations are valid [22]

$$K(t) = K_{\infty} + \dot{K} \exp \left( -\frac{\dot{K}}{\eta} t \right), \quad \mu(t) = G_{\infty} + \dot{G} \exp \left( -\frac{\dot{G}}{\eta_1} t \right)$$

(82)

Using the Laplace transform of a function $f(t)$

$$\tilde{f}(s) = \int_0^\infty f(t)e^{-st}dt,$$

one can write Eqs (78), (79) in the form [22]

$$\sigma = 2s\mu(s) e + sK(s)eI, \quad \tilde{\epsilon} = sM(s)s + sJ(s)\tilde{\sigma}I$$

(83)

Further we consider the same two cases as in Sect. 2.3. In the case of isotropic material behavior one has two material properties describing the viscoelastic behavior. They depend on the thickness coordinate $z$ and on the time $t$

$$K = K(z, t), \quad \mu = \mu(z, t)$$

In addition, a density function must be considered. Let us assume the simplest case – the density depends only on the thickness coordinate $z$

$$\rho_0 = \rho_0(z)$$

Using the analogy between (83) and the Hooke’s law we can extend the identification procedure [3, 4, 48] to the Laplace mapping of the effective relaxation or creep functions, see [2]. The in-plane stiffness tensor components are

$$\tilde{A}_{11} = \frac{1}{2} \left\langle \frac{\tilde{E}}{1-\nu} \right\rangle, \quad \tilde{A}_{22} = \frac{1}{2} \left\langle \frac{\tilde{E}}{1+\nu} \right\rangle = \langle \tilde{\mu} \rangle,$$

the out-of-plane (plate) stiffness tensor components are

$$\tilde{C}_{33} = \frac{1}{2} \left\langle \frac{\tilde{E}}{1-\nu} z^2 \right\rangle, \quad \tilde{C}_{22} = \frac{1}{2} \left\langle \frac{\tilde{E}}{1+\nu} z^2 \right\rangle = \langle \tilde{\mu}z^2 \rangle,$$
and the transverse shear stiffness tensor component is
\[ \bar{\Gamma} = \lambda^2 \bar{C}_{22} \]
with \( \lambda \) following from a Sturm-Liouville problem
\[ \frac{d}{dz} \left( \bar{\mu} \frac{dZ}{dz} \right) + \lambda^2 \bar{\mu} Z = 0, \quad \left. \frac{dZ}{dz} \right|_{z = \frac{h}{2}} = 0 \]
The following relations hold true [14]
\[ \bar{E} = \frac{9\bar{\mu}\bar{K}}{\bar{\mu} + 3\bar{K}}, \quad \bar{\nu} = \frac{3\bar{K} - 2\bar{\mu}}{2(\bar{\mu} + 3\bar{K})} \]
The corresponding relaxation functions \( E(t) \) and \( \nu(t) \) may be used instead of \( \mu(t) \) and \( K(t) \). Let us note that for the viscoelastic plate \( \bar{\mu} = \bar{\mu}(z, s) \). Thus, \( \lambda = \lambda(s) \). The tensors of inertia and the plate density are given by [5, 48]
\[ \rho = \langle \rho_0 \rangle, \quad \rho \Theta_1 = -\langle \rho_0 z \rangle \mathbf{c}, \quad \rho \Theta_2 = \Theta \mathbf{a}, \quad \Theta = \langle \rho_0 z^2 \rangle \]
Considering the symmetry of the thickness geometry and of the material properties of the plate from (84) one gets that \( \Theta_1 = 0 \). \( \Theta \) characterizes the rotatory inertia of the cross-section of the plate.

### 7.2 Examples of Effective Stiffness Relaxation Functions
For the sake of simplicity, let us consider the case \( \nu(t) = \nu = \text{const} \) which is fulfilled in many applications (see arguments in [14] concerning \( \nu(t) \approx \text{const} \)). That means that the following relations hold true
\[ E(t) = 2\mu(t)(1 + \nu), \quad K(t) = \frac{2\mu(t)(1 + \nu)}{3(1 - 2\nu)} \]
For the constitutive equations of the standard viscoelastic solid, the latter relation imply that \( \eta_1 = \eta \), and
\[ K_\infty = \frac{2G_\infty(1 + \nu)}{3(1 - 2\nu)}, \quad \hat{K} = \frac{2\hat{G}(1 + \nu)}{3(1 - 2\nu)} \]
Thus, in this case one gets four independent material constants. They are \( G_\infty, \hat{G} \) (or \( K_\infty, \hat{K} \)), \( \eta \) and \( \nu \).

### 7.2.1 Homogeneous Plate
Taking into account the same considerations like in Sect. 3.1, the non-zero components of the classical relaxation tensors are
\[ A_{11}(t) = \frac{E(t)h}{2(1 - \nu)}, \quad A_{22}(t) = \frac{E(t)h}{2(1 + \nu)} = \mu(t)h, \]
\[ C_{33}(t) = \frac{E(t)h^3}{24(1 - \nu)}, \quad C_{22}(t) = \frac{E(t)h^3}{24(1 + \nu)} = \frac{\mu(t)h^3}{12} \]
The transverse shear relaxation function follows from (29). The solution of (30) with \( \bar{\mu} = \bar{\mu}(s) \) is given by \( \cos \lambda z = 0 \). It yields to the smallest eigenvalue \( \lambda = \pi/h \) which does not depend on \( s \). Finally, one obtains

\[
\Gamma(t) = \frac{\pi^2 \mu(t) h^3}{h^2/12} = \frac{\pi^2}{12} \mu(t) h
\]

(85)

\( \pi^2/12 \) is again similar to the so-called shear correction factor.

It is evident that in the case of homogeneous viscoelastic plates with constant Poisson’s ratio one gets the same relations for the effective stiffness tensors as for elastic plates [3, 4]. There is only one difference – they are now functions of \( t \).

7.2.2 Functionally Graded Material

Now similar assumptions like in Sects 3.3.1 and 3.3.2 are considered. For the description of the symmetric distribution of the porosity of the viscoelastic foam we assume the power law (38)

The properties of a foam strongly depend on the porosity and the cell structure. For the polymer foam in [19] the modification of the standard linear viscoelastic solid it is proposed. For open-cell foam the constitutive law has the form

\[
\dot{\sigma} + \frac{\dot{\bar{K}}}{\bar{\eta}} \sigma = C_1 V(z)^2 \left[ \frac{K_\infty \dot{\bar{K}}}{\bar{\eta}} \dot{\varepsilon} + (K_\infty + \dot{\bar{K}}) \dot{\varepsilon} \right], \tag{86}
\]

while for closed-cell foam the constitutive equation has the form

\[
\dot{\sigma} + \frac{\dot{\bar{K}}}{\bar{\eta}} \sigma = C_2 \left[ \phi^2 V(z)^2 + (1 - \phi) V(z) \right] \left[ \frac{K_\infty \dot{\bar{K}}}{\bar{\eta}} \dot{\varepsilon} + (K_\infty + \dot{\bar{K}}) \dot{\varepsilon} \right], \tag{87}
\]

Here \( C_1 \approx 1, C_2 \approx 1, \phi \) describes the relative volume of the solid polymer concentrated near the cell edges. Usually, \( \phi = 0.6 \ldots 0.7 \), etc. \( K_\infty, \dot{\bar{K}}, \bar{\eta} \) are material constants of the polymer used in manufacturing of the foam.

From Eqs (86), (87) one can see that the corresponding relaxation functions are given by the relations

\[
K = K(z, t) = K(t) \kappa(z), \tag{88}
\]

where \( K(t) \) is defined by Eq. (82), while \( \kappa(z) = C_1 V(z)^2 \) for open-cell foam and \( \kappa(z) = C_2 \left[ \phi^2 V(z)^2 + (1 - \phi) V(z) \right] \) for closed-cell foam, respectively. Analogous to (88) the following relation can be established for the shear relaxation function

\[
\mu = \mu(z, t) = \mu(t) \mu(z) \tag{89}
\]

Equations (88) and (89) have the meaning that the viscoelastic properties of a foam, for example, the time of relaxation, do not depend on the porosity distribution. Note that the representations (88) and (89) are only simple assumptions for spatial nonhomogeneous foams.
Using experimental data presented in [11, 19] one can assume $\nu = \text{const}$. In this case we obtain that $A_{11}, A_{22}, C_{33}, C_{22}$ are related to

$$A_{11} = \frac{1 + \nu}{1 - \nu} A_{22}, \quad C_{33} = \frac{1 + \nu}{1 - \nu} C_{22},$$

(90)

For the open-cell foam $A_{22}$ and $C_{22}$ are given by

$$A_{22} = h \left[ \alpha^2 + \frac{2\alpha(1 - \alpha)}{n + 1} + \frac{(1 - \alpha)^2}{2n + 1} \right] \mu(t),$$
$$C_{22} = \frac{h^3}{12} \left[ \alpha^2 + \frac{6\alpha(1 - \alpha)}{n + 3} + \frac{3(1 - \alpha)^2}{2n + 3} \right] \mu(t),$$

(91)

while for the closed-cell foam by

$$A_{22} = h \left\{ \phi^2 \left[ \alpha^2 + \frac{2\alpha(1 - \alpha)}{n + 1} + \frac{(1 - \alpha)^2}{2n + 1} \right] + (1 - \phi) \left[ \alpha + \frac{1 - \alpha}{n + 1} \right] \right\} \mu(t),$$
$$C_{22} = \frac{h^3}{12} \left\{ \phi^2 \left[ \alpha^2 + \frac{6\alpha(1 - \alpha)}{n + 3} + \frac{3(1 - \alpha)^2}{2n + 3} \right] + (1 - \phi) \left[ \alpha + \frac{3(1 - \alpha)}{n + 3} \right] \right\} \mu(t)$$

(92)

Here we assume that $C_1 = 1$, $C_2 = 1$, and that $\phi$ does not depend on $z$.

From Eqs (91), (92) it is easy to see that the classical relaxation functions differ only by factors from the shear relaxation function. Note that one can easily extend Eqs (86), (87) to the case of general constitutive equations (78) or (80). Thus, using assumption that $\nu = \text{const}$, one can calculate the classical effective stiffness relaxation functions for the general viscoelastic constitutive equations multiplying the shear relaxation function with the corresponding factor similar to Eqs (91), (92). In the more general situation with $\nu = \nu(t)$ or taking into account other viscoelastic phenomena, for example, the filtration of a fluid in the saturated foam, the effective stiffness relaxation functions may be more complex then for the pure solid polymer discussed here.

To obtain the dependence of the transverse shear stiffness relaxation function we have to solve Eq. (30). In the general case the solution of the spectral problem (30) may be performed numerically. For example, in [9] the shooting method [43] was used. For the viscoelastic plate $\lambda = \lambda(s)$. It means that for the determination of $\Gamma(t)$ one has to solve (30) for any arbitrary value of $s$ and with the help of $\lambda = \lambda(s)$ to find numerically the inverse Laplace transform of $\lambda^2(s)\bar{C}_{22}(s)$. But in the special case of Eq. (89) one gets that $\bar{\mu} = \bar{\mu}(s)m(z)$. That means that $\lambda$ does not depend on $s$, and thus $\Gamma(t) = \lambda^2 C_{22}(t)$. For the sake of simplicity, further we will apply the assumption (89).

Let us find the bounds for the values of $\lambda$. Introducing a new independent variable $\zeta$ by the formula

$$\zeta = \int_{-h/2}^{z} \frac{dz}{m(z)},$$
one can transform (30) to the form (see, for example, [23] for details)

$$\frac{d^2Z}{d\zeta^2} + \lambda^2 m^2 Z = 0, \quad \frac{dZ}{d\zeta} \bigg|_{\zeta=0,1} = 0$$ (93)

Here

$$L = \int_{-h/2}^{h/2} \frac{dz}{m(z)}$$

Substituting $\zeta = \zeta/L$, one can transform the spectral problem (93) to the canonical form

$$\frac{d^2Z}{d\zeta^2} + \lambda^2 L^2 m^2 Z = 0, \quad \frac{dZ}{d\zeta} \bigg|_{\zeta=0,1} = 0$$ (94)

The following theorem exists [15]:

**Theorem.** If one has two eigen-value problems

$$\frac{d^2Z}{d\zeta^2} + \lambda_1^2 f_1 Z = 0, \quad \frac{d^2Z}{d\zeta^2} + \lambda_2^2 f_2 Z = 0, \quad \frac{dZ}{d\zeta} \bigg|_{\zeta=0,1} = 0$$ (95)

with two functions $f_1(\zeta)$ and $f_2(\zeta)$ such that $f_1 \leq f_2$, then the following inequality hold true $\lambda_1 \geq \lambda_2$. Here $\lambda_1$ and $\lambda_2$ are the eigen-values corresponding to the functions $f_1(\zeta)$ and $f_2(\zeta)$, respectively.

Using this theorem and the inequality $m_{\text{min}} \leq m \leq m_{\text{max}}$, we obtain the lower and upper bounds of $\lambda$

$$\frac{\pi}{L m_{\text{max}}} \leq \lambda \leq \frac{\pi}{L m_{\text{min}}}$$ (96)

For the homogeneous plate $m_{\text{min}} = m_{\text{max}} = m$, $L = h/m$, and both bounds coincide each other.

Finally, we should mention that in the case of constant Poisson’s ratio and with the assumption (89) the determination of the effective in-plane, bending and transverse shear stiffness tensors of a symmetric FGM viscoelastic plate made of a polymer foam can be realized by the same method as for elastic plates [3, 4, 9]. The relaxation functions for viscoelastic FGM plates can be found from the values of the corresponding effective stiffness of an elastic FGM plate by multiplication with the normalized shear relaxation function of the polymer solid.

### 7.3 Viscoelastic Bending Behavior a Plate made of FGM

Considering the symmetry of the material properties with respect to the mid-plane one gets a decoupling of the in-plane state and the plate state. Let us assume the
Kirchhoff’s plate bending with \( \mathbf{m} = 0 \). Using [9] and the Laplace transform, one can reduce (2) to

\[
\bar{D}_{\text{eff}} \Delta \Delta \bar{w} = \bar{q}_n - \frac{\bar{D}_{\text{eff}}}{t} \Delta \bar{q}_n, \tag{97}
\]

where \( \bar{D}_{\text{eff}} = \bar{C}_{22} + \bar{C}_{33} \) is Laplace transform of the effective bending stiffness relaxation function, \( \bar{w} = \dddot{u} \cdot \mathbf{n} \) is the Laplace transform of the plate deflection, \( \bar{q}_n = \dddot{q} \cdot \mathbf{n} \) is Laplace transform of the transverse load, respectively. Note that here \( \bar{D}_{\text{eff}} = D_{\text{eff}}^0 \bar{\mu}(s) \), where \( D_{\text{eff}}^0 = (C_{22} + C_{33})/\mu(t) \).

To analyze the influence of the transverse shear stiffness on the deflection of the plate let us consider the bending of a rectangular plate made of a functionally graded material. Let us assume that \( x_1 \in [0, a] \), \( x_2 \in [0, b] \), where \( a \) and \( b \) are the length and the width of the plate, respectively. Using the assumption [11, 19] that \( \nu = \text{const} \) and the Eqs (28), (29), and (89) are valid, we can rewrite Eq. (97) in the following form

\[
\bar{D}_{\text{eff}} \Delta \Delta \bar{w} = \bar{q}_n - \frac{2}{1 - \nu} \lambda h^2 \Delta \bar{q}_n \tag{98}
\]

Introducing dimensionless variables by the formulas

\[
W = h^{-1} w, \quad X_1 = h^{-1} x_1, \quad X_2 = h^{-1} x_2, \quad X_1 \in \left[ 0, \frac{a}{h} \right], \quad X_2 \in \left[ 0, \frac{b}{h} \right],
\]

Eq. (98) transforms to

\[
\bar{\mu}(s) \Delta \Delta \bar{W} = Q - \frac{2}{1 - \nu} \lambda h^2 \Delta \bar{Q} \tag{99}
\]

Here \( \Delta = \frac{\partial^2}{\partial X_1^2} + \frac{\partial^2}{\partial X_2^2} \), \( Q = \frac{\bar{q}_n h^3}{\bar{D}_{\text{eff}}^0} \).

Let us consider a sinusoidal load

\[
q_n = Q_0(t) \sin \frac{\pi h X_1}{a} \sin \frac{\pi h X_2}{b}
\]

and the boundary conditions (5). Then

\[
Q = \bar{Q}_0(s) \sin \frac{\pi h X_1}{a} \sin \frac{\pi h X_2}{b}
\]

and the solution of Eq. (99) is given by

\[
\bar{W} = \frac{K}{\eta^2 \bar{\mu}(s)} \sin \frac{\pi h X_1}{a} \sin \frac{\pi h X_2}{b}, \quad K = 1 + \frac{2\eta}{1 - \nu} \frac{1}{\lambda^2 h^2}, \quad \eta = \left( \frac{\pi h}{a} \right)^2 + \left( \frac{\pi h}{b} \right)^2
\]

For the Kirchhoff’s plate theory \( K = K_K \equiv 1 \), for the homogeneous plate modeled in the sense of Mindlin’s plate theory

\[
K = K_M \equiv 1 + \frac{2\eta}{1 - \nu} \frac{1}{\pi^2},
\]
and for the FGM plate
\[
1 + \frac{2\eta}{1 - \nu} \frac{L^2 m_{\text{min}}^2}{\pi^2 h^2} \leq K \leq 1 + \frac{2\eta}{1 - \nu} \frac{L^2 m_{\text{max}}^2}{\pi^2 h^2}
\]

The influence of the shear stiffness on the deflection of the elastic FGM plate was given in [9]. For the viscoelastic plate both the qualitative and the quantitative influence of the shear stiffness is the same as in [9].

For example, let us consider a open-cell foam and following values $\nu = 0.3$, $a = b$, $h = 0.05a$, $\alpha = 0.9$. Using the calculation of [9] we obtain the following values of $\lambda$: $\lambda = 0.83/h$ for $n = 2$, $\lambda = 0.82/h$ for $n = 5$. The corresponding values of factor $K$ are given by

\[K_M \approx 1.014, \quad K \approx 1.20 \quad (n = 2), \quad K \approx 1.21 \quad (n = 5)\]

That means that for the functionally graded plates the influence of transverse shear stiffness may be significant. As well as for elastic FGM plates for the cases of other types of boundary conditions the influence of the structure of viscoelastic plate on the deflection may be greater than for the used simple support type boundary conditions.

8 Summary and Outlook

A plate theory based on Zhilin’s direct approach method in the theory of shells for FGMs is introduced. The basic items of the theory are related to

- the formulation of all balances for a deformable directed surface (àpriory two-dimensional equation) and
- the specific constitutive equation

In addition, for each specific type of plates the identification of the unknown material parameters should be performed. It is clearly shown that based on the assumption of linear elastic or viscoelastic behavior the identification for different foams can be realized. It is helpful that Zhilin’s theory includes elements of symmetry groups for two-dimensional objects and the concept of effective properties. Simple static and dynamic problems are solved and the solutions are compared with a Kirchhoff-type theory and a Mindlin-type theory. We present the analysis of free oscillations of FGM plates based on the generalized equations of motion and taking into account not only the transverse shear stiffness but the rotatory inertia too. We have shown that both parameters play an important role. In particular, the non-zero rotatory inertia possess us to describe the high-oscillated solutions. We established the bounds for the natural frequencies of FGM plates. The presented approach to model FGM plates within the framework of a 5-parametric theory of plates has an advantage with respect to theories of sandwich or laminated plates and can be extended to the case of linear viscoelastic material properties.
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A model for the flow curves of powders. Study of the rheological behavior of monomodal quartz particle beds under stress

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Abstract

A model is proposed that describes the flow curves of powders. The model is based on the adhesive contact of elastic spheres theory developed by Johnson, Kendall, and Roberts (JKR model). The proposed model improves the results by applying the Warren Spring Laboratory equation (WSL) and the Coulomb model. Only two parameters are needed in the present model to describe the flow curve of a powder: powder cohesion ($C$) and the coefficient of friction ($\mu$) of the powder bed. The study verifies the validity of the new equation for describing the flow curves of different powders.

The proposed model has been used to calculate the cohesion and coefficient of friction of monomodal quartz particle beds with different average particle sizes. The study examines the influence of average particle size ($d_S$) and bed compactness ($\phi$) on these parameters. Cohesion is observed to increase by the sixth power of compactness and inverse of the particle Sauter diameter. The bed coefficient of friction increases asymptotically with bed compactness, this relation depending on particle size.

Keywords: flowability, rheology, powders

1 Introduction

In industrial processes that use materials in the form of solid particulates, also known as granular material or simply powder, problems tend to occur more frequently in certain powder processing stages than when fluids are handled [1, 2, 3]. The origin of these problems lies in the fact that the flow characteristics of particulate beds are less well understood and more poorly characterized than those of homogeneous fluid streams [4]. However, it may be noted, first, that there is no universally applicable test or index that allows powder flow characteristics or flowability to be determined.
On the other hand, the relation of the test should also be based on the objective pursued with the flowability measurement.

The tests most commonly used in characterizing powder flowability are those based on the determination of flow curves, measurement of the bulk densities of consolidated particle beds (Hausner ratio, Carr index, etc.), compression tests, measurement of the rest angle, and determination of the flow rate. In this study, the methods based on the determination of the powder flow curves have been used, because they allow determination of the mechanical properties of the beds under different consolidation conditions and provide information for designing equipment used in the handling and storage of powders (silos, hoppers, etc.).

1.1 Flow curves of a powder. Descriptive equations of the phenomenon

The general shape of the flow curves of particle beds, for any state of consolidation, is very similar and displays the following common characteristics: for high normal stress, \( \sigma \), the flow curve consists of a practically straight stretch, whereas for small and even negative normal stress it displays a convex curvature, which becomes more pronounced as the powder becomes more cohesive (Fig. 1).

In 1965 Ashton et al. [5] proposed Equation (1), also termed the Warren-Springs Laboratory (WSLA) equation, in order to describe the flow curve analytically, attempting to justify it by physical arguments based on the attraction and repulsion forces present at the interparticle contact points:

\[
\left(\frac{\tau}{C}\right)^n = \sigma + 1
\]

where \( n \) is the shear index.

Figure 1: Flow curve of a powder bed. Fit of the experimental values to Equation (1), using different values for the parameters.
Although Equation (1) is frequently mentioned in the literature, and its authors attempted to explain it physically, it has never been used in practical applications (silo design, etc.), nor has the shear index \( n \) been used to characterise powder flowability. This is essentially because of the high uncertainty in the estimation of parameters \( T, C, \) and \( n \), which leads to different flow curves for the same experimental values, particularly in the low consolidation stress region (Fig. 1).

Even though, as Jenike [6] already indicated, the flow curve departs significantly from a straight line for small normal stresses, \( \sigma \), other researchers, either because they omitted to work in this stretch of the curve or because they considered that the departures from linearity were mostly small, fitted the experimental results of the yield tests to the Coulomb equation:

\[
\tau = C + \mu \sigma \quad (2)
\]

where \( \mu \) is the internal friction coefficient of the powder, related to the internal friction angle, \( \varphi_i \) by means of the relation \( \mu = \tan \varphi_i \) [8, 9].

1.1.1 Proposed model, based on the adhesive contact of elastic spheres (JKR Model)

In 1986, Kendall [7] used the model describing the adhesive contact of elastic spheres, originally developed by Johnson, Kendall and Roberts (JKR Model) in 1971 [8], to explain the inadequacy of the Coulomb law for quantifying the results of particle bed friction on flat surfaces. However, no study has been found, based on the equation developed by Kendall or on the JKR model, which develops an equation or model that describes the flow curve of both cohesive and non-cohesive powders.

The model proposed in this study [9] is based on the Coulomb fracture criterion. The fracture or yield of the powder in the shear plane on which a total effective normal load, \( \sigma^* \), acts will occur at a value of \( \tau \) that meets the yield condition:

\[
\frac{\tau}{\sigma^*} \leq \mu = \tan \varphi_i \quad (3)
\]

In the Coulomb model, the interparticle surface adhesion force is independent of the external load that is applied. However, in accordance with the JKR model, the force, \( F_{ad} \), which keeps two smooth and elastic spheres of radius \( R \) joined, and the applied external normal load, \( W \), are mutually related, as has been amply demonstrated experimentally [10, 11, 12], in accordance with the equation:

\[
F_{ad}^* = W + 3\gamma\pi R + \left[ 6\gamma\pi RW + (3\gamma\pi R)^2 \right]^{1/2} \quad (4)
\]

where \( \gamma \) is the surface energy of the spheres.

According to this model, the force required to separate the two contacting spheres, when no external load is acting on them, is as follows:
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\[ F_{ad} = \frac{3}{2} \gamma \pi R \]  \hspace{1cm} (5)

Since in the fracture plane of the powder bed there will be a number of contacts per unit apparent surface area, \( n \), the total normal load that acts in this plane will be:

\[ \sigma' = \sigma + 3\gamma \pi R n + \left[ 6\gamma \pi R n \sigma + (3\gamma \pi R n)^2 \right]^{1/2} \]  \hspace{1cm} (6)

The introduction of Equation (6) in the fracture condition, Equation (3), gives:

\[ \tau = \sigma \mu + 3\gamma \pi R n \mu + \left[ 6\gamma \pi R n \sigma \mu^2 + (3\gamma \pi R n \mu)^2 \right]^{1/2} \]  \hspace{1cm} (7)

Application to Equation (7) of the definition of cohesion, i.e. \( \tau = C \), for \( \sigma = 0 \), gives:

\[ C = 6\gamma \pi R n \mu \]  \hspace{1cm} (8)

When this is introduced into Equation (7), one obtains the equation of the flow curve:

\[ \tau = \frac{C}{2} + \sigma \mu + \left( \frac{C}{2} \right)^{1/2} \left[ 2\sigma \mu + \frac{C}{2} \right]^{1/2} \]  \hspace{1cm} (9)

In accordance with Equation (5), the tensile strength of a bed (\( T \)) will be:

\[ T = F_{ad} n = \frac{3}{2} \gamma \pi R n \]  \hspace{1cm} (10)

The combination of this equation with Equation (8) gives the relation between cohesion (\( C \)) and tensile strength of the powder bed (\( T \)):

\[ T = \frac{C}{4\mu} \]  \hspace{1cm} (11)

It may be noted that, though Equation (9) is based on the JKR model, developed for uniformly sized smooth spheres, this expression should, in principle, be equally applicable to real powder beds made up of irregular rough particles of different size, since the effect of these microstructural characteristics on the flow curve would materialise in their influence on \( C \) and \( \mu \), without, for that reason, modifying Equation (9), as will be shown below. In effect, in real powders, the micro-contacts
occur between asperities of neighbouring particles (Fig. 2). For these cases, the expression of the contact force is identical to Equation (4) if the radius of the sphere, \( R \), is replaced with its reduced radius, \( R^* \) [10, 11].

\[
R^* = \frac{R_1 R_2}{R_1 + R_2}
\]

(12)

where \( R_1 \) and \( R_2 \) are the curvature radii of the two contacting asperities.

Analogously, since the geometric characteristics of the contacts differ, the total normal stress, \( \sigma^* \), which acts in the bed fracture plane, is calculated as the sum of the contact forces of the \( n \) contacts between asperities, per unit surface area:

\[
\sigma^* = \frac{1}{A} \sum_{i=1}^{n} \left( W + 3\gamma\pi R_i^* \right. \\
\left. + \left[ 6\gamma\pi R_i W + (3\gamma\pi R_i^*)^2 \right]^{1/2} \right)
\]

(13)

which, when the fracture condition is applied, becomes Equation (9) if it is taken into account that in this case powder cohesion is:

\[
C = 4\mu T = 4\mu \sum_{i=1}^{n} \frac{3/2\gamma\pi R_i^*}{A}
\]

(14)

Equation (9) is graphically represented in Fig. 3 in dimensionless form, for different values of \( \mu \). Examination of the results shows the following:

- The shape of the curves is similar to that of the flow curves that are experimentally obtained and to those described by the Warren equation, Equation (1), though only two parameters (\( C \) and \( \mu \)) are used.

- For values of \( \sigma/C \geq 2 \), independently of the value of \( \mu \), the flow curves exhibit a straight stretch, in accordance with the experimentally observed results.

The tensile strength values predicted by the model are of the same order of magnitude as cohesion, \( C \), the \( C/T \) ratio depending on the value of \( \mu \) (Equation (11)). However, it should be noted that for coefficient of friction values between 0.4 and
0.7, which are the most customary values, the values of the C/T ratio predicted by
the model lie around 2, in accordance with the experimental results obtained by
Farley et al. [13].

On the other hand, the fracture criterion is a law of friction of macroscopic
application, which is why the coefficient of friction, $\mu$, will depend on the fracture
surface or yield characteristics, which will, in turn, depend on the microstructural
characteristics of the bed. Kendall, in his model, erroneously applied the Coulomb
criterion (of macroscopic validity) to sphere contact (a microscopic scale), using a
coefficient of friction that only depended on the mechanical properties of the particle
surface and not on the fracture surface, in clear contradiction to the experimental
results. In effect, for a micro-contact, it has been repeatedly verified that the friction
force is equal to the product of the real area of the micro-contact and its shear
strength [10, 11, 12].

1.1.2 Influence of bed compactness ($\phi$) and average particle size ($d$) on
bed cohesion ($C$)

Two of the best-known models for attempting to relate the mechanical properties
of ideal beds of spherical particles to bed compactness, $\phi$, and average particles
size, $d$, are those of Rumpf [14, 15] and Kendall [16]. If the values of $C$ and $T$
are assumed to be proportional, as deduced from Equation (4), and the adhesive
elastic sphere model (JKR) (Equation (5)) is obeyed in the contacts, the Rumpf and
Kendall models lead, respectively, to the following equations:

$$C \propto \frac{\phi}{1 - \phi} d^{-1}$$  \hspace{1cm} (15)

$$C \propto (\phi)^4 d^{-1}$$  \hspace{1cm} (16)
Comparison of Equations (15) and (16) shows that, though they are two quite different models, for practical purposes they only differ in the function that describes the effect of compactness, owing to the ideal particle packing chosen by both. Both models overestimate the value of $C$ fundamentally because the interparticle contact geometry (rough surfaces) and the particle packing characteristics in the bed (heterogeneities in particle distribution, etc.) are of greater complexity than the models based on ideal particle packings (smooth spheres of equal size).

Other models (Cheng [17, 18, 19], Hartley et al. [20], Shinohara [21], etc.) attempt to explain why the experimental values of $T$, and therefore also of $C$, are smaller than the theoretical values and why the effect of compactness on the latter is greater than that described by Equation (15).

1.1.3 Proposed equation

The proposed model has been developed on the basis of the definition of tensile strength, $T$ (Equation (10)), and the fact that $T$ and $C$ are related (Equation (11)). Taking into account these premises, shear fracture will occur when shear stress exceeds a critical value, $C$, which is given by:

$$C \propto nF_{ad} \quad (17)$$

where $n$ is the number of interparticle contacts per unit fracture surface area.

The adhesion between two rough particles is due to the contact between surface protuberances. When a macroscopic contact occurs between two protuberances of two particles, on a microscopic level the roughness of the protuberances actually causes this contact to comprise $n_{cp}$ micro-contacts. The real number of contacts per unit fracture surface area, $n$, is:

$$n = n_{cp}n_{pp} \quad (18)$$

where $n_{pp}$ is the number of interparticle contacts per unit fracture surface area.

Only a single contact occurs between two very fine particles ($d \leq 1\mu m$), whereas in larger particles the number of micro-contacts between the protuberances of the two particles increases with particle size and the load they are subjected to in order to achieve the contact. Therefore, the number of real micro-contacts per contact between two particles, $n_{cp}$, may be expressed as:

$$n_{cp} \propto d^{n_1}\phi^{n_2} \quad (19)$$

If the particles are not spherical, particle distribution and orientation in a bed will clearly be heterogeneous. They will form groups of particles or agglomerates with different structural characteristics (local compactness, coordination number), which are interconnected and heterogeneously distributed. However, these structural characteristics of the bed (average coordination number of the particles, pore size, etc.) become more uniform as bed compactness increases. As a result, the
distribution of the interparticle adhesion forces and adhesion force orientation during the tension test are also heterogeneous, so that only a relatively small group of columns or particle chains will withstand the applied external load [22, 23, 24]. In addition, the number of columns or particle chains grows with bed compactness.

Therefore, the number of interparticle contacts per unit fracture surface area that withstands the stress, \( n_{pp} \), may be expressed as:

\[
 n_{pp} \propto n_{pi}\phi^{n_3}
\]  

(20)

where \( n_{pi} \) is the number of contacts between smooth spherical particles.

Studies of the packing of spheres of the same size indicate that the relation between average coordination number and compactness [25, 21, 26] is not the sole one, and is much more complicated than Rumpf and Kendall assumed. This will also be the case, therefore, for the number of contacts between smooth spherical particles per unit fracture surface area \( n_{pi} \) (Fig. 4).

Figure 4: Relation between \( n_{pi}d_s^2 \) and compactness, \( \phi \), according to different researchers

In Figure 4, the product \( (n_{pi}d_s^2) \) is plotted on a log–log scale versus compactness, \( \phi \), using different relations between the average coordination number, \( Q \), and \( \phi \), described in the literature [27, 28]. The plot corresponding to the Kendall model is also included.

It may be observed that the relation between \( n_{pi} \) and \( \phi \) of the Rumpf model practically coincides with that obtained by other researchers, and may be assumed to be of the power type, with a slope of practically 2.

Therefore, for not excessively large compactness ranges, \( 0.35 \leq \phi \leq 0.60 \), the relation between \( n_{pi} \), \( d_s \), and \( \phi \) may be expressed as:

\[
 n_{pi} \propto \frac{\phi^2}{d_s^2}
\]  

(21)
If the assumption is made that the adhesive elastic sphere model (JKR) (Equation (5)) is obeyed in the contacts between protuberances, and the relations (18) to (21) are taken into account in Equation (17), one obtains the expression:

$$C \propto \phi^m d^{(1-n)}$$  \hspace{1cm} (22)

This equation describes the combined effect of the two variables in a simpler form than many of the (also empirical) equations in the literature.

The objectives of this study were as follows:

- To verify the validity of the proposed model to describe the flow curves of powders
- To study the influence of the average particle size, $d$, and compactness, $\phi$, of monomodal quartz particle beds on the principal parameters of the proposed model

## 2 Materials and experimental techniques used

Five particle size fractions, obtained from a commercial quartz powder by sieving, were used for the study. The particle size distributions were measured by wet laser diffraction using a He-Ne laser of 633 nm wavelength and measurement range of 600 to 0.1 μm. Table 1 details the average diameter ($d_{50}$), Sauter diameter [29] ($d_s$), and standard geometric deviation (s) of the distributions. The Sauter diameter is the diameter that would correspond to a sphere with the same volume–surface ratio as the complete sample and is a parameter that is used to analyse the flow and packing of particulate materials [30, 31]. Particle shape was characterised by determining the shape factor (FF) and aspect ratio (AR), using an image analyser connected to an optical microscope.

The distributions were found to be very narrow ($s$ close to unity), though the amplitude of the distribution tended to decrease slightly as the average particle size, $d_s$, of the powder fraction increased. Quartz particle shape was very similar for all fractions (Fig. 5 and Table 1). Solid density was measured in a helium pycnometer; the same solid (or real) density value, $2650 \pm 20$ kg/m$^3$, was obtained for all test fractions.

<table>
<thead>
<tr>
<th>Reference</th>
<th>$d_{50}$ (μm)</th>
<th>$d_s$ (μm)</th>
<th>s</th>
<th>FF</th>
<th>AR</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>32.4</td>
<td>25.0</td>
<td>1.66</td>
<td>1.68</td>
<td>1.66</td>
</tr>
<tr>
<td>M2</td>
<td>54.6</td>
<td>50.0</td>
<td>1.46</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>M3</td>
<td>98.7</td>
<td>100.0</td>
<td>1.40</td>
<td>1.44</td>
<td>1.72</td>
</tr>
<tr>
<td>M4</td>
<td>141.5</td>
<td>140.0</td>
<td>1.37</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>M5</td>
<td>409.8</td>
<td>390.4</td>
<td>1.26</td>
<td>1.66</td>
<td>1.58</td>
</tr>
</tbody>
</table>

Table 1: Particle size distribution parameters obtained by wet laser diffraction and particle shape.
A model for the flow curves of powders. Study of the rheological behavior of monomodal quartz particle beds under stress

In order to analyse the densification and flow of the solid particulates subjected simultaneously to normal and shear stresses, a rotational cell like the one schematically illustrated in Figure 6 was used [32, 33]. The experimental procedure followed is the one recommended by the rotational shear cell manufacturer [16, 17], and it allows the flow curves of the test powders and the compaction diagrams to be rapidly and automatically obtained.

A study elsewhere [9] verified the validity of the rotational cell by comparing the flow behaviour of a calcium carbonate powder, determined using the rotational cell, with that obtained by five European laboratories using Jenike cells, whose results were published in a report by the Directorate-General of Telecommunications, Information Industries, and Innovation of the EC Commission [34] in 1992.
3 Results and interpretation

3.1 Validity of the proposed model for describing the flow curves of the powders

The monomodal quartz particle beds and the experimental procedure described above were used to obtain flow curves applying different normal stress, $\sigma_c$ in bed preparation, respectively. In order to verify the validity of the proposed model to describe the flow curves, the experimental values of the flow curves for the M1 fraction, applying 490, 980, 1960, 5880, 7350, 11760 and 14700 Pa normal stress, $\sigma_c$, and their fit to Equation (9) are plotted in Figure 7. The experimental values correspond to the arithmetic mean of at least three measurements.

Very good agreement is observed between the experimental values and the calculated ones (solid lines), no significant deviations being noted between the experimental values and the calculated ones in any stretch of the curve. Similar results were found for the other studied particulate materials, thus corroborating the validity of (9) to describe the flow curves.

Figure 7: Fit of the experimental values to the proposed model (Equation (9)) for test fraction (M1)
3.2 Influence of the properties of the beds ($d_s$ and $\phi$) on bed cohesion ($C$) and coefficient of friction ($\mu$)

The fit of the experimental points of the five studied powder fractions to the proposed model was used to calculate the coefficients of friction ($\mu$) and cohesion ($C$) of the beds for the different maximum consolidation stresses ($\sigma_1$). In addition, the compactness ($\phi$) values of the beds were measured for each maximum consolidation stress.

3.2.1 Cohesion of a particle bed, $C$.

In order to verify the validity of Equation (22), the cohesion, $C$, values have been plotted versus bed compactness in Fig. 8. The fits of the experimental points to Equation (22) for the studied beds are represented by solid lines, yielding:

$$C = \frac{5730}{d_s^{1.15}} \phi^{6.4}$$  \hspace{1cm} (23)

It shows that the agreement between the experimental and the calculated values is very good.

It also shows that the effect of compactness on cohesion is much higher ($m = 6.4$) than that predicted by the theoretical models of Rumpf or Kendall ($m = 4$), mainly owing to the pronounced effect of $\phi$ on the actual number of interparticle microcontacts, as was noted in the introduction.

This value of $m = 6.4$ is very similar to that obtained by fitting the experimental results detailed in the literature [19, 20] for other powders to proposed Equation (22). Indeed, by operating in this manner, the values of $m$ obtained for different materials range from 4 to 8, a value of $m$ close to 6 being the most frequent value.

In regard to the effect of particle size, $d_s$, it may be noted that the value of the exponent obtained ($n = 1.15$) is very close to 1, which is the value predicted by the theoretical models of Rumpf and Kendall (Equations (15) and (16)).

3.2.2 Coefficient of friction ($\mu$)

In order to attempt to relate $\mu$ to powder bed characteristics, $\phi$ and $d_s$, the values of $\mu$ have been plotted versus compactness, $\phi$, for the different studied beds in Fig. 9.

The coefficient of friction is observed to increase with compactness until it reaches a practically constant value at a bed compactness, $\phi^*$, which depends on average particle size. Nevertheless, the variation that $\mu$ follows with $\phi$ is independent of average particle size (parallel curves), as is the value to which the coefficient of friction, $\mu^*$, tends.

In view of the foregoing, it has been attempted to fit the experimental results to an equation of the type:

$$(\mu_f - \mu) \propto (\phi^* - \phi)^s$$  \hspace{1cm} (24)
Figure 8: Comparison of the experimental values for C with those calculated from Equation (23)

This yielded the equation:

\[ 0.67 - \mu = 20.7(\phi^* - \phi)^{1.7} \]  

(25)

Fig. 9 shows that the experimental values and the values calculated according to Equation (25) (solid lines) display good agreement.

On the other hand, it should be noted that the effect of particle size, \( d_S \), and bed compactness, \( \phi \), on the coefficient of friction calculated from Equation (25) is analogous to that described by different researchers using the Coulomb equation (Equation (2)) for the calculation [35, 36, 37, 38, 39] .

4 Conclusions

The study conducted allows the following conclusions to be drawn:

- The validity of the proposed model, based on the adhesive contact of elastic spheres, has been verified for describing the flow curves of all the studied monomodal quartz particle beds, solely using the cohesion and coefficient of friction of the powder as parameters.

- The proposed equation has been shown to appropriately describe the combined effect of average particle size and bed compactness on bed cohesion.
A model for the flow curves of powders. Study of the rheological behavior of monomodal quartz particle beds under stress

Figure 9: Variation of the values of $\mu$ with compactness for the studied monomodal beds. Fit of the experimental results to Equation (25).

- The cohesion of the studied monomodal quartz particle beds increases by the sixth power of bed compactness and decreases with the Sauter diameter.

- The coefficient of friction of the studied monomodal quartz particle beds increases asymptotically with bed compactness, this relation depending on average particle size.

In view of the good results obtained, it would be useful to verify the validity of the developed model to describe the flow functions of other powders used in industrial practice, and attempt to relate the characteristics of these beds to the $C$, $T$, and $\mu$ values that are obtained.

References


A model for the flow curves of powders. Study of the rheological behavior of monomodal quartz particle beds under stress


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The energy approach to formulate the criterion of fatigue strength

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Abstract

The energy and the force methods are the most fundamental approach for receiving the deformation and fracture laws for materials and structures. It is well known that the fracture mechanics as a science was originated by a Griffith's energy concept which allows to formulate the strength criterion. According to this criterion the defects like cracks in a solid body were introduced. In our work a criterion of fatigue strength is formulated. The results of modern experimental investigations on latent energy stored in metallic materials during the active plastic deformation are used.

In the process of plastic deformation the significant changes in metallic materials due to increasing of the interior energy are occurred. During the plastic deformation heat is emitted so the deformation energy is transformed into the heat. But not the whole work is emitted to heat. A part of it called a latent energy of deformation [1-5] is transformed to the potential energy of lattice distortion. The latent energy in average constitutes 10-15 % of full deformation energy.

The methods of measuring of latent energy are reduced to measure with a sufficient accuracy the deformation energy and emitted heat. In this case the energy balance is defined by the first low of thermodynamics, which can be written as $U = E - Q$, where $U$ is interior (latent) energy, $E$ is the deformation energy and $Q$ is the heat.

The results of experiments on latent energy carried out in recent years [6-8] show that the relation of the latent energy or the stored energy is expressed in the form of logistics function. Our experiments [9] conducted on cyclic bending of specimens made of construction materials show that the relations of different physical and mechanical characteristics from number of cycles has two precisely expressed regions. Similarly to the logistics function these relations have the precisely expressed point of inflection. These results are the additional confirmation for the introduction of the logistics function to formulate the fatigue strength criterion.
Let us introduce the parameter $\gamma$, which characterizes the relative changes of latent energy $\gamma = \frac{W}{W^*}$, where $W$ is the current and $W^*$ is the limiting values of latent energy, $\gamma_0 \leq \gamma \leq \gamma_*$, where $\gamma_0, \gamma_*$ are initial and limiting values of parameter $\gamma$ consequently, $\gamma_0 < \gamma_* \leq 1$.

It is well known that the logistics functions describe the different processes which lead to saturation [10-12] and they are the solutions of the following kinetics equation

$$\frac{d\gamma}{d\varepsilon} = A\gamma(\gamma_* - \gamma)$$

(1)

where $A$ and $\gamma_*$ are constants. In the common case $A$ and $\gamma_*$ can be functions of stress $A = A(\sigma)$, $\gamma_* = \gamma_*(\sigma)$.

Taking the initial condition $\varepsilon = 0, \gamma = \gamma_*$, the solution of equation (1) may be written as

$$\gamma = \frac{\gamma_*}{1 + \left(\frac{\gamma_*}{\gamma_0} - 1\right) \cdot e^{-A\gamma_*}}.$$  

(2)

The theoretical curve (2) of latent energy accumulation is shown in fig. 1. The results of experiments on specimens made of aluminium alloy 2024-T351 [8] are shown in this figure by cross points. In calculations the following values of constants were used: $A = 26.852$, $\gamma_0 = 0.02$ and $\gamma_* = 0.94$.

![Figure 1:](image)

It is seen that the experimental points of latent energy accumulation are well described by the logistic function (2).
Introducing the fracture condition in the form \( \gamma = a \gamma_* \) where \( a \) is constant, \( 0.5 \leq a \leq 1 \), from (2) we can receive the following relation

\[
\varepsilon = \frac{1}{A \gamma_*} \ln \left( \frac{a}{a-1} \left( \frac{\gamma_*}{\gamma_0} - 1 \right) \right). \tag{3}
\]

It is known \([13, 14]\) that in process of cyclic loadings, in particular, in cyclic tension regime, the accumulation of plastic deformation from cycle to cycle is occurred. The character of the plastic deformation accumulation is similar to those of creep curves. So to describe such curves the power Norton’s law can be used. This law expressed through the number of cycles can be written in the following form

\[
\frac{d\varepsilon}{dN} = B \sigma^m. \tag{4}
\]

We will assume that the stress in one cycle is constant and is equal to the amplitude of stress \( \sigma \). Using the initial condition \( N = 0, \varepsilon = 0 \) the solution of equation (4) can be found as

\[
\varepsilon = B \sigma^m N. \tag{5}
\]

From relations (3) and (5) follows the fatigue fracture criterion

\[
N = \frac{1}{AB \sigma^m \gamma_*} \ln \left( \frac{a}{a-1} \left( \frac{\gamma_*}{\gamma_0} - 1 \right) \right). \tag{6}
\]

Experiments show that the latent energy decreases when stress is increases. So this relation can be expressed by the decreasing power or exponential functions of stress

\[
\gamma_* = (1 + c \sigma)^{-\beta}, \tag{7}
\]

\[
\gamma_* = e^{-\alpha \sigma}, \tag{8}
\]

where \( \alpha, \beta, c \) are constant.

In view (7) and (8) the fracture criterion (6) will be written as

\[
N = \frac{(1 + c \sigma)^{\beta}}{AB \sigma^m} \ln \left( \frac{a}{a-1} \left( \frac{(1 + c \sigma)^{-\beta}}{\gamma_0} - 1 \right) \right). \tag{9}
\]

\[
N = \frac{1}{AB \sigma^m e^{-\alpha \sigma}} \ln \left( \frac{a}{a-1} \left( \frac{e^{-\alpha \sigma}}{\gamma_0} - 1 \right) \right). \tag{10}
\]

The theoretical fatigue curves (9) and (10) were compared with the experimental results received in axial cyclic tensile tests on sheet specimens made of aluminium alloy 2024-T3 [13]. The mechanical properties of this alloy are most similar to the consequent properties of aluminium alloy used in paper [8].

The theoretical fatigue curves (9) and (10) are shown in fig. 2 by solid and dash lines consequently. The following values of constants were accepted: \( A = 26.852 \), \( m = 4 \), \( B = 3 \times 10^{-15}[\text{MPa}]^{-4}[\text{cycles}]^{-1} \), \( a = 0.9 \), \( \alpha = 7.5 \times 10^{-3}[\text{MPa}]^{-1} \), \( c = [\text{MPa}]^{-1} \), \( \beta = 0.61 \). The experimental results are marked by cross points.
Figure 2:

It is seen that these curves are well describe the experimental points on the whole range of fatigue curves.

References


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Investigation of influence of mechanical characteristics of surface layers on deformation response of interfacially controlled materials

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Abstract

The influence of physical-mechanical properties of surface layers of interfacially controlled materials on strain distribution character in the volume of specimens and value of specimen ultimate strain was theoretically investigated. Computer-aided simulation of outrigger bending test under vibration loading was carried out. Movable cellular automaton method was used for simulation. Analysis of simulation results showed that under bending loading a presence of free surface of the specimen led to formation of periodical character of strain distribution along the specimen and, consequently, led to formation of stress concentrators of different intensity in the specimen. Decrease in Young modulus and elastic limit of surface layers (surface modification) increased in ultimate strain of investigated specimens. This is due to surface modification that to decreases the amplitude of the periodic component of the strain distribution and provides more uniform strain distribution in the volume of specimen. Thus, surface modification led to protraction of strain localization processes, reduces of stress concentrators and greatly increases of ultimate strain of the specimens of interfacially structured materials.

1 Introduction

Investigation of mechanical properties of so-called interfacially structured materials and particularities of their mechanical response under complex loading is the important field of modern materials science. Mechanical response of interfacially structured materials is greatly determined by the processes of localization of irreversible deformations on the interfaces of structural units (grains, blocks, etc.) [1]. The reason of this effect is the difference between physical-mechanical properties of structural units and interfaces and relatively high content of defects or damages in the interfaces. Nanostructured materials are the main representatives of this class
of materials where size of grains greatly suppresses realization of traditional dislocation mechanisms of deformation [2, 3]. Therefore, grain boundary mechanisms play a leading role in deformation processes in this materials [4].

A great number of different factors such as size of structural units, structure and properties of interfaces determines physical-mechanical properties of interfacially structured material (including strength and plasticity) [3]. Change of inner structure of material is very difficult and demands modify of technology and methods of its production. One of the most promising methods of changing physical-mechanical properties of interfacially structured materials is modification of their surface layers [5, 6]. The main advantage of this method is absence of necessity of changing of properties in all volume of material. So, because mechanisms of deformation in interfacially structured materials of different nature could be different it is necessary to investigate influence of main parameters of mechanical response of surface layers on macroscopic properties of material.

It this paper on the base of computer-aided simulation using movable cellular automaton (MCA) method [7] influence of surface modification of preload specimens of interfacially structured materials under vibration loading on their deformation response was theoretically investigated. MCA method allows to consider in relatively simple way changing of properties of elements of simulating medium. It is necessary for theoretical investigation of deformation and fracture processes of complex heterogeneous media [8, 9, 10].

2 Simulation results

A structural model of interfacial structured materials shown on fig. 1a was used for investigation. Simulated specimen had complex inner structure consisted of high-strength elastic blocks and interfaces. Mechanical properties of interfaces allowed taking into account accumulation of irreversible deformations. Elastic characteristics of blocks and interfaces corresponded to proper characteristics of titanium [11]. Response functions of movable automata of blocks and interfaces shown on fig. 1b.

Figure 1: Structure of the specimen (a) and response functions of blocks (1) and interfaces (2) (b)

Ratio of linear dimensions of the simulated specimen was \(L:H=3:1\) (here \(L\) is length of the specimen and, \(H\) is its height). Size of blocks was \(0.051H\). For investigation of influence of physical-mechanical properties of surface layers of interfacially
structured materials on its mechanical response modification of surface layers was carried out. Thickness of modified layers was equal to 0.075\(H\) (fig. 1 a). Modification consisted of simultaneous changing of Young modulus \((E_{\text{surf}})\) and elastic limit \((\sigma_{y\text{surf}})\) of response function of automata of interfaces proportionally to non-dimensional modification parameter \(K\): 

\[
\begin{align*}
E_{\text{surf}} &= KE_0 \\
\sigma_{y\text{surf}} &= K\sigma_0,
\end{align*}
\]

Here \(E_0\) and \(\sigma_0\) are Young modulus and elastic limit of initial material of interfaces. It was supposed that modification did not result in changing of sizes of structural units and interfaces. On the figure 1b four response functions are showed (curves 2). They correspond to unmodified \((K=1)\) and modified \((K=1.2, K=0.8, K=0.6)\) interfaces. As shown on the figure changing of elastic parameters of response function leads to changing of degree of strengthening in region of plastic stains. At the same time strength and deformation limit of interfaces does not change. It is necessary to mention that for nanostructured materials this modification could be achieved by means of grain boundary alloying [4].

Loading conditions were the same as in paper [pJTF2004]. The specimen fixed from the left by immovable clip (fig. 1a). Loading of free right side realized by loader moving and was two-staged. At the first stage, the specimen loaded by constant force \(F_0\), directed vertically downward. Value of the force \(F_0\) defined so as limit of elasticity was achieved in large number of interfaces to the end of the first stage (moment of force equilibrium achievement). At the second stage, vibration loading applied to previously loaded specimen. In the paper was used following law of vibration loading:

\[
\begin{align*}
V_{\text{load}} &= V_A \sin \left(\frac{2\pi t}{T}\right), (k - 1) T < t < (k - 0.5) T \\
F_0, (k - 0.5) T < t < k T.
\end{align*}
\]

Here \(V_A\) is an amplitude of velocity changing, \(t\) is a time, \(T\) is a period of loading, \(k = 1, 2, 3\) is a number of cycle. So, at the first half of period of every cycle of loading coercive displacement assigned to loader vertically downward. At the second half period of loading, the specimen was affected by constant force. In paper [1] it was shown that in the presence of vibration loading a great significance had eigenfrequencies of the specimen. They are defined by elastic waves transmission along length \(L\) and height \(H\) of the specimen. Their values lie in an interval between \(\nu_{\perp L} = V_{\perp}/2L\) and \(\nu_{\parallel H} = V_{\parallel}/2H\), where \(V_{\parallel}\) and \(V_{\perp}\) are velocities of longitudinal and transverse waves in material. For simulated specimen takes place following ratio \(\nu_{\perp L}/\nu_{\parallel H} = 0.23\). In this paper frequency of vibration loading from 0 to 5 and modification parameter \(K\) from 0.6 to 1.2 were varied.

Simulation results show that fracture of specimens is the result of generation and accumulation of damages at the interfaces near clip. In the paper [1] it was shown that frequency of loading \(\nu = 1/T\) greatly influences on value of maximum bend of specimen \(\gamma\). Here \(\gamma\) is equal to maximal vertical displacement of loader \(d_{\text{max}}\) divided to length of the specimen \(L\) \((\gamma = d_{\text{max}}/L)\). Typical curves \(\gamma(\nu)\) have three stages.
At the first stage ($\nu < 2\nu_H$) deformation ability of the specimen almost does not change. At the second stage ($\nu > 2\nu_H$) maximum bend of the specimen greatly increases (up to 2-2.5 times). And under high-frequency vibration loading ($\nu > 3.5\nu_H$) increasing of $\gamma$ stops. This character of dependencies $\gamma(\nu)$ is defined by changing of character of plastic strains distribution in the specimen.

Surface modification lead to changing of deformation ability of the specimens in all interval of load frequencies. Decrease of Young modulus and elastic limit of surface interfaces up to 20% and 40% leads to increasing of up to 10% and 20% respectively. In the case of increasing of modification parameter ($K=1.2$) value of maximum bend of the specimen decreases to 10% in comparison with unmodified specimen.

Analysis of investigation results showed that decrease of modification parameter $K$ led to increasing of value of plastically deformed interfaces under vibration loading and consequently led to increasing of deformation ability of the modified specimens. On figure 3 distributions of irreversible normal and shear strains which are localized on the interfaces along the specimen length are shown ($\nu = 1.6\nu_H$). Figure 3 shows that accumulation of irreversible strains on the interfaces first of all takes place in the left part of the specimen. Decrease of modification parameter $K$ from 1 to 0.6 led to increasing of value of strains accumulated in first quarter of the specimens (in the interval from 0 to 0.25$L$). So, specimens with $K=0.8$ and $K=0.6$ have more higher deformation ability the specimens with $K=1$ and $K=1.2$. Detailed investigations showed that this effect took place mainly for surface layers. This proves a great role of plastic deformation of surface in deformation processes [12].

During investigations of the main factors that define character of deformation and fracture of interfacially structured materials it is necessary to take into account presence of free surface of the specimen. Under complex loading presence of free surface could lead to differences between mechanical behavior of surface layers and material in volume of specimen. This effect could appear in formation of complex character of strains distribution in surface layer and greatly influence on mechanical response of whole material [12]. Analysis of results of simulation of outrigger bending tests showed presence of periodical side-view of strain distributions along
Figure 3: Distributions of normal (a) and shear (b) irreversible strains at the interfaces along the specimen length ($\nu = 1, 6\nu_H^\parallel$).

the specimen length. On the figure 4a showed Fourier spectrum of irreversible shear strains distribution along the specimen length for surface layers of different thickness for $K=1$ and $\nu = \nu_H^\parallel$ (here abscissa axis is spatial period and ordinate axis is amplitude of periodical component of deformation side-view $\varepsilon_{\text{shear}}^\text{ampl}$). On the picture you can see peak which corresponds to maximal period of changing of strain side-view of surface layer $T_x/L = 0.22$ (here $T_x$ is a value of spatial period, $L$ is the length of the specimen) and several smaller peaks with smaller values of $T_x$. It is necessary to mention that occurrence of periodical side-view of strains distribution concerned with presence of free surface of the specimen, because amplitudes of presented peaks decrease along depth of the specimen (curves 2 and 3 in fig. 4a). Character of main peak extinction showed on the figure 4b. On the figure 4b showed dependence of amplitude of strain side-view with $T_x/L = 0.22$ on thickness of surface layer (on the figure thickness of surface layer is normalized on height of the specimen $H$). Velocity of main peak extinction is maximal in the upper part of specimen and decrease with depth. So, free surface forms stress concentrators of different intensity and greatly influence on deformation and fracture processes.

Figure 4: a) Fourier spectra of shear strains distributions along the specimen length for $K=1$ and $\nu = \nu_H^\parallel$ (1 - $h/H = 0.07$, 2 - $h/H = 0.25$, 3 - $h/H = 0.5$); b) dependence of amplitude of strain side-view with $T_x/L = 0.22$ on surface layer thickness.

Fourier analysis of spatial strains distributions showed that decreasing of Young
modulus and limit of elasticity of surface interfaces led to decreasing of amplitude of main periodical component of strain side-view and decreasing of amplitudes all other peaks (fig. 5). This effect takes place for surface layers of material (fig. 5 a) and for whole specimen (fig. 5 b). It is necessary to mention that decreasing of amplitudes of periodical components of strain side-view takes place for all frequencies of vibration loading. Thus, this surface modification led to more uniform distribution of strains in the volume of the specimen. This led to reducing stress concentrators and protracting strain localization processes.

Figure 5: Fourier spectra of shear strains distributions along the specimen length for surface layer with thickness \( h/H = 0.07 \) (a) and for whole specimen (b) (\( \nu = \nu_{||}, 1 - K=1, 2 - K=0.6 \))

It is necessary to mention that it is important to investigate not only spatial character of strains distributions. It is necessary to investigate distributions of strains by their values. On figure 6 showed distributions of normal and shear strains contributions. For construction of these distributions in the paper maximum and minimum values of proper strain were defined and obtained ranges (\( [\varepsilon_{\text{normal}}^{\min}, \varepsilon_{\text{normal}}^{\max}] \) for normal strains and \( [\varepsilon_{\text{shear}}^{\min}, \varepsilon_{\text{shear}}^{\max}] \) for shear strains) were divided to \( N \) intervals. Than pares of automata whose values of strains are corresponded to each interval were defined. Strain contributions of every interval defined by summary value of pares of automata, whose values of strains were corresponded to this interval:

\[
\varepsilon_{\text{normal}}^{N,\text{total}} = \sum \varepsilon_{\text{normal}}^{N,\text{aut}},
\]

\[
\varepsilon_{\text{shear}}^{N,\text{total}} = \sum \varepsilon_{\text{shear}}^{N,\text{aut}}.
\]

Here \( \varepsilon_{\text{normal}}^{N,\text{total}} \) and \( \varepsilon_{\text{shear}}^{N,\text{total}} \) are contributions of normal and shear strains correspondingly in the interval \( N \), \( \varepsilon_{\text{normal}}^{N,\text{aut}} \) and \( \varepsilon_{\text{shear}}^{N,\text{aut}} \) are values of normal and shear strains in the pares of automata which are corresponded to interval \( N \).

Deformation ability of the specimens defines mainly by contributions of relatively small strains, which are distributed on large number of interfaces (fig. 6). For example, normal strains distributions greatly changes in the interval from -0.02 to 0.04. The same effect takes place for shear strains. Contribution of highly strained interfaces is negligible. Increase of deformation ability of the modified specimens
caused mainly by increasing of quantity of weakly strained interfaces (fig. 6). So, investigated type of surface modification leads to increasing of volume of interfaces which takes part in processes of plastic strains accumulation.

Figure 6: Distributions of contributions of normal (a) and shear (b) strains in the specimen ($\nu = \nu_{\text{H}}$).

3 Conclusions

Thus, result of investigations show that free surface of the specimen defines periodical character of strains distributions. Modification of physical-mechanical properties of surface layers leads to changing of strains distribution parameters and greatly influences on deformation and fracture processes. For example, decrease of Young modulus and elastic limit of surface interfaces leads to increasing of deformation ability of interfacially structured material. This is due to that fact that in modified specimens irreversible stains distributed more uniform than in unmodified ones.

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References


79 Application of method of special series for numerical and analytical research


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Numerical modelling and analysis of mechanical systems with impacts and dry friction

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Abstract

The work is devoted to modelling and numerical analysis of technical systems with impacts and dry friction. The model of a mechanical system subjected to unilateral constraints, together with the model of stability, are developed. Examples of analysis are presented for plane triple physical pendulum with rigid limiters motions. The model of the piston-connecting rod-crankshaft system of the combustion engine, as a special case of triple pendulum, is also built and gives results conforming experiments. Then an experimental rig of the triple physical pendulum with the first body periodically forced is built. A mathematical model of the real pendulum is created, where friction in joints is modelled as a composition of dry friction and damping. Good agreement between model and real system is obtained.

1 Introduction

Modern achievements in the development of mathematics, mechanics and associated with them numerical calculation techniques allow for more exact modelling of the real dynamic phenomena that are exhibited by various physical objects. Following historical overview of the natural sciences mentioned, a significant role is played by a physical pendulum, which is the very useful mechanism used in the design of various real processes.

A pendulum as a simple non-linear systems is still a subject of interest of scientists from all the world. It is caused by simplicity of that system on the one hand, and due to many fundamental and spectacular phenomena exhibited by a single pendulum on the other hand. In mechanics and physics investigations of single and coupled pendulums are widely applied. Lately, even the monograph on the pendulum has been published [7]. This is a large study on this simple system also from the historical point of view.

Although a single or a double pendulum (in their different forms) are quite often studied experimentally [8, 9], a triple physical pendulum is rather rarely presented
Numerical modelling and analysis of mechanical systems with impacts and dry friction in literature from a point of view of real experimental object. For example, in the work [10] the triple pendulum excited by horizontal harmonic motion of the pendulum frame is presented and a few examples of chaotic attractors are reported. Experimental rigs of any pendulums are still of interest of many researchers dealing with dynamics of continuous multi-degrees-of-freedom mechanical systems. The model having such a properties has been analysed in work [11]. It consists of a chain of $N$ identical pendulums coupled by dumped elastic joints subject to vertical sinusoidal forcing on its base.

On the other hand, it is well known that impact and friction accompany almost all real behaviour, leading to non-smooth dynamics. The non-smooth dynamical systems can be modelled as the so-called piece-wise smooth systems (PWS) and are interesting also from a theoretical point of view, since they can exhibit certain non-classical phenomena of non-linear dynamics. It was a motivation of the first studies of the authors [1, 2, 3] on a triple physical pendulum. In those studies a numerical model of triple physical pendulum with rigid limiters of motion was formulated. Such a system can exhibit impacts as well as sliding solutions, with permanent contact with the obstacle on some time intervals. Special numerical tools for non-linear dynamics analysis of that system exhibiting discontinuities was developed and tested. In addition, application of the numerical model was presented: the piston - connecting rod - crankshaft system of a combustion engine [2].

In February, 2005, in the Department of Automatics and Biomechanics, the experimental rig of triple physical pendulum was finished and activated. This stand has been constructed and built in order to investigate experimentally various phenomena of non-linear dynamics, including regular and chaotic motions, bifurcations, coexisting attractors, etc. It is clear that to have more deep insight into dynamics of the real pendulum, the corresponding mathematical model is required. In references [4, 6] the suitable mathematical modelling and numerical analysis have been performed, where the viscous damping in the pendulum joints (constructed by the use of rolling bearings) has been assumed. In the next step [5], we have also taken into account the dry friction in the joints with many details and variants. Here we present the model of friction taking into account only essential details.

2 Triple pendulum with rigid limiters of motion

In physics and technology, many dynamical systems can be found, which work in the so called different modes, where the system passes from one region to another very quickly. In such cases it is possible to assume that that passing is immediate and discrete. In such a way the system is modelled as a piece-wise-smooth (PWS) dynamical system and can be described by the use of the following equation

$$\dot{x} = f(x), \quad (1)$$

where $x = x(t) \in \mathbb{R}^n$ represents state of the system in the $t$ instance, whilst the map $f: \mathbb{R}^n \to \mathbb{R}^n$ is the piece-wise smooth function, i.e. the phase space $D \subseteq \mathbb{R}^n$ is divided into a finite number of sub-domains $V_i$ on which the function $f$ is smooth, separated by $(n - 1)$ -dimensional hyper-surfaces $\sum_{i,j}$, which are also (at least) piece-wise-smooth.
If the motion of the system goes on inside one of the sub-domains \( V_i \), then the system behaves like a smooth one. When the orbit crosses one of the surfaces \( \Sigma_{i,j} \), the system undergoes a discontinuity. Piece-wise-smooth systems, dependently on the kind of discontinuity, can be classified as follows:

1. Systems with discontinuous Jacobian \( Df \), with continuous but non-smooth vector field \( f \) and smooth state \( x \) (\( f \) is a \( C^0 \) class function).

2. Systems with discontinuous vector field \( f \) and continuous but non-smooth state \( x \).

3. Systems with discontinuous state \( x \). In this case, every time when the system undergoes a contact with one of the discontinuity surfaces \( \Sigma_{i,j} \), its state undergoes jump \( x^+ = g(x^-) \), where \( x^- \) means state of the system just before the contact with the surface \( \Sigma_{i,j} \), while \( x^+ \) is the system state just after that contact, and \( g(x) \) is a piece-wise-smooth (at least) on surfaces \( \Sigma_{i,j} \) function.

PWS systems of the second group (also first group as a subclass) are sometimes called as Filippov systems, for which a special theory is developed. Some electronic systems with elements possessing characteristics, which can be described as discontinuous (diodes, transistor, etc.) are often modelled as PWS systems. Among the mechanical systems we can often meet dynamical systems with dry friction, which can be modeled as systems with discontinuous damping characteristic (second group). Moreover, mechanical system can also posses discontinuous stiffness characteristic. Particularly, mechanical systems with impacts can be modelled as systems with discontinuous stiffness (second group), if we assume flexible bodies model. However, usually we assume rigid body model for impacting systems. In this case the system is a PWS system of the third group, because during the contact of the system with a surface \( \Sigma_{i,j} \) a jumping change of velocity takes place. Here the Newton’s restitution rule is applied in calculation of the post-impact velocity. Such a system is actually a system with unilateral constraints described by the use of algebraic inequalities. It should be noted that it is equivalent to impulse of the function \( f \) (Dirac’s delta type) on one side of the surface \( \Sigma_{i,j} \). However, as it has been shown many times, model of flexible impacting bodies is convergent to impacting model based on the restitution coefficient, if the stiffness of bodies tends to infinity. Moreover, in some systems, different types of discontinuity can be present simultaneously. As an example we can indicate a mechanical system with impacts and dry friction. Both that phenomena can be independent, or the model of impact can take into account friction phenomena on surfaces of impacting bodies.

When the mathematical model is built, the next problem to be solved is to obtain numerical solution of such defined PWS equations, i.e. simulation of the system. Observe that it can be done by gluing smooth solutions (between the successive points of non-smoothness) obtained by the use of classical methods and the points of non-smoothness should be detected. In each point of non-smoothness it is possible the necessity of mapping of the system state to the another state according to the function \( g \). It is sufficient in the case of finite number of non-smoothness points in a finite time interval. It is however possible that the solution on some time interval has permanent contact with some surface \( \Sigma_{i,j} \) and then it is necessary to
Numerical modelling and analysis of mechanical systems with impacts and dry friction

formally reduce number of degrees of freedom or to describe the problem by the use of differential-algebraic equations (DAEs). Before the permanent contact between the solution and the non-smoothness surface $\sum_{i,j}$, the trajectory can cross this surface infinite number of times. In order to solve this problem numerically, we can artificially determine certain shortest time interval between two successive crossings. If the time between two successive crossings becomes shorter, the permanent contact starts.

Figure 1: Triple physical pendulum model.

The so far presented approach has been used in modelling and numerical analysis of plane triple physical pendulum with rigid limiters of motion [1, 2, 3], shown in Figure 1. The system has been modelled as the system of the third group. The obstacles are the surfaces of non-smoothness in the state space, and crossing of anyone of them by the orbit is detected and the system state undergoes jump according to $g$ function. Function $g$ defines an impact law. Here we have assumed that the obstacle surface is smooth, i.e. there is no dry friction accompanying impact. In other words it is assumed that the impact impulse is perpendicular to the impact surface. This condition and additional equation determining the change of the velocity vector in direction perpendicular to the impact surface according to the so-called restitution coefficient, allow for determining velocities after impact with singular obstacle. In our model also some parts of trajectory can be in permanent contact with obstacles. This is very often preceded by the infinite number of impacts in finite time interval. It has been solved in a way described previously. Permanent
contact demands determination of a reaction force generated by an obstacle.

In the next step the authors build the model of the piston - connecting-rod - crankshaft system of the combustion engine as a special case of triple physical pendulum, where the piston in the cylinder barrel moves with backlash and impact an appear [3]. Figure 2 presents simulation results of this system with restitution coefficient equal to 0.5. This is periodic solution and typical behaviour is seen. Namely, the piston six times moves from one side of the cylinder barrel to the other one during one cycle of the engine work.

![Figure 2: Response of the piston - connecting-rod - crankshaft system for the restitution coefficient $e = 0.5$ ($x_{O3}$ is the pin position coordinate along direction perpendicular to cylinder axis, $\psi_1$ is angular position of the shaft).](image)

The next step is the orbit stability analysis in such kind of systems. In PWS systems, on each part of solution, where the orbit is smooth, the perturbations also behave smoothly according to typical linearized equation. However, in the non-smoothness points we should transform the perturbation state in a special way. Then we can apply classical methods for Lyapunov exponents calculations, periodic orbit stability analysis and classical bifurcation of periodic orbits analysis. In Figure 3 exemplary periodic, quasi-periodic and chaotic solutions exhibited by triple physical pendulum with horizontal barrier and with the first pendulum harmonically forced, are presented. Let us note that because of some parts of the orbit with the permanent contact with the barrier, two Lyapunov exponents (for each orbit) tend to minus infinity.

In PWS systems all kinds of bifurcations typical for smooth systems can be observed and they can be analysed by the use of classical methods with some special modifications described above. Moreover, in PWS systems we can also find non-classical bifurcation, which can be detected only in non-smooth dynamical systems. An example of such a bifurcation is grazing bifurcation. Note also that analysis of
Numerical modelling and analysis of mechanical systems with impacts and dry friction

3 Experimental rig

The experimental rig (see Fig. 4) of the triple physical pendulum consists of the following subsystems: pendulum, driving subsystem and the measurement subsystem. It is assumed that the pendulum is moving in a plane.

Figure 4: Experimental rig: 1, 2, 3 - links; 4 - stand; 5 - rotors; 6 - stators; 7, 8, 9 - rotational potentiometers.

The links (1, 2, 3) are suspended on the frame (4) and joined by the use of radial and axial needle bearings. The first link is forced by a special direct-current motor of our own construction with optical commutation consisting of two stators (6) and
two rotors (5). The construction ensures avoiding the skewing of the structure and forming the forces and moments in planes different that the plane of the assumed pendulum motion. On the other hand the construction allows the full rotations of all the links of the pendulum.

The voltage conveyed to the engine inductors is controlled by the use of special digital system of our own construction together with precise signal generator HAMEG. As a result the square-shape in time forcing (but with some asymmetry - see next sections) with adjustable frequency and desired amplitude is obtained.

The measurement of the angular position of the three links is realized by the use of precise rotational potentiometers (7, 8, 9). Then the LabView measure- programming system is applied for experimental data acquisition and presentation on a computer.

4 Mathematical model

Details on physical modeling, i.e. idealized physical concept of real pendulum presented in Fig. 4, can be found in works [5, 6]. The system is idealized since it is assumed that it is an ideally plane system of coupled links, moving in the vacuum with the assumed model of friction in joints. The system is governed by the following set of differential equations:

\[
\begin{bmatrix}
B_1 & N_{12} \cos(\psi_1 - \psi_2) & N_{13} \cos(\psi_1 - \psi_3) \\
N_{12} \cos(\psi_1 - \psi_2) & B_2 & N_{23} \cos(\psi_2 - \psi_3) \\
N_{13} \cos(\psi_1 - \psi_3) & N_{23} \cos(\psi_2 - \psi_3) & B_3
\end{bmatrix}
\begin{bmatrix}
\dot{\psi}_1 \\
\dot{\psi}_2 \\
\dot{\psi}_3
\end{bmatrix}
+ \begin{bmatrix}
0 & N_{12} \sin(\psi_1 - \psi_2) & N_{13} \sin(\psi_1 - \psi_3) \\
-N_{12} \sin(\psi_1 - \psi_2) & 0 & N_{23} \sin(\psi_2 - \psi_3) \\
-N_{13} \sin(\psi_1 - \psi_3) & -N_{23} \sin(\psi_2 - \psi_3) & 0
\end{bmatrix}
\begin{bmatrix}
\psi_1 \\
\psi_2 \\
\psi_3
\end{bmatrix}
+ \begin{bmatrix}
M_{R1}(\psi_1) - M_{R2}(\psi_1, \psi_2) \\
M_{R2}(\psi_1, \psi_2) - M_{R3}(\psi_2, \psi_3) \\
M_{R3}(\psi_2, \psi_3)
\end{bmatrix}
+ \begin{bmatrix}
M_1 \sin \psi_1 \\
M_2 \sin \psi_2 \\
M_3 \sin \psi_3
\end{bmatrix}
= \begin{bmatrix}
M_c(t) \\
0 \\
0
\end{bmatrix},
\]

where the pendulum position is governed by three angles \(\psi_i (i = 1, 2, 3)\), and where

\[
M_{R1} = T_1 \frac{2}{\pi} \arctan (\epsilon \psi_1) + 2c\psi_1,
\]

\[
M_{R2} = T_2 \frac{2}{\pi} \arctan \left( \frac{\epsilon (\psi_2 - \psi_1)}{2} \right) + c(\psi_2 - \psi_1),
\]

\[
M_{R3} = T_3 \frac{2}{\pi} \arctan \left( \frac{\epsilon (\psi_3 - \psi_2)}{2} \right) + c(\psi_3 - \psi_2),
\]

are the moments of resistance in the corresponding joints and consisting of two parts: dry friction and viscous damping. The dry friction moment does not depend on the loading of the corresponding bearing and the sign function is approximated by the arctan function. The parameter \(c\) is the damping coefficient common for the second and third joint, while in the first joint two times larger damping is taken (since the
first joint is built by the use of four bearings, while each other joint contain two bearings).

In reference [6] more complex model of friction has been investigated, where the dry friction moment consists of two part: the first one being proportional to the normal loading in the bearing, and the second one being constant and present also in the lack of loading. Moreover, the friction is a function of relative velocity due to the Stribeck’s curve. As a result of those investigations we have concluded that in our case the model of friction can be simplified to the one presented by the Eq. (3), without any loss of precision.

The external excitation in the pendulum model can be an arbitrary time function, and in particular, it can be the same function as applied (and recorded to a file) in real system (it is useful in the parameter estimation process). On the other hand, it is possible to apply a forcing due to the following formula:

\[
M_e(t) = \begin{cases} 
q & \text{if } \omega t + \phi_0 \mod 2\pi \leq 2\pi a \\
-q & \text{if } \omega t + \phi_0 \mod 2\pi > 2\pi a,
\end{cases}
\]

which imitates the square-shape in time forcing (applied in the real pendulum), with adjustable angular velocity \(\omega\), initial phase \(\phi_0\), amplitude \(q\) and the coefficient \(a\) (for \(a \neq 0.5\) there is an asymmetry in the forcing).

5 Model parameters

The model parameters are estimated by the global minimum searching of the criterion-function of the model and real system matching. The matching of model and real system is understood as the matching of the corresponding output signals \(\psi_i(t) (i = 1,2,3)\) from model integrated numerically and from the real pendulum, assuming the same inputs to both model and real systems. The sum of squares of deviations between corresponding samples of signals from the model and the experiment, taken for few different solutions serves as a criterion function. Together with the model parameters also initial conditions of the numerical simulation are estimated. A minimum is searched applying the simplex method. In order to avoid the local minima, the simplex method is stopped from time to time and a random searching is then applied. After random searching the simplex method is restarted again.

If we divide final value of criterion-function by the number of samples used in calculation of criterion-function, we obtain average square of deviation between two signals (obtained from the model and the experiment). In what follows we denote this parameter by \(F_{cr}\). Now this parameter can be used for comparison of matching of different sets of experimental data and corresponding numerical solutions.

In Table 1 the part of the results of the parameter estimations performed in work [6] is presented. Three different sets of parameters, correspondingly to three variants of the model of resistance in the joints are presented. The set \(A_1\) corresponds to the model with dry friction only. The model \(B_1\) contains also viscous damping. The next model \((C_1)\) is a development of the previous one \((B_1)\): the parameter \(\varepsilon\) is added to the set of the identified parameters.
In all the identification processes, the same set of experimental solutions is used: five periodic solutions with the forcing frequencies \( f = \omega/2\pi \): \( f = 0.2, 0.35, 0.6, 0.85 \) and \( 1.1 \) Hz (for each the solution the 20 sec of motion was recorded, after ignoring the transient motions) and one decaying solution, which starts from the periodic attractor with forcing frequency \( f = 0.5 \) Hz (after few seconds of the recorded motion, the forcing was switched off and the total length of the recorded motion was 24 sec). Note that in our work, we do not measure actual value of the forcing, but only the control signal is recorded (determining the sign of the forcing), since we assume the constant forcing amplitude \( q = 1.718 \) Nm (determined before the identification experiments).

### 6 Simulation results

In the upper part of Fig. 5 the final model \( C_1 \) and real system matching for vanishing motion (started from the periodic attractor with the forcing frequency \( f = 0.5 \) Hz), obtained during the identification process, is presented. In this scale we see almost perfect matching of the corresponding behaviours. The bottom part of Fig. 5 presents enlargement of the final phase of decaying of the same motion, where in addition the simulation of the model \( A_1 \) is shown. Here we can observe in details certain aspect of the difference between models \( A_1 \) and \( C_1 \).

Figure 6 show results of investigation of the forcing frequency region 0.13-0.14 Hz. It is an example that the developed model with its parameters can predict real pendulum dynamics exhibited also for forcing frequencies \( f \) outside the region 0.2-1.1 Hz (containing all the periodic solutions studied during the identification process).

---

<table>
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<th>( A_1 )</th>
<th>( B_1 )</th>
<th>( C_1 )</th>
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Figure 5: Final model ($C_1$ and $A_1$) and real system matching for vanishing motion
Figure 6: Bifurcation diagrams exhibited by experiment and model (C₁) with the parameter $f$ growing ($\rightarrow$) and decreasing ($\leftarrow$).
7 Concluding remarks

The Aizerman-Gantmakher theory, handling with perturbed solution in points of discontinuity, is used to extend classical method for computing Lyapunov exponents for the multi-degree of freedom mechanical system with rigid barriers imposed on its position. Some examples of identification of attractors in the system of triple pendulum with horizontal barrier are presented, including periodic, quasi-periodic and chaotic attractors with impacts as well as attractors with some segments of trajectory lying on the surface of the obstacle, where the obstacle is permanently active in a certain time interval and the two Lyapunov exponents are degenerated, i.e. their values reach infinity.

Few versions of the model of resistance in the joints have been tested in the identification process. Good agreement between both numerical simulation results and experimental measurements have been obtained and presented for all of the friction model variants. However, one of them (\(C_1\)) seems to be optimal, since it gives relatively good results with simultaneous simplicity of the model itself keeping simultaneously high simulation speed.

The model \(C_1\) is better for simulation (higher simulation speed) than others because the \(\varepsilon\) parameter is much smaller and the characteristic of the friction torque is smooth. Observe that model \(C_1\) gives better results than model \(B_1\), while only the parameter \(\varepsilon\) is modified one (the result is the smaller value of the parameter \(\varepsilon\)).

I should be noted, that examples of numerical and experimental simulations presented in section 6 are selective. However, the presented examples show quite good agreement between numerical and experimental results. It leads to conclusion that the used mathematical model of triple pendulum with its parameters estimated can be applied as a tool for quick searching for various phenomena of non-linear dynamics exhibited by a real pendulum as well as for explanation of its rich dynamics.

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Model of the superdeep penetration of microparticles in solid body

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Abstract

In 1974 an unusual phenomenon called Usherenko effect was observed in impact experiments [1, 2]. Surprisingly large were impact produced craters whose depth varied between 100 and 10000 times the impactor’s size. For materials whose static strength is small or zero, e.g., sand or water, the depth of penetration is no larger than 100 times the size. When a macro-size body impacts on a barrier, it produces a crater whose depth is normally in a ratio of no larger than 6-10 to the body’s size regardless impact parameters.

The papers [1, 3] give overviews of models which were developed to explain the phenomenon. They all try to answer why material resistance to the penetration of micro-size impactors suddenly decreases.

This physical phenomenon is used to solve practical problems in the development of new composite materials or in the experimental verification of aircraft proofing or electronic control system reliability. However none of the proposed models (now about fifteen) has been found as good as to become a theory of superdeep penetration.

We suggest a model that uses the concept of particle entrainment by a shock produced by the impact of a bunch of particles on a barrier. The approach was proposed by V.A. Simonenko [4, 5]. Its advantage consists in the initial account for the collective effect (a shock from the impact of many particles). It is based on calculations by the finite-difference technique TWS [6, 7]. Such an approach shows prospects for further development with account for new experimental results obtained after 1991.

The goal of this paper is to demonstrate feasibility of applying this approach for justification of impactor’s acceleration in solid.

1 Numerical experiment

Using the TWS technique and code, the authors undertook a numerical experiment in the following setup. A perfectly rigid spherical microparticle $10^{-5}$ m in diameter
was given the shock velocity. The initially non-smeared shock passed through its center. In further simulation, the shock smeared, but the particle remained within the width of the smeared shock and could penetrate to any depth if nothing (rarefaction waves from barrier edges, a rarefaction wave from the outer side of HE etc.) could decrease the amplitude of the shock front.

It is important to explain why a particle from a bunch (a powder) impacting on a barrier at a velocity of about $1\text{km/s}$, accelerates to the shock velocity of about $4 - 5\text{km/s}$ (higher than the velocity of longitudinal waves in the barrier). It was earlier supposed that internal (in a powdered material) cumulative effects were responsible for the phenomenon.

We are going to explain such an increase in particle velocity by dynamics of particle motion on the shock front. Construct a model which describes the motion of a perfectly rigid spherical particle on the front of a smeared shock.

The basic assumptions of the model are as follows:

1. The width of the shock front is finite and equal to $H$;
2. All flow parameters on the front are distributed linearly; and
3. A gas "particle" passing the front accelerates to the velocity dictated by the Hugoniot criterion.

Consider a spherical microparticle on the wave front (Figure 1).

![Figure 1: Spherical microparticle on the wave front](image)

Two forces act on the particle: a pressure force $F_y$ from a pressure gradient on the wave front and a drag force $F_c$ due to material flow past the penetrating particle. The first force is expressed as

$$ P_B l^2 - P_A l^2 = l^2 \frac{\partial p}{\partial x} l = \frac{p}{H} l^3 $$

and the second is

$$ F_c = c_x l^2 \rho \frac{(u - u_n)^2}{2} \text{sign}(u - u_n), $$

where $c_x$ is the drag coefficient, $\rho$ is flow density, $u_n$ is flow velocity, $u$ is particle velocity, and $l$ is a characteristic particle size (e.g., radius). Since particle mass is $\frac{4\pi}{3} \rho_s l^3$ ($\rho_s$ is particle density), the equation of its motion takes the form

$$ \rho_s l^3 \frac{du}{dt} = l^3 \frac{p}{H} - c_x l^2 \rho \frac{(u - u_n)^2}{2} \text{sign}(u - u_n), $$
As we are considering particle motion on a wave front, we introduce a variable
\[ \xi = \int_0^t (D - u) \, dt, \]
where \( D \) is wave velocity.

Then Eq. (1) can be rewritten as
\[ \rho_s (D - u) \frac{du}{d\xi} = \frac{P}{H} - \rho c_s \frac{1}{2} l^2 (u - u_n) |u - u_n|. \] (2)

and its solution is sought for \( \xi \in [0, H] \).

By virtue of the second assumption, we assume that
\[ u_n = u_2 \frac{\xi}{H}, \]
\[ \rho = \rho_0 \left( 1 - \frac{\xi}{H} \right) + \rho_2 \frac{\xi}{H}, \]
where \( \rho_0 \) is the initial density of barrier material, \( u_2 \) is Hugoniot velocity, i.e., particle flow velocity behind the shock front, and \( \rho_2 \) is material density behind the front.

Take all necessary equations:
\[ u_2^2 = \frac{P \left( \frac{\rho_2}{\rho_0} - 1 \right)}{\rho_2}, \quad D = \frac{\rho_2 u_2}{\rho_2 - \rho_0}. \] (3)

Our further consideration is limited to the "cold" equation of state for barrier material:
\[ P = \frac{\rho_0 c_0^2}{n} \left( \frac{\rho}{\rho_0} \right)^n - 1, \] (4)
where \( c_0^2 \) is the squared velocity of sound in barrier material and \( P \) is pressure.

Introduce the following dimensionless parameters and variables:
\[ a_1 = \frac{\rho_s}{\rho_0}, \quad \lambda = \frac{P}{\rho_0 D^2}, \quad m = \frac{H}{T}, \quad \rho_2 = d, \quad V = \frac{u}{D}, \quad \xi = \eta H, \quad \eta \in [0, 1]. \]

Then Eq. (2) takes the form
\[ (1 - V) a_1 \frac{dV}{d\eta} = \lambda - c_s \frac{m}{2} (V - V_2 \eta) |V - V_2 \eta| (1 - \eta + \eta d). \] (5)
Here $V_2$ is a dimensionless Hugoniot velocity of the flow behind the wave front. Eq. (3) takes the form

$$V_2^2 = \frac{(d^n - 1)(d - 1) c_0^2}{nD^2}.$$  

In real barriers, $D^2 \approx c_0^2$ and

$$V_2 = \sqrt{\frac{(d^n - 1)(d - 1)}{nd}}. \quad (6)$$

Then Eq. (4) takes the form

$$P = \frac{\rho_0 c_0^2}{n}(d^n - 1)$$

and

$$\lambda = \frac{d^n - 1}{n}.$$  

Finally the equation of particle motion takes the form

$$(1 - V) a_1 \frac{dV}{d\eta} = \frac{1}{n}(d^n - 1) - c_x \frac{m}{2} \left( V - \sqrt{\frac{(d^n - 1)(d - 1)}{nd}} \eta \right) \cdot \left| V - \sqrt{\frac{(d^n - 1)(d - 1)}{nd}} \eta \right| (1 - \eta + \eta d). \quad (7)$$

For a simple equation of state, i.e., $n = 1$, Eq. (7) takes the form

$$(1 - V) a_1 \frac{dV}{d\eta} = (d - 1) - c_x \frac{m}{2} \left( V - \frac{d - 1}{\sqrt{d}} \eta \right) \left| V - \frac{d - 1}{\sqrt{d}} \eta \right| (1 - \eta + \eta d).$$

This equation was solved on a computer with different sets of parameters and initial velocities. The only point was in question. What is the initial velocity $V_0$ at which the particle on the wave front reaches the shock velocity, i.e., $V = 1$ in the range $[0, 1]$?

Lots of calculations were run, but there is no use in discussing all results in this paper. Everyone who wants can easily repeat our calculations. Below we briefly summarize our conclusions.

1. If the differential in pressure across the wave is large ($d - 1 = 0.6, a_1 = 1$), the particle with zero initial velocity reaches the shock velocity when the drag coefficient $\frac{c_x m}{2} \leq 0.5$. In most experiments, the initial particle velocity was about 1 km/s and the wave velocity was 4–5 km/s, i.e., $V_0$ was equal to 0.25. Therefore constraints on problem parameters become much weaker.

2. When $d - 1 = 0.3$ and $a_1 = 1$, the particle reaches the shock velocity if its initial velocity $V_0 = 0.4$ for $\frac{c_x m}{2} \leq 0.25$ or $V_0 = 0.3$ for $\frac{c_x m}{2} \leq 0.05$. 

To prove the above assumptions and conclusions on the mechanism that governs particle entrainment by the strong shock, we have simulated the SDP process by the finite-difference code TWS [4].

The setup was as follows. A perfectly rigid particle $10^{-5}$m in size was placed in a barrier at a depth equal to its 5 diameters. Its motion was modeled in a noninertial cylindrical frame of reference $(z, r)$ whose origin was in the center of the particle and the $OZ$ axis was pointed into the barrier.

Boundary conditions can be chosen arbitrary because rarefaction waves running from the barrier edges are of no effect on particle penetration at the time of interest. We chose them to be as follows. The right boundary ($z = 20\varnothing$; $\varnothing$ is particle diameter) was defined as a free surface. The side surface ($r = 20\varnothing$) was defined as a perfectly rigid wall. On the left boundary ($z = -60\varnothing$) we defined time-invariant Hugoniot conditions for a shock moving at velocity $D = 5$km/s.

At the initial time the wave front was on the surface $z = 0$, i.e., in the particle center.

Barrier material rheology was described with the Prandtl-Reuss elastic-plastic model. The equation of state was taken in the form

$$p = c_0^2(\rho - \rho_0).$$

The thermal pressure was not accounted for. The barrier material had the volume velocity of sound $c_0 = 3$km/s, the initial density $\rho_0 = 7.8$g/cm$^3$, Poisson’s ratio $\nu = 0.3$, shear strength $\tau = 0.36$GPa, and breaking strength $0.2$GPa.

TWS is peculiar in its tracking discontinuities through a fixed finite-difference mesh with use of random sampling [6].

Calculated results are illustrated below in Figs. 2-10 that provide a record of the penetration process.

In the figures, $d$ stands for material density, $Z$ for the $Z$ axis, $R$ for the $r$ axis, $U_s,n$ for particle velocity, and $Z_s,n$ for the depth of penetration. Units of measurement are as follows. Unit length is $10^{-5}$m; unit time is $10^{-8}$s; unit mass is $10^{-8}$g. The derived units are: unit density $0.1$g/cm$^3$; unit velocity $1$km/s; and unit pressure $0.1$GPa.
The shock front is at \( Z = 0 \); for \( t > 0 \), Hugoniot conditions for strong shock moving at \( D = 5 \text{km/s} \) were defined on the left boundary at \( Z = -6\varnothing \).
Particle velocity is $U_{sn} = 5.20$. The depth of particle penetration is $Z_{sn} = 5.2$.

An eddy is seen behind the spherical particle (its shape in the figure is distorted because of different scales of the coordinate axes). What is happening around the particle is observed in the center-of-particle coordinates. The barrier seems to lap on the particle and therefore the velocity field in front of it is nonzero.

Figure 4: A vector field of relative velocities at $t = 1.1$, $U_{sn} = 5.32$, $Z_{sn} = 5.6$

Figure 5: Velocity field at $t = 5.14$, $U_{sn} = 5.2$, $Z_{sn} = 26.2$
Figure 6: Density field at $t = 8.04$, $U_{sn} = 5.25$, $Z_{sn} = 40.5$

Figure 7: Density field at $t = 8.04$, $U_{sn} = 5.25$, $Z_{sn} = 40.5$
Two eddies are now seen behind the particle.

Figure 8: Density field at $t = 18.06$, $U_{sn} = 5.07$, $Z_{sn} = 88.6$

The number of eddies is three. The third is seen on the boundary. If the left boundary were farther from the particle, we would see more eddies.

Figure 9: Velocity field at $t = 18.06$
Conclusions

So the velocity of the spherical particle oscillates about 5km/s, exactly the shock velocity. During the time $t = 22$ the particle has penetrated to a depth of 109 diameters and will go on moving till our assumptions and boundary conditions remain applicable.

The above figures demonstrate eddy flows behind the particle. This is normal because under pressures that realize on the front of the almost stationary strong shock, the elastic-plastic behavior of metal is similar to that of viscous liquid whose viscosity is described by the plasticity equation for barrier material. And it is known that the flow of liquid past a body usually produces eddy behind it.

It is important here to note the following. It was proposed that the impact of a particle flow on the surface of a target produces such conditions for each individual particle that correspond to the strong shock. The shock front interacting with the surface is plane. In actual situations, particle velocity varies between 0.3 and 3km/s. The density of particle flow also varies in space.

Experimental evidence suggests that fibrous structures are present in the target material, where phase transitions occur. It is clear that the plane shock and the constant-in-space material density behind its front cannot anyhow describe the fibrous structure in the target.

It would seem possible to improve the hypothesis of particle entrainment by the wave if refuse the assumption that material properties behind the shock front are uniform. In this case the mathematical problem becomes three-dimensional in spatial variables, which strongly complicates numerical simulations.

One more hypothesis can be proposed. The impact of a bunch of particles on
a target produces local strong shocks for individual particles. Then the particle entrained by the shock front penetrates deeper leaving a vortex wake behind. Pressures behind the shock front are as high as to allow phase transitions in metal to occur, and they will occur. What allows the particle to penetrate is the energy of the particle flow incident on the target.

What could reproduce the actual superdeep penetration conditions better is the direct simulation of HE detonation, generation of the cumulative jet and the impact of particle flow on target. But it is impossible to describe the distribution of particle velocities in the flow in all details and we will inevitably have to use simplifying assumptions.

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Forces and moments acting on the rapidly rotating floating bearing

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Abstract

An extension of the classical short-bearing theory for rotating shafts is presented. While the classical short-bearing theory was derived for rotating solid shafts being beard in a fixed circular solid housing, the gap between the two solids being filled by flowing oil, we here consider the fundamental case of a pre-stressed oil flow between a rotating cylinder, whose rotation axis is fixed in space, and the rotating bearing. As a main result, analytic formulations for the forces and moments acting in this fundamental case are derived, where the effect of centrifugal forces is retained, since the latter becomes crucial for rapid rotations. The presented fundamental results therefore can be used in the more complex case of rapidly rotating floating bearings, which consist of a fixed cylindrical housing, a circular solid ring with an own rotational speed, and a rapidly rotating shaft, the two gaps between the three solids being filled by pre-stressed flowing oil.

Introduction

The present contribution is concerned with an extension of the current state-of-the-art of the modelling of reactive forces and moments that act on rotating shafts supported by oil bearings. Comprehensive presentations of methods for describing the reaction forces transmitted to rotating shafts via the flow of pre-stressed oil contained in classical bearings can be found in the books by Childs [1], Gasch, Nordmann, Pfuetzner [2] and Kraemer [3]. In classical bearings, the housing of the
bearings can be assumed as fixed in space. Based on both, constructive and computational considerations, the so-called classical short-bearing theory enjoys particular interest in practice. This theory allows deriving analytic expressions for the forces transmitted to the rotating shaft as functions of its current position, and of the rate of change of the latter. Such an analytic formulation, avoiding the direct solution of the hydrodynamic field equations for the oil flow in the gap between shaft and housing, is perfectly suited for setting up the equations of motion for a co-rotating solid body (the rotor) that is supported by the shaft. The basic considerations of the short-bearing theory date back to a fundamental study by Dubois and Ocvirk [4]. As long as the rotation speed is comparatively low, classical bearings and the corresponding short-bearing theory turned out to lead to excellent design performance. Due to the increased use of rapidly rotating shafts, and also in order to improve the maintenance of industrial rotors, floating bearings have been introduced, see Li [5] and Szeri [6]. In floating bearings, a solid ring is situated between the fixed housing and the rotating shaft, the ring being allowed to rotate, where a pump provides pre-stressed oil to fill the gap between the rotating shaft and the solid ring (generally rotating with an own speed), as well as the gap between the ring and the fixed housing. The present work is an attempt to extend the short-bearing theory for classical bearings towards floating bearings. Our work is organized as follows. In Section 1, we present the hydrodynamic field equations valid for the rotating oil present in the gap between two rotating cylindrical solids. This results in approximate Navier-Stokes equations in cylindrical coordinates, the oil in the gap being assumed to be an incompressible Newton fluid. Because of the lack of space, we then restrict to one of the gaps in floating bearings, where we study the fundamental case of a flow between a rotating cylinder whose rotation axis is fixed in space and the rotating bearing. (Recall that the classical short-bearing theory in contrast deals with a cylindrical housing fixed in space.) Section 2 represents corresponding integrals of the hydrodynamic field relations given in Section 1 above. In the Section 3, extensions of the classical Reynolds equations are derived for the considered case of a flow between a rotating cylinder whose rotation axis is fixed in space and the rotating bearing. Since we deal with rapidly rotating shafts, the centrifugal forces are retained in our formulations, this also representing an extension to the literature. The short bearing approximation is introduced into our formulations in Section 4, resulting in the desired forces and moments in Section 5. The case of classical bearings is contained as a special case. By proper extension to the case of two gaps, the presented fundamental solution will allow to model a full floating bearing consisting of a fixed housing, a rotating ring and a rapidly rotating shaft. This will be shown in full length in a future contribution.

1 Velocity and pressure in the gap of rotating shaft

The motion of the oil in the gap of a rotating shaft is governed by the balance of linear momentum

\[ \nabla \cdot \tau - \rho \ddot{\mathbf{v}} = 0, \]  

(1)
in which $\tau$ is the stress tensor and $\rho$ is the mass density. The velocity vector $v$ and the Hamilton operator $\nabla$ in a cylindrical coordinate system are

$$v = e_r u + e_\phi v + e_z w, \quad \nabla = e_r \frac{\partial}{\partial r} + e_\phi \frac{1}{r} \frac{\partial}{\partial \phi} + e_z \frac{\partial}{\partial z}. \quad (2)$$

The oil in the gap is assumed to be an incompressible Newton fluid; i.e.

$$\tau = -pE + s, \quad s = 2\mu (\nabla v), \quad p \geq 0, \quad (3)$$
in which $p$ denotes the oil pressure, $s$ is the deviator of $\tau$ and $\mu$ is the dynamic viscosity. We assume a quasi-stationary flow and obtain the material time-rate of the velocity in the form

$$\dot{v} = \frac{dv}{dt} = \frac{\partial v}{\partial t} + v \cdot (\nabla v) = v \cdot (\nabla v), \quad (4)$$

Calculating the symmetric part of the velocity gradient $(\nabla v)^s$ by means of eq. (2) and inserting the result into eq. (1) yields the Navier-Stokes equation in cylindrical coordinates. For instance the equation in the radial direction is given by

$$\frac{\partial p}{\partial r} = \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \phi^2} + \frac{\partial^2 u}{\partial z^2} - \frac{r}{r^2} \frac{\partial u}{\partial z} - \frac{2}{r^2} \frac{\partial v}{\partial r} \right]$$

$$- \rho \left( u \frac{\partial u}{\partial r} + \frac{v}{r} \left( \frac{1}{r} \frac{\partial u}{\partial \phi} - \frac{v}{r} \right) + w \frac{\partial u}{\partial z} \right). \quad (5)$$

Next, we assume a laminar flow and we neglect the radial component $u$ of the velocity vector in comparison with the other components. The gap is very narrow and the velocity changes drastically in the gap, which allows one to make the following assumptions: the dependence of the velocity vector on $\phi$ and $z$ is very weak, i.e. $\partial / (r \partial \phi) \ll \partial / \partial r$ and $\partial / \partial z \ll \partial / \partial r$. These approximations result in three scalar equations

$$e_r : \quad \frac{\partial p}{\partial r} = \rho \frac{\partial v^2}{r},$$

$$e_\phi : \quad \frac{\partial p}{\partial \phi} = \rho \left( \frac{1}{r} \frac{\partial u}{\partial \phi} - \frac{v}{r} \right),$$

$$e_z : \quad \frac{\partial p}{\partial z} = \frac{1}{r} \frac{\partial u}{\partial \phi} \left( \frac{r}{\partial \phi} \right), \quad (6)$$
in which $\nu$ is the kinematic viscosity.

### 2 Flow in the gap

The further consideration is limited to one of the two gaps of the floating bearing. Because of the lack of space, we study the flow between a rotating cylinder whose rotation axis is fixed in space and the floating bearing. The boundary conditions for the boundary value problem are

$$r = R : \quad u_o = 0, \quad v_o = R \omega, \quad w_o = 0,$$

$$r = r_o = R - h_o : \quad u_o = -h_o, \quad v_o = \Omega_B (R - h_o), \quad w_o = 0. \quad (7)$$
Here \( h_o \) is the gap height, \( \omega \) and \( R \) are the angular velocity and the internal radius of the rotating cylinder, whereas \( \Omega_B \) and \( r_o \) are the angular velocity and the external radius of the bearing. Equation (7) assumes that the axes of rotation of the housing and the floating bearing are coincident.

Integration of the first equation in eq. (6) yields

\[
p_o = \int \rho \frac{\nu_o^2}{r} \, dr + P_o(\varphi, z),
\]

while integrating the second and third equations of eq. (6) and neglecting the weak dependence of the velocity on \( \varphi \) and \( z \) we obtain

\[
v_o = \frac{1}{4} \frac{\partial P_o}{\partial \varphi} r + C_{o1} \ln(r) + C_{o2}, \quad w_o = \frac{1}{4} \frac{\partial P_o}{\partial z} r^2 + K_{o1} \ln(r) + K_{o2}.
\]

The integration constants are to be determined from the boundary conditions for \( v_o \) und \( w_o \), see eq. (7). The solution is

\[
v_o = \frac{1}{4} \frac{\partial P_o}{\partial \varphi} f_{ov}(r) + g_{ov}(r), \quad w_o = \frac{1}{4} \frac{\partial P_o}{\partial z} f_{ow}(r),
\]

where

\[
f_{ov}(r) = \frac{\ln \left( \frac{R}{r} \right)}{\ln \left( \frac{R}{R-h_o} \right)} h_o + (R-r), \quad g_{ov}(r) = \frac{\ln \left( \frac{r}{R-h_o} \right)}{\ln \left( \frac{R}{R-h_o} \right)} R\omega + \frac{\ln \left( \frac{R}{r} \right)}{\ln \left( \frac{R}{R-h_o} \right)} (R-h_o)\Omega_B,
\]

\[
f_{ow}(r) = \frac{1}{4} \left( r^2 - R^2 + \frac{\ln \left( \frac{R}{r} \right)}{\ln \left( \frac{R}{R-h_o} \right)} h_o (2R - h_o) \right).
\]

The radial velocity can not be determined in the framework of the present analysis. For this reason, we assume a linear distribution satisfying the boundary conditions

\[
u_o(r) = -\frac{\dot{h}_o}{h_o} (R-r).
\]

3 Continuity and Reynolds equations

Integration of the local form of the continuity equation for the incompressible fluid \( \nabla \cdot \mathbf{v} = 0 \) yields the continuity equation for the gap \( r_o \leq r \leq r_o + h_o \)

\[
\int_{\mathbf{v}(t)} \nabla \cdot \mathbf{v} \, dV = \int_{\partial \mathbf{v}(t)} \mathbf{v} \cdot \mathbf{n} \, dS = 0.
\]

We first apply this equation for the areas \( R \, d\varphi \, dz \) and \( (R-h_o) \, d\varphi \, dz \) to get

\[
Q_{or} = ([v_o(R)] R \, d\varphi \, dz - [v_o(R-h_o)] (R-h_o) \, d\varphi \, dz) \cdot \mathbf{e}_r \approx
\]

\[
\approx ([u_o(R)] R - [u_o(R-h_o)] (R-h_o)) \, d\varphi \, dz.
\]
Due to the linear approximation for the radial velocity $u_o(R) = 0$, $u_o(R - h_o) = -\partial h_o/\partial t$ we obtain $Q_{or} = (R - h_o) d\phi dz \partial h_o/\partial t$. In a similar manner one obtains the expressions for the flow through the other surfaces of the control volume in the gap. This leads to the following continuity equation

$$\frac{1}{R} \frac{\partial}{\partial \phi} q_{o\phi} + \frac{\partial}{\partial z} q_{oz} + \frac{R - h_o}{R} \frac{\partial h_o}{\partial t} = 0,$$

where

$$q_{o\phi} = \int_{R-h_o(\phi)}^{R} v_o dr = \frac{1}{\nu} \frac{\partial P_o}{\partial \phi} F_{ov}(h_o) + G_{ov}(h_o), \quad q_{oz} = \int_{R-h_o(\phi)}^{R} \omega_o \frac{R}{R} dr = \frac{1}{\nu} \frac{\partial P_o}{\partial z} F_{ow}(h_o).$$

(15)

Substituting these expressions into the continuity equation results in the so-called Reynolds equation which we generalised to the case of the considerable centrifugal forces,

$$\frac{\partial^2 P}{\partial z^2} F_{ow}(h_o) + \frac{1}{R} \left[ \frac{\partial^2 P_o}{\partial \phi^2} F_{ov}(h_o) + \frac{\partial P_o}{\partial \phi} \frac{\partial F_{ov}(h_o)}{\partial h_o} \frac{\partial h_o}{\partial \phi} \right] =$$

$$= -\frac{\nu}{R} \left[ (R - h_o) \frac{\partial h_o}{\partial t} + \frac{\partial G_{ov}(h_o)}{\partial h_o} \frac{\partial h_o}{\partial \phi} \right],$$

since

$$\frac{\partial q_{o\phi}}{\partial \phi} = \frac{1}{\nu} \frac{\partial}{\partial \phi} \left( \frac{\partial P_o}{\partial \phi} F_{ov}(h_o) \right) + \frac{\partial G_{ov}(h_o)}{\partial h_o} \frac{\partial h_o}{\partial \phi}, \quad \frac{\partial q_{oz}}{\partial z} = \frac{1}{\nu} \frac{\partial^2 P_o}{\partial z^2} F_{ow}(h_o).$$

(16)

Expansion in a Taylor series in terms of $h_o$ yields

$$\frac{h_o^3 \partial^2 P_o}{6 \partial z^2} + \frac{h_o^3}{6 R^2} \left[ \frac{\partial^2 P_o}{\partial \phi^2} + \frac{\partial P_o}{\partial \phi} \frac{3 \partial h_o}{\partial \phi} \right] = \nu \left[ 2 \frac{\partial h_o}{\partial t} + (\omega + \Omega_B) \frac{\partial h_o}{\partial \phi} \right].$$

(17)

4 Short bearing approach

Under the assumption that the change in pressure in the circumferential direction ($\phi$) is much smaller than in the axial direction ($z$), i.e. $|\partial P_o/\partial \phi| << |\partial P_o/\partial z|$ and neglecting the term $h_o/R$ in eq. (19) we simplify the Reynolds equation to the form

$$\frac{h_o^3 \partial^2 P_o}{6 \partial z^2} = \nu \left[ 2 \frac{\partial h_o}{\partial t} + (\omega + \Omega_B) \frac{\partial h_o}{\partial \phi} \right].$$

(20)

The pressure distribution is given by the equation

$$p_o = P_o + \rho \int_{z=0}^{2} \frac{v_o^2}{r} dr,$$

where the integration constant is obtained from the boundary conditions. For a symmetric bearing they are as follows

$$z = 0, \quad r = R, \quad p_o = p_{in}.$$
where $p_{\text{in}}$ denotes an external input pressure and the pressure symmetry $p_o(z) = p_o(-z)$ is assumed.

The integral in eq. (21) is independent of $z$, that is, the above symmetry condition should be satisfied only for $p_o$. We obtain $p_o$ from the Reynolds equation by means of twofold integration and taking into account the symmetry condition

$$p_o = \frac{6\nu}{h_o^3} \left[ 2 \frac{\partial h_o}{\partial t} + (\omega + \Omega_B) \frac{\partial h_o}{\partial \varphi} \right] \left( \frac{1}{2} z^2 + C_o \right). \tag{23}$$

The pressure in the gap is given by eq. (21) and it allows one to determine the integration constant $C_o$ and obtain the sought-for pressure distribution

$$p_o(r, \varphi, z, t) = p_{\text{in}} - \rho R \int_r^R \frac{v_o^2(r)}{r} dr + \frac{3\nu}{h_o^3} \left[ 2 \frac{\partial h_o}{\partial t} + (\omega + \Omega_B) \frac{\partial h_o}{\partial \varphi} \right] z^2. \tag{24}$$

In the case in which the pressure delivered by this formula becomes negative, one should put $p = 0$. Calculating the pressure at the end of the bearing $x = \pm L/2$

$$p_{\text{oo}} = p_{\text{in}} - \rho \int_r^R \frac{v_o^2(r)}{r} dr + \frac{3\nu}{h_o^3} \left[ 2 \frac{\partial h_o}{\partial t} + (\omega + \Omega_B) \frac{\partial h_o}{\partial \varphi} \right] \frac{L^2}{4} \tag{25}$$

yields

$$p_o = p_{\text{oo}} - 3\nu h_o^{-3} \left[ 2 \frac{\partial h_o}{\partial t} + (\Omega_B + \Omega) \frac{\partial h_o}{\partial \varphi} \right] \left( z^2 - \frac{L^2}{4} \right). \tag{26}$$

### 4.1 Gap pressure distribution

As the next step, one should express the gap height in terms of the kinematical parameters of the rotating bearing. To this end, we put

$$h_o = h_{\text{oo}} - e_B(t) \cos(\varphi - \gamma_B(t)), \tag{27}$$

where $h_{\text{oo}}$ denotes the nominal gap, $e_B$ is the eccentricity of the bearing centre and $\gamma_B$ is the angle describing the position of the line between the center of bearing and rotating cylinder. Taking the derivatives with respect to time $t$ and angle $\varphi$ and inserting them into eq. (26) we have

$$p_o = p_{\text{oo}} + 3\nu h_o^{-3} \left[ 2 \frac{\partial h_o}{\partial t} + (\Omega_B + \Omega) \frac{\partial h_o}{\partial \varphi} \right] \left( z^2 - \frac{L^2}{4} \right). \tag{28}$$

### 5 Forces and moment acting on the floating bearing

As we intend to stay in the framework of the classical short bearing theory we will consider only the bracketed term in eq. (28). This assumption corresponds to the
case that the pressure vanishes at both ends of the floating bearing. The integration over $z$ provides us with the force of the length unit. By introducing $\sigma_B = \varphi - \gamma_B$ we have

$$q_{oB} = \int_{-L/2}^{L/2} (p_o - p_{oo}) dz = \frac{\nu L^3 (\Omega_B + \omega)}{2h_{oo}^3} q_{oB},$$  \hspace{1cm} (29)$$

where

$$q_{oB}(\sigma_B, t) = \frac{\varepsilon_B \left( \frac{2\gamma_B}{\Omega_B + \omega} - 1 \right) \sin \sigma_B + \frac{2\epsilon_B}{\Omega_B + \omega} \cos \sigma_B}{\left( 1 - \epsilon_B \cos (\sigma_B) \right)^3}, \hspace{1cm} \varepsilon_B = \frac{e_B h_{oo}}{h}. \hspace{1cm} (30)$$

For determining the pressure acting on the inner surface of the bearing one should repeat the similar calculations for the corresponding inner gap. In the case of stationary rotation eq. (30) is simplified to

$$q_{oB}(\sigma_B) = -\varepsilon_B \sin (\sigma_B) \frac{1}{\left( 1 - \epsilon_B \cos (\sigma_B) \right)^3}. \hspace{1cm} (31)$$

In order to determine the force acting on the floating bearing we need to integrate the pressure over the surface of positive pressure $\pi \leq \sigma_B \leq 2\pi$. If the pressure given by eq. (30) or (31) is negative, then it is assumed to be equal to zero. We take two orthogonal directions $\xi_B, \eta_B$, for which the direction $\xi_B$ corresponds to $\sigma_B = 0$ ($\varphi = \gamma_B$). The result of the integral evaluation is

$$F_{\xi_B} = \int_{\pi}^{2\pi} q_{oB} \cos \sigma_B d\sigma_B =$$

$$\frac{\nu L^3 (\Omega_B + \omega)}{2h_{oo}^3} \left[ \left( 1 - \frac{2\gamma_B}{\Omega_B + \omega} \right) \frac{2\epsilon_B^2}{(1 - \epsilon_B^2)^2} + \pi \frac{\epsilon_B}{\Omega_B + \omega} \frac{1 + 2\epsilon_B^2}{(1 - \epsilon_B^2)^{5/2}} \right],$$

(32)

$$F_{\eta_B} = \int_{\pi}^{2\pi} q_{oB} \sin \sigma_B d\sigma_B =$$

$$\frac{\nu L^3 (\Omega_B + \omega)}{2h_{oo}^3} \left[ \frac{\pi}{2} \left( 1 - \frac{2\gamma_B}{\Omega_B + \omega} \right) \frac{\epsilon_B}{(1 - \epsilon_B^2)^{3/2}} + \frac{\epsilon_B}{\Omega_B + \omega} \frac{4\epsilon_B}{(1 - \epsilon_B^2)^2} \right].$$

The forces acting on the floating bearing from the inner chamber are calculated by analogy and it allows one to obtain the expression for the total force acting on the bearing.

The torque acting on the floating bearing is nothing else than the integral of the shear stresses. Clearly, the integration should be performed over the regions of the positive pressure on both sides of the bearing. Under the above assumptions (i.e. neglecting the radial component of the velocity) we obtain the following expressions for the shear stresses for the inner and external chambers

$$\tau_{r\varphi}^i = \mu \left( \frac{\partial v_i}{\partial r} - \frac{v_i}{r} \right), \hspace{1cm} \tau_{r\varphi}^o = \mu \left( \frac{\partial v_o}{\partial r} - \frac{v_o}{r} \right).$$

(33)
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References

A discrete thermodynamic approach to high frequency dynamics of structures

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1 Introduction. High frequency dynamics

There exist many different types of dynamics. The dynamics of rigid bodies deals with zero eigenfrequencies. The frequencies, which the dynamics of solids deals with, can be referred to as the natural frequencies of the solid under consideration. Thermodynamics should also be considered as a relevant dynamics in which the frequencies of thermal motions are essentially higher than the frequencies of mechanical vibrations. Classical thermodynamics is based upon a kinetic-statistical approach to thermal processes ("the mechanical theory of heat") which linked thermodynamic processes to dynamics. Quantum thermodynamics should also be considered as a relevant dynamics. The quantum effects are considerable only at very high frequencies, at least at the frequencies essentially higher than those of the thermal motion of the molecules. The dynamics of rigid body can be derived from vibration theory since the rigid body motions correspond to zero eigenfrequencies within vibration theory. The equations governing the dynamics of solids can be obtained from rigid body dynamics provided that the solid is modelled by a regular spatial array of elemental mass-spring systems. This means that the dynamics of rigid bodies and the dynamics of solids can be considered as two neighbouring dynamics. Classical thermodynamics and quantum thermodynamics may also be considered as two neighbouring dynamics. The difficulties encountered when attempting to link the dynamics of solids to thermodynamics indicate that there exists a gap between these theories which "reserves" a place for a new dynamics. The latter is in fact a low frequency limit of thermodynamics and a high frequency limit of the dynamics of solids. The new dynamics that fills this gap will be referred to here as high frequency dynamics, and the corresponding frequencies will be referred to as high frequencies of mechanical vibration or, for short, high frequencies. If high frequency dynamics is the high frequency limit of vibration theory and the low frequency limit of thermodynamics then the conventional methods of vibration theory and thermodynamics
can be applied there. In particular, the high frequency dynamics should be governed by the equations typical for thermodynamics.

Complex mechanical structures like ships, buildings, spacecraft and aircraft are actually assemblies of substructures. Attempts to pedantically describe all details and peculiarities of real structures are doomed to failure for the following reasons. Firstly, at higher frequencies, the existence of many inherently uncontrolled factors plays a principle role. Review papers by Ibrahim [1] and Fahy [2] give a very deep insight into the problem of uncertainties in dynamics. In structural dynamics, uncertainties arise from stiffness, mass and damping fluctuations caused by variations in material properties as well as variations resulting from manufacturing and assembly. The latter factor causes vagueness in the boundary conditions for each structural member since the high-frequency dynamic properties of joints between structural members are especially uncertain. Secondly, the essential heterogeneity and presence of complicated interiors, i.e. secondary systems, have to be taken into account. Thirdly, even if it were possible to obtain an ”exact” boundary-value problem in which all the complexity of the structure was taken into account and we could solve this problem, the very interpretation of this ”exact” result would present great difficulty. The reason for this is that the field of vibration of a complex structure (for instance, under a broad-band excitation) is a very complicated function of time and spatial coordinates since a great many modes are excited in the structure. Summarising, one can say that the blind extension of conventional methods of modal analysis to higher frequencies at the expense of computational cost reaches a deadlock because the results become unreliable and ”indigestible”.

The present paper suggests another approach to tackling the problem.

2 Energy Balance

A complex structure is assumed to consist of $N$ substructures. Let us consider a substructure $n$, where $n = 1, 2, ..N$. Its dynamics is governed by the following equation

$$\mathbf{r} \in V_n, \nabla \cdot \mathbf{\tau} + \mathbf{h} - \rho \mathbf{\ddot{u}} = 0,$$  \hspace{1cm} (1)

where $\mathbf{r}$ is the position vector, $\mathbf{\tau}$ is stress tensor, $\rho$ is the mass density, $\mathbf{u}$ is the absolute displacement, $\mathbf{h}$ is a body force, $\nabla$ is the Hamiltonian operator and dot denotes the time derivative. Multiplying eq. (1) by velocity $\dot{\mathbf{u}}$ and integrating over the volume of substructure $V_n$ one obtains

$$\int_{V_n} (\nabla \cdot \mathbf{\tau} + \mathbf{h} - \rho \mathbf{\ddot{u}}) \cdot \dot{\mathbf{u}} dV = 0.$$  \hspace{1cm} (2)

Using the chain rule $(\nabla \cdot \mathbf{\tau}) \cdot \dot{\mathbf{u}} = \nabla \cdot (\mathbf{\tau} \cdot \dot{\mathbf{u}}) - \mathbf{\tau} \cdot (\nabla \dot{\mathbf{u}})$ and applying the Ostrogradsky-Gauss theorem and the rule of differentiation of an integral over the material volume with respect to time [3] yields

$$\int_{V_n} \mathbf{h} \cdot \dot{\mathbf{u}} dV + \int_{S_n} \mathbf{f} \cdot \dot{\mathbf{u}} dS - \int_{V_n} \mathbf{\tau} \cdot \dot{\mathbf{e}} dV - \mathbf{\bar{T}} = 0,$$  \hspace{1cm} (3)
where $\varepsilon = (\nabla \mathbf{u})^s$ is the linear strain tensor, $\mathbf{f} = \mathbf{N} \cdot \mathbf{\tau}$ is the traction vector on the substructural surface $S_n$ with exterior unit normal $\mathbf{N}$, $T = \frac{1}{2} \int_{V_n} \rho \mathbf{u} \cdot \mathbf{u} dV$ denotes the kinetic energy of the subsystem and $\cdot \cdot$ stands for the double scalar product. The latter equation is in fact an integral form of the first law of thermodynamics [3], ensuring the power balance at any time instant. The power balance, averaged over the period $P$ of a periodic process is given by

$$\frac{1}{P} \int_t^{t+P} \left[ \int_{V_n} \mathbf{h} \cdot \mathbf{\dot{u}} dV + \int_{S_n} \mathbf{f} \cdot \mathbf{\dot{u}} dS - \int_{V_n} \mathbf{\tau} \cdot \cdot \mathbf{\dot{\varepsilon}} dV - \dot{T} \right] dt = 0. \quad (4)$$

It is clear that

$$\langle \dot{T} \rangle = \frac{1}{P} \int_t^{t+P} \dot{T} dt = \frac{1}{P} [T(t+P) - T(t)] = 0, \quad (5)$$

where $\langle \rangle$ denotes the above time averaging. In order to account for the energy dissipation in the structure, let us make use of the theory of microplasticity [3]. This implies the following splitting the stress and strain tensors into spherical and deviatoric parts

$$\mathbf{\tau} = \sigma \mathbf{E} + \mathbf{s}, \quad \varepsilon = \frac{\vartheta}{3} \mathbf{E} + \mathbf{e}, \quad (6)$$

where $\mathbf{E}$ is the unity tensor. Here $\mathbf{s}$ and $\mathbf{e}$ are stress deviator and strain deviator, respectively, and $\sigma$ and $\vartheta$ denote respectively the mean normal stress and the dilatation. The spherical parts of the stress and strain tensors exhibit elastic behaviour, that is, the constitutive equation for the mean normal stress and the dilatation is given by

$$\sigma = k \vartheta,$$

where $k$ is the bulk modulus.

The deviatoric parts are known to be governed by constitutive equations of elastoplasticity. Palmov [3] proved that the Ishlinsky rheological model is the most appropriate one to this aim. The model consists of an infinite number of the Prandtl elastoplastic elements in parallel and is governed by the following equation

$$\mathbf{s} = 2G \left[ \mathbf{e} - \int_0^\infty \mathbf{e}_y p(y) dy \right], \quad (7)$$

where $G$ is the shear modulus, $p(y)$ is the distribution function of a continuous spectrum of nondimensional yield stress $y$. The plastic strain $\mathbf{e}_y$ in the Prandtl element with an yield stress $y$ is as follows

$$\begin{align*}
\dot{\mathbf{e}}_y &= 0, \quad \sqrt{\frac{1}{2}(\mathbf{e} - \mathbf{e}_y) \cdot (\mathbf{e} - \mathbf{e}_y)} \leq y, \\
\dot{\mathbf{e}}_y &\neq 0, \quad y \dot{\mathbf{e}}_y / v_y = \mathbf{e} - \mathbf{e}_y.
\end{align*} \quad (8)$$
where \( v_y = \sqrt{\frac{1}{2} \hat{e}_y \cdot \hat{e}_y} \) is the intensity of shear strain rate, see [3] for detail.

The time averaging yields

\[
\left\langle \int_{V_n} \tau \cdot \dot{\varepsilon} dV \right\rangle = \int_{V_n} \left( \left\langle \frac{d}{dt} \left[ \frac{1}{2} k \dot{\varepsilon}^2 + 2 G e \cdot \varepsilon \right] \right\rangle - \left\langle 2 G \dot{\varepsilon} \cdot \int_0^\infty e_y p(y) dy \right\rangle \right) dV
\]

\[
= - \left\langle \int_{V_n} 2 G \dot{\varepsilon} \cdot \int_0^\infty e_y p(y) dy dV \right\rangle,
\]

where the term with time rate of the conservative term vanishes by analogy with eq. (5). Eq. (4) takes the form

\[
\left\langle \int_{V_n} h \cdot \dot{u} dV \right\rangle + \left\langle \int_0^\infty 2 G \dot{\varepsilon} \cdot \int_0^\infty e_y p(y) dy dV \right\rangle + \left\langle \int_{S_n} f \cdot \dot{u} dS \right\rangle = 0.
\]

The physical sense of this equation is obvious, it expresses the average power balance. The first term is the power received by the system, the second one gives the power dissipated in the system, whereas the third describes the power, transmitted to the neighbouring subsystems.

Let us make a remark. The very fact that Eq. (10) is fulfilled for any periodic process implies that it is met in average for any harmonic which in turn means that the conventional methods of the theory of stationary random processes can be applied to further analysis. The correspondence principle [3] suggests a way for obtaining a boundary value problem for harmonic vibration of elastoplastic bodies. To incorporate the effects of internal friction one replaces the elastic moduli in the dynamic theory of elasticity by their complex values. Let us demonstrate how this principle works in the particular case of the dynamical elastoplasticity.

The effects of internal friction are described by eqs. (7) and (8). To linearise a nonlinear tensorial constitutive equation (8) we assume that the strain tensors obey a harmonic law, i.e.

\[
e = \hat{e} e^{i \omega t}, \quad e_y = \hat{e}_y e^{i \omega t}.
\]

In order to use the method of harmonic linearisation we replace the only nonlinearity \( v_y^{-1} \hat{e}_y \) in Eq. (8) by a linear function \( v_y^{-1} \hat{e}_y \approx K_y \hat{e}_y \) where \( K_y = \frac{4}{\pi \omega \Gamma_y} \) is a scalar linearisation factor and \( \Gamma_y = \sqrt{\frac{1}{2} \hat{e}_y \cdot \hat{e}_y} \) and asterisk denotes the complex conjugate. Repeating the reasonings of [3] we arrive at the following constitutive equation

\[
s = 2 G c e,
\]

where

\[
G_c = G \left[ 1 - \int_0^1 \left[ 1 - \eta^2 - i \eta \sqrt{1 - \eta^2} \right] p \left( \frac{\pi \Gamma}{4 \eta} \right) \frac{\pi \Gamma}{4} d\eta \right],
\]

is referred to as a complex shear modulus and \( \eta = 4y/\pi \Gamma \) is a nondimensional yield stress with \( \Gamma = \sqrt{\frac{1}{2} \hat{e} \cdot \hat{e}^*} \) denoting the amplitude of the shear stress intensity.
3 Kinetic Energy of Substructures

Outside of the region of these global resonances, the vibration localizes within each substructure or groups of substructures. This allows one to look for the vibration field in the subsystems by means of Galerkin’s approach (modal analysis), i.e.

\[ u(r, t) = \sum_{k=1}^{\infty} U_k(r)q_k(t), \]  

(13)

where \( U_k(r) \) is referred to as the basic functions (orthonormalised vibration modes) and \( q_k(t) \) are the generalised coordinates. The normal modes of elastic vibrations are known to be orthonormal, i.e.

\[
\int_{V_n} \rho U_k \cdot U_l dV = \delta_{kl}, \quad \int_{V_n} (k \theta_k \theta_l + 4G e_k \cdot e_l) dV = \Omega_k^2 \delta_{kl},
\]

where \( \delta_{kl} \) is the Kronecker delta and \( \Omega_k \) is referred to as the \( k \)-th eigenfrequency of the substructure. Multiplying the equation for dynamics (1) by \( U_k(r) \), integrating over the substructural volume \( V_n \) and taking into account the above property of the normal modes one arrives at the following equation for the generalised coordinate

\[
\ddot{q}_k + \Omega_k^2 q_k + \sum_{l=1}^{\infty} D_{nl} q_k = \int_{V} h \cdot U_k dV, \tag{14}
\]

cf. [3]. Here the complex exponential form of the variables is used and

\[
D_{nl} = \int_{V} 2 (G - G_c) e_k \cdot e_l dV, \tag{15}
\]

where \( e_k \) is referred to as the deviatoric part of the strain tensor corresponding to \( U_k \). As mentioned in [3] the effect of plastic deformation is normally very small in application problems, so \( |D_{nl}| < \Omega_k^2 \). The asymptotically leading part of the solution of (14) is governed by the following equation

\[
\ddot{q}_k + (\Omega_k^2 + D_{kk}) q_k = \int_{V} h \cdot U_k dV. \tag{16}
\]

By means of spectral decomposition of the external forces and generalised coordinates

\[
h(r, t) = \int_{-\infty}^{\infty} \hat{h}(r, \omega) e^{i\omega t} d\omega, \quad q_k(r, t) = \int_{-\infty}^{\infty} \hat{q}_k(r, \omega) e^{i\omega t} d\omega \tag{17}
\]

we come to the following spectrum of the generalised coordinate

\[
\hat{q}_k(r, \omega) = \frac{1}{-\omega^2 + \Omega_k^2 (1 + i\psi)} \int_{V} h \cdot U_k dV, \tag{18}
\]
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where

\[
\psi = \int_0^1 \eta \sqrt{1 - \eta^2} \frac{\pi \Gamma}{4 \eta} \frac{\pi \Gamma}{4} d\eta. \tag{19}
\]

The expression for mean value of the kinetic energy of n-th subsystem

\[
\langle T_n \rangle = \frac{1}{2} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \langle \dot{q}_{nk} \dot{q}_{nl} \rangle \int_{V_n} \rho U_k \cdot U_l dV =
\]

\[
= \frac{1}{2} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \int_{V_n} \rho U_k \cdot U_l dV \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{V} \left( h_r(r, \omega) h^*_r(r_1, \omega_1) \right) \cdot U_l(r_1) dV(r) \int_{-\infty}^{\infty} \omega \omega_1 e^{i(\omega - \omega_1)t} d\omega d\omega_1 dV(r)dV(r_1)
\]

\[
\left[ -\omega^2 + \Omega_k^2 (1 + i\psi) \right] \left[ -\omega_1^2 + \Omega_1^2 (1 - i\psi) \right].
\]

We next assume that the external distributed load is a stationary delta-correlated isotropic spatial white noise, spectral density of which is constant within each subsystem, i.e.

\[
r \in V_j, \langle h_r(r, \omega) h^*_r(r_1, \omega_1) \rangle = S_j(\omega) \delta (r - r_1) \delta (\omega - \omega_1) E. \tag{20}
\]

This allows one to simplify the equation for \( T \)

\[
\langle T_n \rangle = \frac{1}{2} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \int_{V_n} \rho U_k \cdot U_l dV \int_{V} \left( S_j(\omega) \omega^2 \right) d\omega
\]

\[
= \int_{-\infty}^{\infty} \left[ -\omega^2 + \Omega_k^2 (1 + i\psi) \right] \left[ -\omega_1^2 + \Omega_1^2 (1 - i\psi) \right] \left[ -\omega^2 + \Omega_k^2 (1 + i\psi) \right] \left[ -\omega_1^2 + \Omega_1^2 (1 - i\psi) \right] \tag{21}
\]

The further advance is possible under the assumption that the system in question belongs to the class of weakly coupled systems, i.e. \( U_k(r) \) coincides with k-th orthonormal vibration mode within this particular substructure. Adopting the assumption that the mass density of each substructure is constant leads to a drastic simplification of the result

\[
\langle T_n \rangle = \frac{1}{2} \sum_{k=1}^{\infty} \sum_{j=1}^{N} \frac{1}{\rho_j} \int_{-\infty}^{\infty} \frac{\omega^2 S_j(\omega) d\omega}{(-\omega^2 + \Omega_k^2)^2 + \psi^2 \Omega_k^4} \tag{22}
\]

Let us consider a broad band loading and assume a small damping. Then, due to Bolotin’s method [4] one can replace the spectral density at the resonance frequency beyond the integral and evaluate the integral obtained. The result is

\[
\langle T_n \rangle = \frac{\pi}{2} \sum_{k=1}^{\infty} \sum_{j=1}^{N} \frac{1}{\rho_j} \frac{S_j(\Omega_k)}{\psi \Omega_k}. \tag{23}
\]
In the case of high modal overlap the sum above may be replaced by an integral over frequency [bolotin]

\[ \langle T_n \rangle = \frac{\pi}{2} \sum_{j=1}^{N} \frac{1}{\rho_j} \int_{0}^{+\infty} \frac{S_j(\Omega)}{\psi \Omega} \nu_j(\Omega) \, d\Omega, \]  

(24)

where \( \nu_j \) is referred to as the asymptotic modal density of \( j \)-th subsystem. Introducing the spectral density of the averaged kinetic energy of \( n \)-th subsystem \( \langle \Sigma_n \rangle \), we obtain

\[ \langle \Sigma_n(\Omega) \rangle = \frac{\pi}{4} \sum_{j=1}^{N} \frac{\nu_j(\Omega)}{\psi \Omega} S_j(\Omega). \]  

(25)

In fact we obtained an expression for the average modal energy \( E \) of \( n \)-th subsystem having a frequency \( \Omega \) since the spectral density of the averaged kinetic energy of \( n \)-th subsystem \( \langle \Sigma_n(\Omega) \rangle \) can be viewed as this energy.

4 The Input, Dissipated and Transmitted Power

Let us now transform the other terms in Eq. (10). To begin with, we consider the average input power, i.e.

\[ \left\langle \int \mathbf{h} \cdot \mathbf{\dot{u}} dV \right\rangle = \left\langle \sum_{k=1}^{\infty} \int_{-\infty}^{\infty} \frac{i \omega e^{i(\omega-\omega_1)t} d\omega d\omega_1}{-\omega^2 + \Omega_k^2 (1 + i \psi)} \right\rangle \]

\[ \int \int V_n U_k(r) \cdot \langle \mathbf{h}(r, \omega) \mathbf{h}^*(r_1, \omega_1) \rangle \cdot U_l(r_1) dV(r) dV(r_1). \]

By virtue of the above assumptions we can simplify the latter expression, to give

\[ \left\langle \int \mathbf{h} \cdot \mathbf{\dot{u}} dV \right\rangle = \frac{1}{\rho_n} \sum_{k=1}^{\infty} \int_{-\infty}^{\infty} \frac{S_n(\omega) i \omega d\omega}{-\omega^2 + \Omega_k^2 (1 + i \psi)}. \]

Transforming the integral in such a way that integration is performed only over the positive frequencies and performing an asymptotic evaluation of the integral yields

\[ \left\langle \int \mathbf{h} \cdot \mathbf{\dot{u}} dV \right\rangle = \frac{\pi}{\rho_n} \sum_{k=1}^{\infty} S_n(\Omega_k). \]

When modal density is high one may replace the sum by an integral over the frequency

\[ \left\langle \int \mathbf{h} \cdot \mathbf{\dot{u}} dV \right\rangle = \frac{\pi}{\rho_n} \int_{0}^{+\infty} S_n(\Omega) \nu_n(\Omega) d\Omega. \]
and introduce the spectral density of the input power
\[ \Sigma_n^{\text{input}} = \frac{\pi}{2\rho_n} \mathbf{v}_n(\Omega) S_n(\Omega). \] (26)

The power dissipated in the substructure is given by Eq. (9)
\[ \left\langle \int_{V_n} 2G \mathbf{e} \cdot \mathbf{e} p(y) dy dV \right\rangle = - \left\langle \int_{V_n} \tau \cdot \dot{\mathbf{e}} dV \right\rangle = - \left\langle \int_{V_n} (k\dot{\mathbf{\theta}} + s \cdot \dot{\mathbf{e}}) dV \right\rangle. \]

Using the series (13) in terms of the normal forms and introducing the complex shear modulus \( G_c \), yields
\[ \left\langle \int_{V_n} \tau \cdot \dot{\mathbf{e}} dV \right\rangle = \int_{V_n} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \left( (k\dot{\mathbf{\theta}}_l + 2G_{c_k} \mathbf{e}_k \cdot \mathbf{e}_l) \right) q_k \dot{q}_l dV \] (27)

where \( \dot{\mathbf{\theta}}_k \) are \( \mathbf{e}_k(r) \) are dilatation and the strain deviator corresponding to \( U_k(r) \), respectively. Using the spectral decompositions for generalized coordinates (17) and (18), simplifying the result under the above assumptions and taking into account that the correlation function of a stationary random function and its time derivative vanishes (i.e. \( \langle q_k \dot{q}_k \rangle = 0 \)) one can cast the latter expression in the form
\[ \left\langle \int_{V_n} \tau \cdot \dot{\mathbf{e}} dV \right\rangle = I_1 + I_2, \]

where
\[ I_1 = \int_{V_n} dV \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \sum_{j=1}^{N} \frac{1}{\rho_j} \int_{-\infty}^{\infty} S_j(\omega) \left( k\dot{\mathbf{\theta}}_l + 2G_{c_k} \mathbf{e}_k \cdot \mathbf{e}_l \right) (-i\omega) d\omega dV, \]
\[ I_2 = \int_{V_n} dV \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \sum_{j=1}^{N} \frac{1}{\rho_j} \int_{-\infty}^{\infty} S_j(\omega) 2i\psi G_{c_k} \mathbf{e}_k \cdot \mathbf{e}_l (-i\omega) d\omega dV. \]

Clear that \( I_1 = 0 \) because of the orthogonality condition
\[ \int_{V_n} (k\dot{\mathbf{\theta}}_k + 4G_{c_k} \mathbf{e}_k \cdot e_l) dV = \Omega_k^2 \delta_{kl}. \]

Transforming \( I_2 \) in the above manner we can introduce the spectral density of the power dissipated in the substructure (details are omitted)
\[ \Sigma_n^{\text{diss}} = \sum_{j=1}^{N} S_j(\omega) \frac{2G_{c_j}}{\rho_j} \int_{V_n} dV \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \left\{ \mathbf{e}_k \cdot \mathbf{e}_l + \frac{(-\omega^2 + \Omega_k^2) (-\omega^2 + \Omega_l^2)}{(-\omega^2 + \Omega_k^2)^2 + \psi^2 \Omega_k^4} \mathbf{e}_k \cdot \mathbf{e}_l \right\} \frac{dV}{(-\omega^2 + \Omega_k^2)^2 + \psi^2 \Omega_k^4}. \] (28)
The power transferred to another substructures through the surface of the n-th substructure is given by

\[
\left\langle \int_{S_n} \mathbf{f} \cdot \mathbf{u} dS \right\rangle = \left\langle \int_{S_n} \mathbf{N} \cdot \mathbf{t} \cdot \mathbf{u} dS \right\rangle = \int_{S_n} \mathbf{N} \cdot \langle \mathbf{t} \cdot \mathbf{u} \rangle dS = \int_{S_n} \mathbf{N} \cdot \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} (k \delta_k \mathbf{U}_l + 2G \mathbf{e}_k \cdot \mathbf{U}_l) \langle q_k q_l \rangle dS
\]

Again we represent the power as a sum of two integrals

\[
J_1 = \int_{S_n} \mathbf{N} \cdot \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} (k \delta_k \mathbf{U}_l + 2G \mathbf{e}_k \cdot \mathbf{U}_l) \langle q_k q_l \rangle dS,
\]

\[
J_2 = \int_{S_n} \mathbf{N} \cdot \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} 2 \langle (G - G) \mathbf{e}_k \cdot \mathbf{U}_l q_k q_l \rangle dS.
\]

with the condition \( \langle q_k q_k \rangle = 0 \) being taken into account. Repeating the above derivation we finally arrive at the following expression for the spectral density of the power transmitted to the neighbouring substructures

\[
\Sigma_n^{(\text{trans})} = \sum_{j=1}^{N} S_j(\omega) \frac{\omega \psi_j}{\rho_0} \int_{S_n} dS \mathbf{N} \cdot \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{2 (k \delta_k \mathbf{U}_l + 2G \mathbf{e}_k \cdot \mathbf{U}_l) (\Omega_k^2 - \Omega_l^2) \omega^2 + 2G \mathbf{e}_k \cdot \mathbf{U}_l (-\omega^2 + \Omega_k^2) (-\omega^2 + \Omega_l^2)}{((-\omega^2 + \Omega_k^2)^2 + \psi^2 \Omega_k^4) \left((-\omega^2 + \Omega_l^2)^2 + \psi^2 \Omega_l^4\right)}.
\]

Now one can view the spectral densities of the input of each subsystem \( \Sigma_n^{(\text{input})} \) given by eq (26) as an entry of a row, and solve the matrix equation for this entry. The result can be conveniently written in the form which was first suggested in [5]

\[
\Sigma_n^{(\text{input})} = \omega \eta_n \Sigma_n + \sum_{j \neq n} \omega \eta_j \nu_j(\omega) \left( \frac{\Sigma_n}{\nu_n(\omega)} - \frac{\Sigma_j}{\nu_j(\omega)} \right).
\]

Here \( \eta_n \) and \( \nu_{nj}(\omega) \) are referred to as the loss factors and the coupling loss factors. Further, \( \Sigma_n/\nu_n(\omega) \) may be understood as the modal energy of the substructure, since the modal density \( \nu_n(\omega) \) gives actually a number of modes which are resonant over a unit frequency band with as the centre frequency \( \omega \).

**5 Conclusions**

Equation (29) is fully analogous to the Fourier law in the theory of thermal conductivity for a system of bodies in thermal equilibrium. The first term in eq. (29) describes the energy absorbed in the substructure whereas the sum models the energy exchange between the neighbouring substructures. Equation (29) serves as a substantiation of the continuous approaches to high-frequency dynamics known as the vibration conductivity approach, e.g. [6] and [7].
6 Acknowledgment

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References


Determination of macroscopic characteristics for graphene layer using angle-depending atomic interactions

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Abstract

The purpose of this investigation is to construct a stable model of graphene (monolayer of graphite) using microstructure analysis and to connect parameters of this model with the macro parameters such as Young modulus and Poisson ratio. It is well-known that usage of central interaction can lead to instability of graphene lattice. A model of interaction containing the terms describing the central and angular interaction is considered. The relation between the model parameters and macro characteristics is found. Parameters describing stiffnesses of the bonds are determined using experimental data. It is planned to use the models considered above for description of the deformation processes in graphene layers.

1 Introduction

Graphene is a monolayer of graphite crystal lattice and it attracts a great deal of attention among physicists. It is primarily connected with its unusual electronic and mechanical properties. In the majority of researches graphene is considered to be two-dimensional material with hexagonal lattice and almost ideal location of atoms, which is particularly the reason of great free run’s distance of charge carriers (till one micron). As a matter of fact experimentally obtained monolayer of graphene [1] is not absolutely flat: there are some deformations in transverse direction and it the condition of stability [2]. However in this work the fact mentioned above is not taken into consideration and graphene is considered in two-dimensional space.

There are several reasons why mechanical properties of graphene are so interesting. Firstly the carbon nanotubes that are more and more widely applied in medicine and technics are layers of graphene wrapped in one or another way. Secondly the questions concerning the development of composite materials based on graphene
are discussed. Other possible applications of graphene’s mechanical properties are widely discussed in the literature. Thus construction of a rational mechanical model of graphene is extremely important.

It is typically to introduce effective interaction potentials to model the interaction between the atoms of crystal lattices. Pair interaction potentials such as Lennard-Jones and Morse potentials are successfully applied for close packed lattices. However when trying to apply these potentials to a model of material with directed crystal bonds one can reveal that it turns out to be unstable. To solve this problem many-body potentials depending on the angles between the bonds are applied. Such potentials for modeling of carbon compounds were proposed by Tersoff and Brenner [3, 4]. Family of MM-potentials and MM3-potential in particular are also efficiently applied. At the same time Brenner and MM3 potentials are the most-used for modeling of carbon nanotubes.

The method of applying many-particle potentials has some difficulties concerned with complex structure of such potentials and large quantity of interaction parameters. That is why another methods are also applied. One of alternatives taking into account the moment contribution in interatomic interaction. In [6, 7] non-central interaction consisting of two components — force described by a force vector and torque described by a torque vector — is used to model lattice of graphite. Torque component is able to carry in additional transversal stiffness in the system which provides with the stability of hexagonal lattice.

There are some other methods of introducing additional stiffness in the system. In [8] a mechanical model of carbon nanotube is proposed. This model is based on applying elastic rods and springs connecting the atoms to provide stability of the system. Another approach introducing rotatory degree of freedom for describing the moment interaction is used in [9] and [10].

Current research is based on theoretical appliance proposed in [11]. Common representation of energy of interaction containing dependence on angles between interatomic bonds is considered. On basis of of this potential and geometry of the lattice macro parameters such as Young modulus, bulk modulus and Poisson ratio are obtained.

Application of developed models in investigation of deformation and oscillation processes that happen in graphene sheets is presumed.

## 2 Stiffness tensor of two-atomic lattice

Let us consider ideal complex crystal lattice and assume that elementary cell of this lattice contains two atoms. Such kind of lattice is typical for diamond, graphite, hexagonal close-packed (HCC) crystals. Let us assume that each atom interacts only with its closest neighbours and introduce the following notations: $\alpha$ is an index describing the closest neighbours of the selected atom and corresponding bonds, index $\beta$ describes adjacent atoms and bonds. The energy accounting for one particle can be represented in the following way:

\[
W = \frac{1}{V_0} \left( G_1 \sum_\alpha \kappa_\alpha^2 + G_2 \sum_{\alpha,\beta} \xi_{\alpha\beta}^2 + G_3 \sum_{\alpha,\beta} (\kappa_\alpha + \kappa_\beta) \xi_{\alpha\beta} \right) \tag{1}
\]
Here $V_0$ is volume of the elementary cell, $\kappa_\alpha$ and $\kappa_\beta$ are deformations of the bonds $\alpha$ and $\beta$, $\xi_{\alpha\beta}$ is change of the angle between the bonds. Prime next to sum means that summation is carried out by adjacent bonds. It is taken into account that the elementary cell contains two particles and that in the result of summation it is allowed for the same bonds twice. If the interaction is carried out by linear springs with stiffness $c$ and by angular springs with stiffness $\gamma$, then

$$G_1 = \frac{1}{2}ca^2, \quad G_2 = \frac{1}{2} \gamma, \quad G_3 = 0,$$

(2)

where $a$ is length of the linear spring.

It is well-known that every complex lattice can be represented as a combination of two simple sublattices. Let us assume that deformation of the crystal consists of small homogeneous deformation of its both sublattices. The obtained configuration won’t be in equilibrium position but will be tending to this position at the expense of displacement of one sublattice relative to another upon some discrepancy vector $\zeta$.

Therefore strain energy that on one hand appears to be the quadratic form of strain tensor can be represented as the sum of quadratic and bilinear forms of the strain tensor $\varepsilon$ and the discrepancy vector $\zeta$ on the other hand:

$$W = \frac{1}{2} \varepsilon : 4 C : \varepsilon = \frac{1}{2} \varepsilon : 4 C : \varepsilon + \frac{1}{2} \varepsilon : C : \zeta + \frac{1}{2} \zeta : C : \varepsilon$$

(3)

Let us assume that the crystal undergoes small strain $\varepsilon$. The discrepancy vector should provide here with the displacement of the sublattices so that to implement a minimum of the strain energy. This allows to obtain a relation between the discrepancy vector and the strain tensor.

$$\frac{\partial W}{\partial \zeta} = 0 \Rightarrow C : \zeta + 3 \zeta : 3 C = 0 \Rightarrow \zeta = -C^{-1} \cdot 3 \zeta : 3 \varepsilon$$

(4)

Using the last relation one can express the stiffness tensor:

$$4 C = 4 C : 3 C : C^{-1} \cdot 3 C$$

(5)

It is shown in Appendix A that deformations of the bonds can be represented in the following way:

$$\kappa_\alpha = \bar{n}_\alpha \bar{n}_\alpha \varepsilon + \bar{n}_\alpha \cdot \zeta, \quad \kappa_{\alpha\beta} = \bar{n}_\alpha \bar{n}_\beta \varepsilon + \frac{1}{2} (\bar{n}_\alpha + \bar{n}_\beta) \cdot \zeta,$$

$$\xi_{\alpha\beta} = \frac{(\kappa_\alpha + \kappa_\beta) \cos \varphi - 2 \kappa_{\alpha\beta}}{\sin \varphi}.$$

(6)

After putting formula (6) in (1) the stiffness tensors from (3) can be expressed:

$$4 C = \frac{2}{V_0} \left( H_1 \sum_{\alpha} \bar{n}_\alpha \bar{n}_\alpha \bar{n}_\alpha + H_2 \sum_{\alpha, \beta}^{'} \bar{n}_\alpha \bar{n}_\alpha \bar{n}_\beta \bar{n}_\beta \right) +$$

$$+ \frac{2}{V_0} \left( H_3 \sum_{\alpha, \beta}^{'} \left( \bar{n}_\alpha \bar{n}_\beta \bar{n}_\beta \bar{n}_\alpha + \bar{n}_\alpha \bar{n}_\beta \bar{n}_\alpha \bar{n}_\beta \right) \right),$$

$$3 C = \frac{1}{V_0} H_4 \sum_{\alpha} \bar{n}_\alpha \bar{n}_\alpha \bar{n}_\alpha,$$

$$2 C = \frac{2}{V_0} H_5 \sum_{\alpha} \bar{n}_\alpha \bar{n}_\alpha,$$

(7)
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where constant coefficients $H_k$ can be calculated using the following formula:

\begin{align*}
H_1 &= G_1 - 6M_1G_2 \cot^2 \varphi - 2M_1G_3 \cot \varphi, \\
H_2 &= 2G_2 \cot^2 \varphi + 2G_3 \cot \varphi, \\
H_3 &= 2G_2(1 + \cot^2 \varphi), \\
H_4 &= 2G_1 + 4G_2M_1 \cot \varphi \left(1 - \cos \varphi \right)^2 + 2G_3M_1 \cot \varphi \left(2\varphi - \cos \varphi \right), \\
H_5 &= G_1 + 2G_2M_1(1 - \cos \varphi) - 2G_3M_1 \sin \varphi.
\end{align*}

While obtaining (7)–(8) formula (50) from Appendix B was used. $M1$ is number of bonds adjacent with the selected one, $d$ is dimensionality of space. Formula (7) applying (49) and (52) from Appendix B and taking into consideration symmetry can be represented in the following way:

\begin{gather*}
\sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha = M_1^2, \\
\sum_\alpha n_\alpha n_\alpha n_\alpha = \frac{H_4^2}{V_0^2} \left( \frac{d + 1}{d} \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha - \frac{M_2^2}{d^2} \right), \\
\sum_\alpha n_\alpha n_\alpha n_\alpha = \frac{2}{V_0} \left( (H_1 + M_1P(H_2 + 2H_3)) \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha + H_2QJ_1 + H_3Q \left( J_{z_2} + J_{z_3} \right) \right); \\
Q = \frac{M_1M \sin^2 \varphi}{d(d - 1)}, \\
P = \cos^2 \varphi - \frac{\sin^2 \varphi}{d - 1}.
\end{gather*}

After putting (9) in (5) the stiffness tensor of the complex lattice can be expressed as

\begin{align*}
\sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha = \kappa' \sum_\alpha n_\alpha n_\alpha n_\alpha + \lambda' J_{z_1} + \mu' \left( J_{z_2} + J_{z_3} \right),
\end{align*}

where

\begin{align*}
\kappa' &= \frac{2}{V_0} \left( (H_1 + M_1P(H_2 + 2H_3)) - \frac{1}{2MH_5} \right), \\
\lambda' &= \frac{2}{V_0} QH_2 + \frac{MH_5^2}{2d^2H_5V_0}, \\
\mu' &= \frac{2}{V_0} QH_3.
\end{align*}

Let us consider tensor $\sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha$. In case of orthotropic material with cubic symmetry this tensor can be represented in the following way:

\begin{align*}
\sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha n_\alpha = M_\kappa \xi_k \xi_k \xi_k \xi_k \xi_k + M_\mu \left( J_{z_1} + J_{z_2} + J_{z_3} \right),
\end{align*}

where $\xi_k$ are unit vectors of cubic sublattice’s axes in case of crystals with cubic symmetry or unit vectors of a arbitrary orthonormal basis in case of isotropy of elastic properties; $M_\kappa$ and $M_\mu$ — dimensionless coefficients defined by formula

\begin{align*}
M_\kappa &= 2 \frac{1 - \eta_c}{d(\eta_c + 2)} M, \\
M_\mu &= \frac{\eta_c}{d(\eta_c + 2)} M,
\end{align*}
where \( \eta_c \) — anisotropy parameter of tensor \( \sum_{\alpha} \eta_\alpha \eta_\alpha \). It coincides with anisotropy parameter of considered material’s stiffness tensor in case of purely force interaction. Anisotropy parameter is usually defined via elastic moduli

\[
\eta \overset{\text{def}}{=} \frac{2C_{44}}{C_{11} - C_{12}} = \frac{2\mu}{\kappa + 2\mu}.
\]

(15)

For isotropic material \( \eta = 1 \). Thus one can rewrite the expression for the stiffness tensor in the following way:

\[
\begin{align*}
4C & = \kappa \epsilon_k \epsilon_k + \mu(J_{z1} + J_{z3}), \\
\kappa & = \kappa'M_k, \quad \lambda = \kappa'M_\mu + \lambda', \quad \mu = \kappa'M_\mu + \mu',
\end{align*}
\]

(16)

where \( \kappa, \lambda, \mu \) are generalised Lame parameters.

In case of isotropy of elastic properties

\[
M_\kappa = 0, \quad M_\mu = \frac{1}{d(d + 2)} M
\]

(17)

and the stiffness tensor takes the canonical form

\[
\begin{align*}
4C & = \lambda J_{z1} + \mu(J_{z2} + J_{z3}), \\
\lambda & = \frac{M}{d(d + 2)} \kappa' + \lambda', \quad \mu = \frac{M}{d(d + 2)} \kappa' + \mu',
\end{align*}
\]

(18)

where \( \lambda, \mu \) are Lame parameters, which in our case can be expressed in the form

\[
\begin{align*}
\lambda & = \frac{M}{d(d + 2)} \kappa' + \lambda', \\
\mu & = \frac{M}{d(d + 2)} \kappa' + \mu',
\end{align*}
\]

(19)

where \( \kappa', \lambda', \mu' \) have the form (12). For two-dimensional isotropic material such as sheet of graphene all the stiffness tensor’s moduli can be expressed in the following way:

\[
\begin{align*}
C_{11} & = \lambda + 2\mu, \quad C_{12} = \lambda, \quad C_{44} = \mu; \quad K = \lambda + \mu, \\
E & = \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu}, \quad \nu = \frac{\lambda}{\lambda + 2\mu}.
\end{align*}
\]

(20)

3 Determination of elastic characteristics for graphene lattice

Let us consider crystal structure with graphene lattice. An example of such lattice can be found on Figure 1. In case of graphene lattice

\[
d = 2, \quad M = 3, \quad M_1 = 2, \quad \varphi = \frac{2\pi}{3}, \quad Q = \frac{9}{4}, \quad P = -\frac{1}{2},
\]

(21)

the coefficients \( H_i \) can be calculated using the following formula:

\[
\begin{align*}
H_1 & = G_1 - 4G_2 + \frac{4\sqrt{3}}{3}G_3, \quad H_2 = \frac{2}{3}(G_2 - \sqrt{3}G_3), \quad H_3 = \frac{8}{3}G_2, \\
H_4 & = 2(G_1 - 6G_2), \quad H_5 = G_1 + 6G_2 - 2\sqrt{3}G_3,
\end{align*}
\]

(22)
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Figure 1: Graphene lattice

and coefficients \( \kappa' \), \( \lambda' \) and \( \mu' \) are

\[
\kappa' = \frac{2}{V_0} \left( H_1 - H_2 - H_3 - \frac{H_4^2}{4H_5} \right), \quad \lambda' = \frac{3}{4V_0} \left( 6H_2 + \frac{H_4^2}{2H_5} \right), \quad \mu' = \frac{9}{2V_0} H_3
\]

respectively. The volume of the elementary cell is \( V_0 = \frac{3\sqrt{3}}{2} a^2 \).

Let us assume that the interaction is carried out in correspondence with (35). Here the bulk modulus, Young modulus and the Poisson ratio can be expressed via stiffnesses \( G_1 \) and \( G_2 \) using (16) and (19):

\[
E = \frac{72G_1G_2}{V_0(G_1 + 18G_2)}, \quad \nu = \frac{G_1 - 6G_2}{G_1 + 18G_2}, \quad K = \frac{3G_1}{2V_0}.
\]

As one can see the bulk modulus does not depend on the stiffness of the angle interaction \( G_2 \) but only on the tension stiffness of the bond as would be expected. After putting (2) in (24) and introducing a notation \( c_\gamma = \frac{\gamma}{a^2} \) the following formulae are obtained:

\[
E = 8\sqrt{3} \frac{c c_\gamma}{c + 18c_\gamma}, \quad \nu = \frac{c - 6c_\gamma}{c + 18c_\gamma}, \quad K = \frac{\sqrt{3}}{6} c.
\]

Let us consider the matrix of the stiffness tensor according to (20)

\[
\begin{bmatrix}
\lambda + 2\mu & \lambda & 0 \\
\lambda & \lambda + 2\mu & 0 \\
0 & 0 & \mu
\end{bmatrix},
\]

where Lame parameters can be calculated applying formula (19)

\[
\lambda = \frac{\sqrt{3}}{6} \frac{c - 6c_\gamma}{c + 6c_\gamma}, \quad \mu = \frac{2\sqrt{3}c c_\gamma}{c + 6c_\gamma}.
\]
The 2D stability criterion can be expressed like this:

\[
\begin{cases}
\lambda + \mu > 0 \\
\mu > 0
\end{cases}
\]  

(28)

After putting (27) in (28) the criterion can be obtained:

\[
\begin{cases}
c \gamma > 0 \\
c \gamma < -\frac{c}{6} \\
c > 0
\end{cases}
\]  

(29)

The same results can be obtained from equations (25) taking into consideration the fact that

\[K > 0, \quad -1 < \nu < 1.\]

(30)

According to [12] elastic moduli of this lattice’s stiffness tensor are:

\[\frac{C_{11}}{h} = 1060 \text{ GPa}, \quad \frac{C_{12}}{h} = 180 \text{ GPa}, \quad a = 0.142 \text{ nm}, \quad h = 0.34 \text{ nm},\]

(31)

where \(h\) is a distance between the graphene planes in graphite crystals. Let us remind that the stiffness coefficients (20) correspond to two-dimensional theory and therefore are measured in N/m whereas obtained experimentally values for graphite correspond to three-dimensional theory and are measured in Pa=N/m². Distance \(h\) is a coefficient of proportionality between two-dimensional and three-dimensional elastic moduli (since the volume of three-dimensional graphite crystal’s elementary cell is equal to the composition of the volume of two-dimensional graphene’s one and the distance \(h\)). Putting the experimental data in (20) one can obtain:

\[\lambda = 61.2 \text{ N/m}, \quad \mu = 149.6 \text{ N/m}, \quad K = 210.8 \text{ N/m}\]

\[E = 350.0 \text{ N/m}, \quad \nu = 0.17.\]

(32)

Stiffnesses \(c\) and \(c_\gamma\) for graphene lattice can be calculated applying (32) and the latter relations:

\[c = 730.2 \text{ N/m}, \quad c_\gamma = 66.9 \text{ N/m}.\]

(33)

As one can see from (33) criterion (29) holds true.

4 Conclusion

In this work the general representation for the energy of interatomic interaction including the angles between the atomic bonds was considered. The interaction is carried out by means of linear and angular springs. Representation for complex two-atomic lattice’s stiffness tensor is obtained on the basis of proposed model. The elastic characteristics of graphene crystal lattice as well as stiffnesses of torsion and linear springs are determined applying the experimental data. It was shown
that considered model allows to obtain the correct values of the components of the macroscopic stiffness tensors and satisfies the necessary stability conditions.

The performed investigation permitted to build the model of interatomic interaction that can be used for analytical modeling and computer simulations by methods of particle and molecular dynamics to investigate deformation and oscillation processes that happen in graphene sheets.

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Appendixes

A Determination of interatomic bonds’ deformations.

Let us consider a deformation of the bonds between the selected particle and its closest neighbours that are indicated with index $\alpha$. The bond vectors $A_\alpha$ in the current configuration can be expressed in the following way:

$$A_\alpha = a_\alpha + u_\alpha - u + a_\zeta,$$

(34)

where $a_\alpha$ is a vector of the bond between the selected particle and the particle $\alpha$ in the initial configuration, $u_\alpha$ and $u$ – displacements of the particle $\alpha$ and the selected particle respectively, $\zeta$ – discrepancy vector ($a$ – length of the bond in the initial configuration).

Taking into account long-wave approach one can express

$$u_\alpha - u = a_\alpha \cdot \nabla u.$$  

(35)

Then casting out small terms and applying (34):

$$A_\alpha = a_\alpha + a_\alpha \cdot \nabla u + a_\zeta,$$

$$A_\alpha^2 = a_\alpha^2 + 2a_\alpha a_\alpha \cdot \xi + 2a_\alpha a_\zeta$$

(36)

The modulus of the bond vector in the current configuration can be expressed in the following way:

$$A_\alpha \approx a(1 + n_\alpha n_\alpha \cdot \xi + n_\alpha \cdot \zeta).$$

(37)

Here the deformation of the bond

$$\kappa_\alpha = \frac{A_\alpha - a_\alpha}{a_\alpha} = n_\alpha n_\alpha \cdot \xi + n_\alpha \cdot \zeta.$$  

(38)

Let us evaluate the change of the angle $\varphi$ between the bonds. After introducing the notation $\xi_{\alpha\beta}$ that defines the increment of the angle between the bonds $\alpha$ and $\beta$ the following equations can be obtained:

$$\cos(\varphi + \xi_{\alpha\beta}) = \frac{A_\alpha \cdot A_\beta}{A^2} = \cos \varphi - \sin \varphi \xi_{\alpha\beta}.$$  

(39)
Taking into consideration that \( \cos \phi = (\mathbf{a}_\alpha \cdot \mathbf{a}_\beta)/a^2 \) and
\[
A_\alpha \cdot A_\beta = a_\alpha \cdot a_\beta + 2a_\alpha a_\beta \cdot \xi + 2(a_\alpha + a_\beta) \cdot a_\zeta,
\]
one can come to the following relation:
\[
\cos \phi - \sin \phi \xi_{\alpha\beta} = (\cos \phi + 2\kappa_{\alpha\beta})(1 - \kappa_\alpha)(1 - \kappa_\beta).
\]
Here
\[
\kappa_{\alpha\beta} = n_\alpha n_\beta \cdot \xi + \frac{1}{2}(n_\alpha + n_\beta) \cdot \zeta.
\]
And now let us transform (41) and obtain as a result of this transformation
\[
\xi_{\alpha\beta} = (\kappa_\alpha + \kappa_\beta) \cos \phi - 2\kappa_{\alpha\beta} \sin \phi.
\]

**B Some relations for components of the stiffness tensor**

Let us consider unit vectors \( \mathbf{n}_\alpha \) and \( \mathbf{n}_\beta \) that specify the direction of the adjacent bonds. Then let us represent \( \mathbf{n}_\beta \) as a sum of two items: one is parallel and another is perpendicular to \( \mathbf{n}_\alpha \):
\[
\mathbf{n}_\beta = \mathbf{n}_\alpha \cos \phi + \mathbf{n}_a^b \sin \phi,
\]
where \( \mathbf{n}_a^b \) is a unit vector normal to \( \mathbf{n}_\alpha \). Let us assume that the following identities hold true owing to the symmetry of the lattice
\[
\sum_{\beta(\alpha)} n_a^b = 0, \quad \sum_{\beta(\alpha)} n_a^b n_a^b = \frac{M_1}{d-1} (\mathbf{E} - n_\alpha n_\alpha), \quad \sum_\alpha n_\alpha n_\alpha = \frac{M}{d} \mathbf{E},
\]
where the summation by \( \beta(\alpha) \) means the summation by all the bonds that are adjacent to \( \mathbf{n}_\alpha \); \( d = 2, 3 \) — dimensionality of space; \( \mathbf{E} \) — unit tensor corresponding to the space dimension, \( M \) — the number of closest neighbours for selected atom, \( M_1 \) — the number of the bonds adjacent to the selected one. These identities hold true for the graphite lattice and at least for the following crystal lattices: triangular, simple cubic, square, BCC. Applying formulae (44)–(45) one can obtain
\[
\sum_{\beta(\alpha)} \mathbf{n}_\beta \mathbf{n}_\beta = M_1 P \mathbf{n}_\alpha \mathbf{n}_\alpha + \frac{M_1}{d-1} \mathbf{E}, \quad P = \cos^2 \phi - \frac{\sin^2 \phi}{d-1}.
\]
Then the following tensors can be transformed:
\[
\sum_{\alpha,\beta} n_\alpha n_\alpha n_\beta n_\beta = M_1 P \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha + Q I_1,
\]
\[
\sum_{\alpha,\beta} (n_\alpha n_\beta n_\alpha n_\beta + n_\alpha n_\beta n_\beta n_\alpha) = 2M_1 P \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha + Q \left( I_2 + I_3 \right),
\]
where $J^k$ — isotropic tensors of forth rank

$$
J^1 = e_ke_k e_ne_n = EE, \quad J^2 = e_ke_n e_ne_k, \quad J^3 = e_ke_ne_k e_n,
$$

(48)

where $e_k$ are vectors of some orthonormal basis. Here and further the summation by the recurring Latin index is applied. The following notation was introduced:

$$
Q = M_1 M \sin^2 \varphi / d(d - 1). \quad (49)
$$

The following identities are useful for derivation of the formula for the stiffness tensor:

$$
\sum_{\alpha, \beta} n_\alpha n_\alpha = M_1 \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha, \quad \sum_{\alpha, \beta} n_\alpha n_\alpha = M_1 \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha,
$$

(50)

$$
\sum_{\alpha, \beta} n_\alpha n_\alpha n_\alpha n_\beta = M_1 \cos \varphi \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha, \quad \sum_{\alpha, \beta} n_\alpha n_\beta = M_1 \cos \varphi \sum_\alpha n_\alpha n_\alpha.
$$

It is not difficult to obtain the formula

$$
a_m \cdot a_n = \begin{cases} a^2 / \mu, & \mu = \nu; \\ -a^2 / d, & \mu \neq \nu \end{cases} \iff a_m \cdot a_n = \frac{1}{d} a^2 \left( (d + 1) \delta_{mn} - 1 \right) \quad (51)
$$

if one takes into account the symmetry of the lattice. Here $\delta_{mn}$ — Kronecker symbol. Applying formula (51) allows to express the following composition:

$$
\sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha \cdot \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha = \frac{d + 1}{d} \sum_\alpha n_\alpha n_\alpha n_\alpha n_\alpha - \frac{1}{d} \left( \sum_\alpha n_\alpha n_\alpha \right) \left( \sum_\alpha n_\alpha n_\alpha \right). \quad (52)
$$

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**References**


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Nonlinear effects in vibrating vessels with fluid and granular medium

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Abstract

The results of the experiments on studying behaviour of fluid and granular medium in vertically vibrating vessels performed on the vibrating stand of "Mekhanobr" institute have been given. Then on the basis of single approach - vibrational mechanics and the method of direct separation of motions - the theory of detected effects has been offered.

In the first part of the report the phenomena taking place with vibration influence on an open vessel with fluid have been considered. It has been noted, that the problem was investigated by many researchers, including outstanding scientists. The special place among those works is occupied by the article of academician V.N.Chelomey; the authors have devoted their report to his memory.

The initial differential equation of particle motion in the field of standing wave is nonlinear and non-autonomous; the analytical solution of this equation is not obviously possible. At the same time on its basis using the method of direct separation of motions rather simple equation of slow motions is obtained. It is autonomous and corresponds to conservative system - to an original pendulum with the occurrence of displacing moment. The analysis of this last equation has allowed to come to rather simple conditions of dipping gas bubbles in to the fluid and floating heavier particles. In these cases the system tends to the maximum of potential energy as to the steady state. Peculiar "vibrating unestablishability" of stable without vibration of state of gas - fluid and fluid - heavy particles systems in the field of gravity has been revealed. The "slow" self-oscillating phenomena in system have been described. The results are in good agreement with experimental data of the authors and other researchers.

In the second part of the report nonlinear effects at behaviour of granular medium in vibrating communicating vessels are considered. It has been noted, that in some cases medium behaves as a viscous fluid and in other cases it behaves rather differently. As an example two cases of peculiar behaviour of
granular medium in a tube dipped in a vibrating vessel with granular medium
have been studied. In the case of the straight tube - medium is quickly
transported down the tube. In the second case when the configuration of the
tube is, seemingly, rather slightly changed, almost the same level of medium
as in the vessel are settled in it. The model describing observable effects on the
basis of the vibrational displacement theory and the approach of vibrational
mechanics has been offered. The concepts of input and output resistances of
medium have been introduced; they play an essential role in explanation of
discovered effects.

1 "Anomalous" phenomena in fluid under the
action of vibration

1.1 Preliminary remarks
Peculiar nonlinear effects, in particular, the sucking of gas bubbles deep into the
depths of the vessel and on the contrary, floating of bodies, which are heavier than
fluid are observed under vibration in gas medium of the vessel with fluid. In other
words, the "anomalous" behaviour of system exists: it evolves to the states corre-
sponding with maximal or close to them values of potential energy.

These and allied questions were considered in many publications also written
by outstanding scientists; the list [1 - 15] is far from being full. The given work
develops and completes the mentioned researches: conditions of dipping bubbles
and floating a "heavy" body have been received with rather simple assumption by
using of vibrational mechanics approach and by the method of direct separation of
motions. The results have been compared with experimental data.

The significant impulse to the researches in this area was given by the publication
of V.N.Chelomey (Paradoxes in mechanics, caused by vibrations // Dokl. Academy
of Sciences of the USSR, 1983, volume 270, 1, pp. 62-67). The authors devote this
part of the report to his memory. The authors are deeply grateful to D.A.Indeytsev
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1.2 Experimental research
Glass cylindrical vessel with internal diameter 60 mm was fixed on the table of the
vibrating stand of Mekhanobr institute (Fig. 1).

The vessel was filled with water up to the level of H = 180 mm, then vertical
harmonious oscillations with constant amplitude A = 6.5 mm were imparted to
it. The change of system behaviour with slow increase of frequency \( \omega \), observed at
normal and stroboscopic lighting, is schematically presented in Fig. 2. In an interval
\( 0 < \omega < \omega_1 = 170s^{-1} \) fluid remained clear (the area I). The fluid layer saturated
with bubbles of various sizes arised near the surface gradually growing with increase
in frequency. With \( \omega > \omega_1 = 170s^{-1} \) there were intensive chaotic oscillations of the
fluid surface, and separate splashes amounted to 180 mm (the area II).

With frequency \( \omega = \omega_2 \approx 190s^{-1} \) the dipping of bubbles into the depths of the
vessel was observed and at that bubbles with diameter of nearly 1-2 mm were more
or less uniformly disposed in the volume (the area III). With $\omega = 200 - 210\text{s}^{-1}$ the drift of such and smaller bubbles downwards was so intensive that the whole volume of fluid notably grew turbid, reminding milk with water.

Dipping bubbles were forming an air space ("cushion") near the bottom of the vessel. When the cushion amounted to the certain volume ($\omega = \omega_4 \approx 220\text{s}^{-1}$) an air bubbles swarm, forming "cushion", with characteristic noise uprushed and out-croped. After that at the same frequency situation repeated: bubbles were dipped, again forming a cushion etc. In other words the asynchronous excited self-oscillations arised (the area IV). Their period was 2-3 s. At that the general rate of fluid-gas mixture in the vessel was raising to 290 mm which corresponded to gas content $\alpha = 38\%$. In the interval of frequencies $220 - 230\text{s}^{-1}$ ($\omega_5 < \omega < \omega_6$) there was the floating of particles (the area V), which density were more than density of water (rubber pieces of 5 mm size and balls of 10 mm size). With frequency $\omega = \omega_3 = \lambda$, close to $\omega_2$, the passage through a resonance corresponding to the frequency of free oscillations of water column on the air cushion took place. At that Sommerfeld effect was observed (see, for example, [10]). The other experiments are considered below.
1.3 The equation of particle motion

The equation of particle motion (Fig. 3), we write down in the form

\[(ρ + \frac{1}{2} ρ_0)\ddot{v} = -k\dot{x} + (ρ - ρ_0)v(\ddot{ξ} + g)\]  

(1.1)

Here \(x\) - coordinate of a particle relative to a vessel, counted from undisturbed fluid surface downwards; \(v\) - volume of a particle, \(ρ\) - its density, \(ρ_0\) - medium density; \(g\) - gravity acceleration, \(k\dot{x}\) - medium resistance force, assumed either linear or linearized. The value of \(\frac{1}{2} ρ_0v\) approximately considers the additional medium mass. Absolute medium acceleration in the place of particle location is denoted by \(\ddot{ξ}(x, ωt)\) (we consider, that medium is deformable and \(\ddot{ξ}\) changes along \(x\) relatively slowly).

We’ll be finding acceleration \(\ddot{ξ}\) from the supposition, that medium is saturated with gas with volume concentration \(α\) at some depth \(h ≤ H\) and can be considered as an elastic rod. Sound speed in such rod for air bubbles with radius \(a > 10^{-3} \text{sm}\) to an accuracy of less than 5% can be determined by the formula (see [6]) \(c ≈ 10/\sqrt{α(1 - α)} \text{ (m/s)}\). This speed is paradoxically low [6]. So, at \(α = 0.3 \div 0.7\) we have \(c ≈ 20 \text{ m/s}\), i.e. more than lower degree than sound speed in the air (see Fig. 4). This circumstance plays the important role at explanation of the phenomena involved.

From the solution of the wave equation \(\ddot{ξ} = c^2\ddot{ξ} + g\) under boundary conditions \(\dot{ξ}|_{x=0} = 0\); \(\ddot{ξ}|_{x=h} = A\sinωt\) (we consider, that at \(h ≤ x ≤ H\) fluid oscillates as a solid body together with the vessel), we find:

\[\ddot{ξ} = -Ψ(x)\sinωt, \quad Ψ(x) = Aω^2\cos(ωx/c)/\cos(ωh/c)\]  

(1.2)

Allowing for these expressions the equation (1.1) takes the form

\[\ddot{x} = -k_1\dot{x} + κ[-Ψ(x)\sinωt + g],\]  

(1.3)
Figure 4: Sound speed dependence on concentration of bubbles in water.

\[ k_1 = k / (\rho + \frac{1}{2} \rho_0) \nu, \quad \kappa = (\rho - \rho_0) / (\rho + \frac{1}{2} \rho_0) \]  

(1.4)

1.4 The equation of slow motion (the basic equation of vibrational mechanics). Some motion regularities

We search for the solution of equation (1.3) by of the method of direct of separation motion [10, 15] in the form of \( x(t) = X(t) + \psi(t, \omega t) \), where \( X \) - basic "slow", and \( \psi \) - "fast", \( 2\pi \) - periodical over \( \omega t \) constituent with a zero average over period. For \( X \) the equation is written as

\[ \ddot{X} = -k_1 \dot{X} + \kappa g + V(X), \]  

(1.5)

where

\[ V(X) = -\frac{1}{2} \frac{\kappa^2}{\omega^2 + k_1^2} \psi'(X) \psi(X) = -\frac{1}{2} \frac{\kappa^2}{\omega^2 + k_1^2} [\psi^2(X)]' = \]

\[ = \frac{1}{4} \frac{\kappa^2}{\cos^2(\omega h/c)} \cdot \frac{\omega^2}{\omega^2 + k_1^2} \cdot \frac{A \omega}{c} \cdot \Lambda \omega^2 \sin \frac{2X \omega}{c}, \quad (X \leq h) \]  

(1.6)

- vibrational force (in this case - acceleration but we conventionally use the term "force").

The difference between expression (1.6) and the expression received in the book [10] for the particle in the field of standing wave (pp. 340-344) lies in the using expression (1.2) and also in the fact that in the solution of fast motion equation the viscous resistance force \( k_1 \dot{\psi} \) is considered; it is essential in case of fine particles at rather low frequencies \( \omega \). It is noteworthy, that equitation (1.5) corresponds to potential system (in the presence of dissipation) whereas the initial equation (1.3) answers essentially non-conservative system; such systems refer to the class of potential on average systems [10].

If \( V(X) \ll \kappa g \), then a particle in the steady mode moves with an almost constant speed \( \dot{X} = \kappa g / k_1 \) (floats in case of bubble and dips in case of a particle, more density, than medium). If \( V(X) \gg \kappa g \) the particle "is attracted" as to the stable positions.
to nodes of wave $X_0$, where $X_0$ - the roots of equation $\Psi(X_0) = 0$, i.e. it moves in the line of decrease function $|\Psi(X)|$. In intermediate cases a particle is attracted to points $X_*$, where $V(X_*) = \kappa g$ and at that $V'(X_*) < 0$ at $\kappa g \ll V(X_*)$; these points lay near to nodes.

For the expressions such as (1.6) resulted in previous researches, the presence of multiplier $\sin(2\omega x/c)$ is also typical (see for example, [1-4, 7, 8, 11, 15]). However coefficients with this multiplier are essentially various; it is explained by distinction in initial suppositions, which sometimes are rather complicated. As a result various conclusions concerning "extent" of particles to wave nodes or antinodes occur; some experimental data are also conflicting (see, for example, [4, 7]).

Vibration force (1.6) can be interpreted as radiation pressure determined with the fast constituent of particle motion $\psi$.

If medium density $\rho_0$ changes along coordinate $X$ then the role of $\Psi(x)$ plays function $\kappa(x)\Psi(x)$, at that $\Psi(x)$ must be determined from the wave equitation with variable coefficients. Studying such cases is an independent problem. Here we in the main consider step change $\rho_0$ along $x$.

### 1.5 A condition of gas bubble dipping. The phenomenon of vibrational unstability of an equilibrium position of gas-fluid system in the field of gravity

For air bubble $\rho \ll \rho_0$ and $\kappa \approx -2$. Then, according to (1.5) if at the boundary of the front of gas phase propagation $X = h$ the inequality $V(h) > 2g$ or, allowing for (1.6), the relation

$$Q = \frac{\omega^2}{\omega^2 + k^2} \cdot \frac{A\omega}{c} \cdot \frac{A\omega^2}{g} \cdot \frac{h\omega}{c} > 1,$$  

(1.7)

is satisfied, then bubbles, formed in a layer with thickness $h$, will propagate deep into the depths of the vessel. Inequality (1.7) is possible to consider as a condition of vibrational unstability of separate state of gas-fluid system in the field of gravity. At not very high frequencies $\omega$, as in our experiments, it can be satisfied only with availability of a gas-saturated layer definite thickness $h$ near to a fluid surface, when sound speed $c$ is comparatively low in this layer (see above). Thus, for explanation of the discussed unstability and bubbles dipping an important point is turbulization of some fluid layer near the free surface with formation of bubbles. Various points of view about physical reason of such layer formation are expressed (see, for example, [5, 12]). We consider this layer to be vibrating generator of the bubbles. According to work [13] and publications of G.M.Ostrovsky, the radius of generated bubbles is stable enough and is about 0.7 mm that also corresponds to our observations. Such bubbles at frequencies $\omega < 200s^{-1}$ can be considered as rigid particles. In Fig. 5 the shaded areas of changing parameters $A\omega^2/g$ and $A\omega/c$ are specified with condition (1.7) for $h = 5A$ and $h = 10A$, $\alpha = 0.4$ and $k^2 \ll \omega^2$; the last one corresponds at frequency $\omega \approx 200s^{-1}$ to bubbles with radius $a > 0.4$ mm and to resistance by Stokes formula. The sign * marks the point corresponding to the beginning of dipping bubbles in our experiments. Evidently, at $h = 10A$ the agreement is rather good.
The significance of the layer saturated with bubbles for the initiation of dipping bubbles deep into the vessel is proved by additional experiments. In one case the air was blown in through the tube in the upper layer fluid, in another case the air balloon in thin rubber covering was placed in it (see also [3]). As a result bubbles dipping into the depths of the vessel was observed already at $\omega \approx 130 \text{s}^{-1}$.

In another experiment fluid surface was closed with polyethylene film; at that no described effects was observed, fluid moved as a solid whole together with the vessel.

1.6 The bubbles, drifting to standing wave antinodes

The present consideration covers the case when the particle can be taken as solid-state. This condition at frequencies $\omega < 200 \text{s}^{-1}$ is satisfied by air bubbles with radius less than 1 mm. Such bubbles are "attracted" to the amplitude nodes $|\Psi(X)|$ of a standing wave. As follows, in particular, from works [11, 15], bigger bubbles which frequencies of free oscillations are close or less $\omega$, in the certain ranges of changing $\omega$ are gravitated to the amplitude antinodes $|\Psi(X)|$.

1.7 Conditions of floating particles, more denser, than fluid

If the column of fluid is uniformly saturated with air bubbles than a condition of floating a particle laying at the bottom of the vessel, according to (1.5), is inequality $\kappa g = V(H) < 0$, or, allowing for (1.6),

$$\frac{1}{2} \frac{\omega^2 \kappa}{\omega^2 + k_1^2} \frac{A \omega}{c} g \frac{H \omega}{c} < -1 \quad (1.8)$$

When this condition is fulfilled, the amplitude node $|\Psi(X)|$ is above the bottom of the vessel, and antinode is as though below the bottom.

If deformability of medium is defined by a water-air cushion, and fluid above it is practically rigid (see 1.2), then at the account of the formula for frequency of free
oscillations of such system \( \lambda \) (see [8], p. 105), and also equations (1.5), the following condition particles detachment from the bottom of the vessel is obtained

\[
R \equiv \frac{1}{z^2} \kappa \frac{\omega^2}{\omega^2 + k^2} \frac{A}{Y_1 \zeta^2 - 1} \frac{A \omega^2}{9} > 1, \quad (z > \sqrt{2})
\]  

(1.9)

where

\[
Y_1 = \frac{Y_0}{\alpha} = z^2 \frac{\zeta p_0}{\alpha \rho_0 H} \frac{1}{\omega^2}
\]

height of a water-air layer, and \( p_0 \) - atmospheric pressure, \( Y_0 \) - height of purely air space, \( \zeta \) - polytropic coefficient, \( z = \omega / \lambda \). The height of lifting a particle above the bottom of the vessel

\[
h_* = Y_1 \frac{z^2 - 1}{R} \frac{R - 1}{R}, \quad (z > \sqrt{2})
\]

At \( z > \sqrt{2} \) and at any attenuation the fluid column oscillates with the amplitude, smaller than and (without attenuation) opposite in phase with fluctuations of the vessel.

1.8 The "breakthrough" of an air "cushion" and self-oscillating cycle of system behaviour

When water-air "cushion" reaches the certain volume corresponding value \( z \), exceeding a little \( z = \sqrt{2} \), the growth of "cushion" stops, as the bubbles do not dip any more. The increase of \( z \) results in further decreasing of oscillations amplitude of the fluid column. At \( \omega = \omega_5 \), \( z = \omega_5 / \lambda \) (Fig.2) amplitude decreasing becomes so significant, that air is not kept any more by vibrational force near the bottom of the vessel, and it breaks upwards. This breakthrough can occur and with smaller values of \( z \) and \( \omega \) if there are enough disturbances [7]. After the breakthrough of cushion at the fixed values of frequency \( \omega \) in the certain range the whole cycle of system change repeats (in our experiments - each 2 - 3 s). In other words, so-called asynchronous excitation of self-oscillations takes place.

2 Some nonlinear effects of granular medium behaviour in communicated vibrating vessels

2.1 Preliminary remarks

Contrary to the frequent statement, granular medium under vibration behaves not as viscous fluid, or more precisely, not quite as viscous fluid. Namely, along with the liquation, owing to vibration additional slow volumetric and surface forces (vibrational forces) occur in the medium, which cause effects of vibrational movement and displacement [10, 16]. Vibrational transportation can exemplify the first effect, and the second effect can be exemplified by vibrobunkerization and inequality of medium levels setting in communicated vibrating vessels.
It is possible to consider established, that the physical reason of the mentioned effects is asymmetry of system or of oscillation trajectory. The various types of asymmetry resulting in vibrational movement and displacement are analyzed in book [10].

In this section two unusual, apparently, unstudied cases of granular medium behaviour in communicated vibrating vessels are considered.

The other cases of peculiar granular medium behaviour in such vessels and on the basis of other theoretical models are considered in works [16, 17]. Notice, that now it’s put more emphasis on the problem of modeling granular bodies as peculiar "non-classical" bodies (see, for example, work [18]).

2.2 Conditions and results of experiments

Experimental researches were carried out with two kinds of tubes, dipped in a vibrating vessel with sand. In the first case a straight tube opened at the top and at the bottom with passage section diameter of 6 mm was put into the vessel of square section with side of 150 mm and was rigidly connected with it (Fig.6, a). In the second case such tube but with a 90° bend of the bottom end was put into the vessel (Fig.6, b). Top ends of the tubes were above the free surface level of granular medium in the vessel.

The granular medium represented dry sand of less 0.3 mm fraction. The space between the tube bottom end and the bottom of the vessel was 150 mm. Vertical vibration with amplitude $A = 0.55$ mm and frequency up to $240s^{-1}$ was imparted to the vessel.

Experimental researches consisted in observation of the behaviour of sand in the tubes at different depths of dipping $H$ of the tubes in the vessel. With gradual increase in vibration frequency in the vessel the circulation flows of granular medium occur with increasing intensity. At frequency $180s^{-1}$ it was observed that there is
an outflow of sand from the bottom end of the straight tube filled with sand into the vessel up to its practically full emptying.

The speed of the outflow of sand from the tube was determined from the time of movement of free surface or tinted particles on the fixed area (100 mm).

Behaviour of sand in the case of dipping the empty tube in the sand with a bend of the bottom end was another. Reaching vibration frequency of $180 \text{s}^{-1}$ the sand started to flow inside the tube, amounting to some certain level. With the increase in vibration frequency this level grew and at frequency $210 \text{s}^{-1}$ became equal to the free surface level of the sand in the vessel.

![Experimental installation](image)

Figure 7: Experimental installation (on the left - an axial section of the straight channel, on the right - an axial section of the bend channel).

In Fig.7 there is a photo of experimental installation illustrating detected effect. The plank with cylindrical straight and bend channels (their axis coincides with a surface of the plank) is pressed to the front transparent wall of the vessel.

At vertical vibrations the sand completely poured out of the left (straight) channel to the vessel while the sand ran into the right (bend) channel from the vessel and fills it practically up to the sand level in the vessel.

Detected effects are also observed at increase of the passage section diameter up to 12 mm. The further increase of the tube diameter results in disappearance of the detected effects. The described effects also occur when the tubes are fixed in space and are not connected with the vibrating vessel.

### 2.3 To the theory of the detected effects

According to the classification introduced in book [10], it is possible to say, that vibrational displacement and drift in the considered case are caused by constructive asymmetry of system.

We’ll try to explain theoretically and to describe mathematically the behaviour of granular medium in both described cases. For this purpose we’ll consider the movement of a medium column in tubes. We’ll describe this movement by the equation

$$\rho S \ddot{x} = -\rho g S x + \rho S x A \omega^2 \sin \omega t + F(\dot{x}, x) + R_e(\dot{x}, x, \omega t)$$  \hspace{1cm} (2.1)
Here $x$ - height of the medium column in the tube, counted from its bottom section, $S$ - section area of the tube, $\rho$ - medium density, $g$ - gravity acceleration. Expression $F(\dot{x}, x)$ denotes the force of dry friction between medium and internal surface of the tube which we’ll consider defined with relations

$$F(\dot{x}, x) = \begin{cases} -F(x) & \text{when } \dot{x} > 0 \\ F(x) & \text{when } \dot{x} < 0 \end{cases} \quad (2.2)$$

$$-F(x) < F(\dot{x}, x) < F(x) \quad \text{when } \dot{x} = 0$$

Expression $R_e(\dot{x}, x, \omega t)$ denotes the force acting on the bottom section of the medium column in the tube. This force is supposed to consist of two components

$$R_e(\dot{x}, x, \omega t) = R_0(\omega t) + R(\dot{x}, x) \quad (2.3)$$

Component $R_0$ refers to the force acting on the bottom section of the granular medium column in the tube from the side of medium in the vessel, and $R(\dot{x}, x)$ refers to the force which we’ll call the force of face resistance at medium passing of outlet section of the tube. Force $R_0$ will be considered below. As for force it’ll be defined with relations

$$R(\dot{x}, x) = \begin{cases} -R_+(x) & \text{when } \dot{x} > 0 \\ R_-(x) & \text{when } \dot{x} < 0 \end{cases} \quad (2.4)$$

$$-R_+(x) < R(\dot{x}, x) < R_-(x) \quad \text{when } \dot{x} = 0$$

Unlike force $F$, resistance force $R$ is supposed to be different at movement of the medium column inside of the tube and out of the tube, i.e. consider, that $R_+ \neq R_-$. This supposition which foundation we’ll take below, is essential, as it, basically, will serve as an explanation of the detected effects.

Reactive force caused by variability of medium mass in the tube, in this case is equal to zero as this mass starts moving with zero initial speed.

We’ll solve equation (2.1) by the method of direct separation of motions [10], suppose

$$x = X(t) + \psi(t, \omega t), \quad (2.5)$$

where $X(t)$- basic slow component, and $\psi(t, \omega t)$ - fast small component with a zero average for period $T = 2\pi/\omega$ over ”fast time” $\tau = \omega t$:

$$\langle \psi \rangle = 0 \quad (2.6)$$

(angle brackets denote averaging for period $2\pi$ over $\tau$).

Plugging expression (2.5) into equation (2.1) and making averaging at the account of (2.6) and considering only linear summand according to $\psi$, we’ll obtain the following equation of slow motions

$$S\rho X\ddot{X} + S\rho \langle \psi \dot{\psi} \rangle = -S\rho gX + S\rho A\omega^2 \langle \psi \sin \omega t \rangle +$$

$$\langle F(X + \psi, X) \rangle + \langle R_0(\omega t) \rangle + \langle R(X + \psi, X) \rangle \quad (2.7)$$
As for the equation of fast motion, as is known [10], it is possible to be confined only with its rather approximate solution, without introducing big error into the solution of slow motion equation (2.7). In this case we’ll be confined with so-called merely inertial approximation, defining fast constituent \( \psi \) from equation

\[
\ddot{\psi} = A\omega^2 \sin \omega t
\]

i.e. considering other members in this equation to be small. Periodical over \( \tau = \omega t \) solution of equation (2.8) is

\[
\psi = -A \sin \omega t
\]

Plugging this expression into formulas (2.2) - (2.4) and making operation of averaging, we’ll obtain (at calculation of integrals from time intervals where \( \dot{x} > 0 \) and \( \dot{x} < 0 \), it is possible to use directly formulas (2.10) p. 202 books [10]):

\[
\langle F(\dot{X} + \dot{\psi}, X) \rangle = \begin{cases} 
-F(X) & \text{when } \dot{X} \geq A\omega \\
-\frac{2}{3} F(X) \arcsin \frac{\dot{X}}{A\omega} & \text{when } |\dot{X}| \leq A\omega \\
F(X) & \text{when } \dot{X} \leq -A\omega 
\end{cases}
\]

\[
\langle R(\dot{X} + \dot{\psi}, X) \rangle = \begin{cases} 
-R_+ & \text{when } \dot{X} \geq A\omega \\
\frac{1}{2}(R_- - R_+) - \frac{1}{3}(R_+ + R_-) \arcsin \frac{\dot{X}}{A\omega} & \text{when } |\dot{X}| \leq A\omega \\
R_- & \text{when } \dot{X} \leq -A\omega 
\end{cases}
\]

As for force \( \langle R_0(\omega t) \rangle \), assuming that granular medium in the vessel is in corresponding sense liquated owing to the action of vibration, we’ll consider it to be defined as "hydrostatic pressure", similar to the first summand in the right part of equation (2.7):

\[
\langle R_0(\omega t) \rangle = \rho g HS
\]

Here \( H \) denotes the height of the medium level in the vessel above the level of outlet section of the tube. It can be considered to be not dependent on coordinate \( X \) if the section area of the tube \( S \) is much less than the section area of the vessel outside the tube \( S_0 \). Otherwise values \( X \) and \( H \) are connected by relation (a condition of volume preservation)

\[
S_0 H = SX
\]

Then

\[
H = H(X) = \frac{S}{S_0} X
\]

At last, we’ll find force \( F(X) \) as the force of dry friction of the medium column on walls of the tube, considering, that this force for a layer of thickness \( dx \) in section \( x \) is defined by equality

\[
dF = fp(x) dx
\]

where

\[
p(x) = \rho g x
\]
- medium pressure on the wall in this section, \( l \) - perimeter of section, and \( f \) - constant of dry friction. Then integrating equality (2.14) between \( x = 0 \) and \( X \), we’ll find

\[
F = \frac{1}{2} f \rho g l X^2 \tag{2.16}
\]

In view of equality (2.10) - (2.12) and (2.16) equation of slow motion (2.7) after not complicated transformations has the following form

\[
S \rho X \ddot{X} = S \rho g (H - X) - \frac{1}{2} (R_+ - R_-) - \frac{1}{\pi} [f \rho g l X^2 + (R_+ + R_-)] \arcsin \frac{\dot{X}}{A \omega} \quad (| \dot{X} | < A \omega) \tag{2.17}
\]

It should be noted that with relation to vibrational mechanics penultimate summand in the right part of equation (2.17) represents moving force, and the last - inverted vibrational force. This last one is a force of nonlinear-viscous friction.

Autonomous nonlinear equation of second order allows for a global research on the phase plane. Without stopping on such research, notice that this equation allows for the stationary solution

\[
X = X_* = H - \frac{1}{2} \left( \frac{R_+ - R_-}{S \rho g} \right) \tag{2.18}
\]

corresponding to quasi-equilibrium state of medium in the tube (i.e. to the balance state by slow constituent of motion \( X \)). For the research of stability of this state we suppose that in equation (2.17) \( X = X_* + \delta \), we linearize the equation by \( \kappa \) and use relation (2.18). Then we’ll come to the following equation in variations

\[
S \rho X_* \ddot{\delta} + S \rho g \delta + \frac{1}{\pi} [f \rho g l X_*^2 + (R_+ + R_-)] \frac{\dot{\delta}}{A \omega} = 0 \tag{2.19}
\]

At \( X_* > 0 \), i.e. on conditions that in quasi-equilibrium state there is medium in the tube, all factors of this equation are positive. Therefore quasi-equilibrium position (2.18) is asymptotically steady.

Supposing that the speed of medium motion in the tube \( \dot{X} \) varies with time comparatively slowly, i.e. \( \dot{X} \) is small, then from the condition of equality to zero of the right part of equation (2.17) we find the following simple approximate expression for the rate of change of medium column height in the tube

\[
\dot{X} = A \omega \sin \left[ \pi \cdot \frac{S \rho g (H - X) - \frac{1}{2} (R_+ - R_-)}{f \rho g l X^2 + (R_+ + R_-)} \right] \tag{2.20}
\]

In view of notation (2.18) expression (2.20) can have the following form

\[
\dot{X} = -A \omega \sin \left[ \pi \cdot \frac{S \rho g (X - X_*)}{f \rho g l X_*^2 + (R_+ + R_-)} \right] \tag{2.21}
\]

From formula (2.21) follows, as well as should be, that speed \( \dot{X} \) decreases in process of approaching layer height in the tube \( X \) to equilibrium value \( X_* \). At that for \( X > X_* \) speed \( \dot{X} < 0 \), and for \( X < X_* \) we have \( \dot{X} > 0 \).
2.4 Discussion of results. Input and output resistances in the tube

First of all, mention that the basic role in the offered theoretical explanation of discussed effects is played by the supposition about inequality in the general case of resistance force \( R_+ \) and \( R_- \) at input and output of medium out of the tube. Let \( R_+ \) denote input resistance, and \( R_- \) - output resistance. It is obvious to suppose, that for the tube with not very big section \( R_+ > R_- \), i.e. input of medium into the tube is harder, than output from the tube. Notice that such effect is well-known in hydraulics concerning fluid flow (see, for example, [19]).

In this supposition from formula (2.18) at once follows, that always \( X_* < H \), i.e. the level of stationary position of medium in the tube is below the level of medium in the vessel. At satisfying inequality

\[
R_+ - R_- < 2SH\rho g
\]  
(2.22)

coordinate \( X_* \) becomes negative, i.e. the tube completely becomes empty (Fig.6, a). If \( R_+ \approx R_- \), that is for the tube with comparatively big section, and also as it is natural to suppose, for the tube with bend end (Fig.6, b) then \( X_* \approx H \). In case when \( R_+ < R_- \) it turns out \( X_* > H \), i.e. the granular level in the tube is higher, than in the vessel.

Thus, the offered theoretical description explains the concerned regularities. This description is phenomenological in a sense: the reasons leading to the inequality or equality of resistances \( R_+ \) and \( R_- \) are not explained in detail in it. (Notice that the attempt of such “explanation” is essentially made for other cases in works [16, 17]). At the same time from the position of vibrational mechanics such description is natural: whatever real physical reasons of considered effects would be, they cannot lead to anything else, but to the occurrence of corresponding vibrational forces in the equation of type (2.17). These forces just consider influence of the mentioned effects on slow motion in the integrated form.

It should be noted further, that, introducing notations

\[
R_+(X) = R_+ + \frac{1}{2} f\rho g lX^2
\]  
(2.23)

it is possible to present equation (2.17) and relations (2.18) and (2.20-2.21) correspondingly in the form

\[
S\rho Xx' = S\rho g(H - X) - \frac{1}{2} [R_+(X) - R_-(X)] - \frac{1}{\pi} [R_+(X) + R_-(X)] \arcsin \frac{\dot{X}}{A\omega} \quad (|\dot{X}|, A\omega)
\]  
(2.17)'

\[
X_* = H - \frac{1}{2} \frac{[R_+(X) - R_-(X)]}{S\rho g}
\]  
(2.18)'

\[
\dot{X} \approx A\omega \sin \left[ \pi \cdot \frac{S\rho g(H - X) - \frac{1}{2} [R_+(X) - R_-(X)]}{R_+(X) + R_-(X)} \right]
\]  
(2.20)'

\[
\dot{X} \approx -A\omega \sin \left[ \pi \cdot \frac{S\rho g(X - X_*)}{R_+(X) + R_-(X)} \right]
\]  
(2.21)'
Values \( R_\pm(X) \) and \( R_-\pm(X) \), considering not only input and output resistances of medium at sliding along the tube sides, are named accordingly as input and output summary resistances of the tube.

It should be emphasized, that like equation (2.17), all next relations, are true in supposition, that vibration of the vessel is rather intensive, so slippage of medium along the tube sides is provided (relation \( A\omega > |\dot{X}| \) in formulas (2.10) and (2.11)), and adequate accuracy of merely inertial approximation for determination of fast motion (2.9) is provided too (significant dominance of inertial forces over resistant forces).

It should be noted in conclusion, that the concerned regularities allow to refer granular media at vibration to so-called vibrational dynamic materials - to nonlinear media which properties in relation to slow or constant actions essentially change under influence of fast (vibrational) action [20].

### 2.5 Results of additional experiments

The results of measuring the speed of sand outflow from the straight tube with keeping its constant level of filling with sand - \( 0.25 \text{m} \) and vibration frequency \( 210 \text{s}^{-1} \) are shown in Fig.8 with triangular marks.

At lowering of medium level in the vessel to value \( H = 0.15 \text{m} \) sand outflow from the tube starts. As evident from the figure, the further lowering of sand level in the vessel leads to the growth of outflow speed to value \( 0.04 \text{ m/s} \) at \( H = 0 \) (the level of sand in the vessel coincides with the level of the bottom end of the tube).

With increase of the sand level in the vessel the sand outflow from the tube stops at value \( H = 0.18 \text{m} \). Difference in the values of sand levels in the vessel, corresponding to the beginning and the termination of the sand outflow from the tube, can be explained by the presence of dry friction forces in this process.

![Figure 8: Dependence of the sand outflow speed (from the straight tube) \( \dot{X} \) from the medium level in the vessel \( H \) at vibration frequency \( 210 \text{s}^{-1} \) (▽ -experimental points, • - the results of calculation).](image)

According to the experimental results shown in Fig. 8, at \( H \approx 0.15 \text{ m} \) equilibrium position of sand \( X = X_\ast = 0.25 \text{ m} \) is reached. Plugging these values into relation (2.18)' we'll obtain

\[
R_+ - R_- = -0.068 \text{ N}
\]
We find the second relation for the forces of face resistance from expression (2.20) with use of experimentally found value of sand outflow speed $V = \dot{X} = 0.04 \text{ m/s}$ in case when the bottom end of the tube is located at the level of free surface of sand in the vessel ($H = 0$). Plugging experimentally found parameters into $(2.20)'$ and neglecting at that the force of sand dry friction along the walls of the tube, we’ll find

$$R^*_+ + R^*_- = 0.328 \text{ N}$$

The obtained relations for the forces of face resistance are used for definition from $(2.20)'$ of calculated values of sand outflow speed at $H = 0.05 \text{ m}$ and $H = 0.1 \text{ m}$. The results of calculations are shown in Fig.8 with circle.

Thus, the resulted theoretical consideration not only allows to explain the basic detected effects, but also to be in good agreement with quantitative experimental data. In particular, it was proved, that the introduced parameters $R_+$ and $R_-$, at least, in the conditions of experiment, can be considered to be constant. At the same time, as the experiments show, that with the increase of the tube size the effect of ”emptiness” disappears, then it is possible to consider, that at that values $R_+$ and $R_-$ become identical.

### 3 Conclusion

Summing up it should be noted, that two analyzed groups of effects have essential nonlinearity of corresponding systems in common. Both can be considered as effects of vibrational displacement - occurrence of the directional on the average ”slow” motion due to the non-directional on the average ”fast” vibrational actions [10]. Vibrational displacement is always caused by asymmetry of system or of vibrational action nature. Namely, dipping of bubbles and floating of particles in fluid are caused by so-called gradient asymmetry, and ”anomalous” behaviour of granular medium in communicated vessels is caused by constructive asymmetry.

The next similar moment is that under vibration influence one or another system can tend not to minimum, but to maximum of system potential energy.

Finally, both the first, and the second group of effects accept rather simple explanation and mathematical description within the limits of the approaches called vibrational mechanics and the method of direct separation of motions.

At the same time the considered effects are rather individual.

The physical basis of effects in fluid is the saturation with air bubbles at vibration its and considerable decrease of sound speed in such medium (up to 20 m/s). In turn specified saturation occurs owing to peculiar unstability of a separate state of fluid-gas system in the field of gravity. This unstability takes place at occurrence of rather thick layer saturated with gas near the free surface of fluid.

As for the described cases of peculiar behaviour of granular medium in communicated vibrating vessels, they are explained and described here phenomenologically in the certain degree - on the basis of the concept about input and output resistances of one of the vessels.
Later on it is supposed to carry out additional experiments both with fluid vessels, and with granular medium.

Finally, we emphasize, that from the positions of the dynamic materials concept granular medium under the action of vibration represents a distinct vibrational dynamic material [20].

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Dynamic equilibrium in aggregating and shattering systems

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Abstract

In a variety of astrophysical applications one encounters a problem of a steady-state size distribution of particles, which suffer fragmentative as well as aggregative collisions. To attack the problem we study a simplified model. Namely, we consider a system, composed of big particles which carry on their surface smaller ones, attached by adhesive forces. When the big particles (carriers) collide with each other at large impact velocities, the small particles (dust) detach from the carriers due to inertial forces. When the dust particles collide with carriers at low speeds they attach back to the carriers surface. As the result a dynamical equilibrium between the dust particles sitting on the carriers and free dust particles is established. For simplicity only interactions between the dust and carriers are taken into account, while dust-dust and carrier-carrier aggregation is neglected. We develop an analytical theory for the particle size distribution for such system and analyze its dependence on the system parameters. Application to the planetary rings is discussed.

1 Introduction

In various astrophysical applications, one encounters systems where particles suffer aggregative and fragmentative collisions. The latter occur when the impact velocity of colliding particles is large, while the former may happen if particles approach each other with a small velocity. If the particles interact with attractive forces, e.g. with adhesive or gravitational forces [1], they may agglomerate. Hence, debris, produced in fragmentative collisions, play a role of a building block in subsequent aggregative collisions. One can expect that a closed system, lacking a particle source, will eventually evolve to a steady state with a stationary particle size distribution.

A general solution of this problem is very complicated. Keeping in mind the astrophysical application, namely, the application to the particle size distribution in planetary rings, we consider the following simplified model, which still has the
main ingredients of a real system. We assume that there exist large bodies of the size $R$, called in what follows "carriers" (for simplicity we assume that all particles are of spherical shape), embedded in a sea of smaller particles, "dust", with a size distribution $N_d(r)$, where the $N_d(r)dr$ gives a number of particles in a unit volume of size within the interval $(r, r + dr)$; the maximal size of the dust particles $r_{\text{max}}$ is much smaller than the size of carriers, that is $r_{\text{max}} \ll R$. We also assume that the characteristic collisional velocity is not large enough, neither to break the carriers nor the dust particles themselves. The shattering of the aggregates formed by carriers and dust particles is, however, possible. Let the concentration of dust is such that it covers the carriers only with one layer, moreover we neglect the formation of hierarchical structures, when larger dust particles, covered by smaller dust particles are attached to the carriers. When the carriers collide we neglect the influence of the surface dust on their collision. Due to aggregation of the carriers and dust, a significant part of the dust is located on the carriers surface. Let $n_s(r)$ be the surface density of the attached dust particles of size $r$, while $n_v(r)$ be the respective distribution of free, unattached dust particles. The mass conservation then reads,

$$N_d(r) = n_v(r) + 4\pi R^2 n_s(r)N,$$

where $N$ is the number density of carriers. For a polydisperse system of carriers $R^2N$ in the above equation is to be substituted by $\int R^2N(R)dR$.

Consider now a collision of two carriers of radius $R_1$ and $R_2$ and masses $m_1$ and $m_2$, with

$$R_{\text{eff}} = \frac{R_1R_2}{R_1 + R_2} \quad m_{\text{eff}} = \frac{m_1m_2}{m_1 + m_2}$$

(2)

The force acting between them at the collision may be approximated by the Hertz force [2]:

$$F_H = \sqrt{R_{\text{eff}}}D\xi^{3/2} \quad D = \frac{3\left(1 - \nu^2\right)}{2Y}$$

(3)

where $\xi = R_1 + R_2 - |\vec{r}_{12}|$ is the compression and $\nu$ and $Y$ are respectively the Poisson ratio and Young modulus of the colliding particles [2]. From the equation of the relative motion follows the acceleration:

$$\ddot{\xi} = \frac{F_H}{m_{\text{eff}}}$$

(4)

and the force of inertia acting on the dust particle, sitting on the surface of a carrier, $F_{\text{inert}} = m_d(r)\vec{r}_1$, where $m_d(r) = (4\pi/3)r^3\rho_d$ is the mass of the dust particle of radius $r$ with the material density $\rho_d$. Since

$$\ddot{\vec{r}}_1 = \frac{1}{2}\ddot{\vec{r}}_{12} = \ddot{\xi},$$

(5)

we finally obtain for the maximal inertial force acting on the dust particle:
\[
F_{\text{inert max}} = \frac{1}{2} \frac{m_d}{m_{\text{eff}}} \frac{\sqrt{R_{\text{eff}}}}{D} \xi_0^{3/2}
\]

where \( \xi_0 \) is the maximal compression, which in the approximation of the Hertzian collision reads [3],

\[
\xi_0 = \left( \frac{5}{4} \frac{D m_{\text{eff}}}{R_{\text{eff}}^{1/2}} \right)^{2/5} g^{4/5}.
\]

Here \( g \) is the normal component (that is, the component along the inter-particle centers) of the relative velocity of the colliding particles. Hence we obtain,

\[
F_{\text{inert max}} = \frac{m_d}{2} \left( \frac{5}{4} \right)^{\frac{3}{5}} \left( \frac{R_{\text{eff}}}{m_{\text{eff}}^2 D^2} \right)^{1/5} g^{6/5}
\]

The inertial force given above refers only to the dust particles located on the line. If a dust particle sits away from this line, so that its location may be specified by the azimuthal angle \( \theta \) with respect to the collision line, one should use the corresponding projection of the force on that line, that is,

\[
F_{\text{inert max}}(\theta) = \frac{m_d}{2} \left( \frac{5}{4} \right)^{\frac{3}{5}} \left( \frac{R_{\text{eff}}}{m_{\text{eff}}^2 D^2} \right)^{1/5} g^{6/5} \cos \theta.
\]

If a dust particle of radius \( r \) is kept on a big particle of radius \( R \gg r \), by the adsorption forces, the maximal external force, which the adsorption can resist reads in the JKR theory[4],

\[
F_{\text{sep}} = \frac{3}{2} \pi \gamma r
\]

where \( \gamma \) is the adhesion coefficient. Naturally, if the maximal inertial force exceeds the maximal force which the adhesion may overcome, the dust particle releases from the surface. Therefore, the total number of the dust particles of size \( r \) produced at the collision of two carriers of radii \( R_1 \) and \( R_2 \), colliding with the normal velocity \( g \) reads,

\[
\Delta n_s(r; R_1, R_2, g) = 2\pi \int_0^{\pi/2} n_s(r) \sin \theta d\theta (R_1^2 + R_2^2) \Theta [F_{\text{inert max}}(\theta) - F_{\text{sep}}],
\]

where \( \Theta(x) \) is the Heaviside step-function and we take into account that the dust releases from both particles, from the side directed to the collision partner. We also ignore the process of re-attachment of a dust particle, released from one collisional partner to the other one.

Using the above expressions for the maximal inertial force and for the separation force, we arrive at the following yield:

\[
\Delta n_s(r; R_1, R_2, g) = 2\pi n_s(r)(R_1^2 + R_2^2) \Theta(g - g_c) \times \left( 1 - \left( \frac{g_c}{g} \right)^{6/5} \right),
\]

where \( g_c \) is the critical velocity.
where $g_c$ is the critical velocity, which characterizes the collision velocity which leads to the release of the dust particles of size $r$:

$$g_c(R_1, R_2, r) = \left(\frac{9\gamma}{4\rho_d r^2}\right)^{5/6} \frac{m_{\text{eff}}^{1/3} D^{1/3}}{R_{\text{eff}}^{1/6}} \frac{2}{\sqrt{5}} \sim r^{-5/3}$$

(13)

As it follows from Eq. (13), the smaller the particle, the larger the impact velocity of carriers is needed to release it by a collision.

2 Dust production rate at collisions

We assume for simplicity that the granular gas of carriers is uniform and kept (e.g. by shearing in planetary rings) at constant temperature. We also assume that the velocity distribution of all species is Maxwellian and that particles of different sizes have the same granular temperature, $T$. Hence, the production rate for dust particles of size $r$ due to a collision of two carriers of radii $R_1$ and $R_2$ reads:

$$I_+(r, R_1, R_2) = (R_1 + R_2)^2 \frac{1}{\pi^3} \frac{N(R_1) N(R_2)}{V_{T,1}^3 V_{T,2}^3} \times \int d\vec{V} d\vec{g} d\vec{e} \exp \left(-\frac{MV^2}{2T} - \frac{m_{\text{eff}} g^2}{2T} \right)$$

$$\times \Theta(-\vec{g} \cdot \vec{e}) |\vec{g} \cdot \vec{e}| \Theta(|\vec{g} \cdot \vec{e}| - g_c) \left(1 - \left(\frac{g_c}{g}\right)^{6/5}\right) \left[n_s(r) 2\pi (R_1^2 + R_2^2)\right]$$

(14)

where $M = m_1 + m_2$, and $V_{T,1/2}^2 = 2T/m_{\text{eff}}$ is the thermal velocity of the colliding carriers; the expression in Eq. (14) has the form of the collision integral [2]. Evaluating the above integral we obtain,

$$I_+(R_1, R_2, r) = 8\pi^{3/2}(R_1 + R_2)^2 N(R_1) N(R_2) V_{T,12}^2 (R_1^2 + R_2^2) n_s(r) F(\alpha),$$

(15)

where

$$V_{T,12}^2 = \frac{2T}{m_{\text{eff}}}$$

(16)

is the thermal velocity of the relative motion and

$$F(\alpha) = \frac{1}{4} (5\alpha + 2) \exp(-\alpha) + \alpha^{\frac{5}{4}} \Gamma\left(\frac{7}{5}; \alpha\right)$$

(17)

with

$$\Gamma(z; \alpha) \equiv \int_{\alpha}^{\infty} dy y^{z-1} e^{-y}, \quad \alpha = \frac{m_{\text{eff}} g_c^2}{2T}$$

(18)

3 Dust adsorption

For the adsorption rate of the dust of size $r$ by particles of size $R$ we obtain:

$$I_-(r, R) = K(R, r) N(R) n_v(r)$$

(19)
Here the rate kernel \( K(R, r) \) within the JKR theory \([4]\) and for \( R \gg r \) reads \([1, 5]\)

\[
K(R, r) = 2\pi R^2 \left( \frac{2T\pi}{m_d(R)} \right)^{1/2} \left[ 1 - \left( 1 + \frac{W(r)}{\epsilon^2 T} \right) e^{-W(r)/\epsilon^2 T} \right],
\]

(20)

where \( \epsilon \) is the restitution coefficient \([2]\) which characterizes the collision of the dust particles with the carriers and \( W \) is the adhesion barrier \([6]\),

\[
W(r) = q_0 \left( \pi^5 \gamma^5 D^2 \xi^4 \right)^{1/3} \approx 1.57.
\]

(21)

4 \ Fragmentation-aggregation kinetics and the steady state

Let us assume for simplicity that all carriers have equal radius \( R \), mass \( m \) and density \( \rho_d \)

\[
\frac{dn_v(r)}{dt} = I_+(r, R, R) - I_-(r, R); \quad n'_v(r) = N_d(r) - n_v(r)
\]

(22)

where we introduce \( n'_v(r) = 4\pi R^2 N n_s(r) \). It may be written, using Eqs. (1), (15) and (19) and the dimensionless time \( \tau = t/\tau_E \), measured in the collision time of the carriers, \( \tau_E^{-1} = \frac{32}{3} \pi R^2 \sqrt{\pi T/m} \) as

\[
\frac{dn_v(r)}{dt} = -n_v(A + B) + BN_d
\]

(23)

where

\[
A(r) = \frac{3\pi}{8\sqrt{2}} \frac{r}{(r/R)^{3/2}} \left[ 1 - \left( 1 + \alpha_{agg}(r/R)^{4/3} \right) \exp \left( -\alpha_{agg} (r/R)^{4/3} \right) \right]
\]

(24)

\[
\alpha_{agg} = q_0 \left( \pi^5 \gamma^5 D^2 \xi^4 \right)^{1/3} \frac{R^{4/3}}{\epsilon^2 T}
\]

(25)

and

\[
B(r) = 3F(\alpha), \quad \alpha = \frac{\alpha_{frag} (r/R)^{-10}}{\tau},
\]

(26)

\[
\alpha_{frag}^{-1} = \frac{4}{5} \frac{1}{V_{12}} \left( \frac{9\gamma}{4\rho} \right)^{5/2} \frac{m^{3/2} D^{1/2} \xi^{1/2} R}{2^{3/2}}
\]

(27)

Here \( F(\alpha) \) is given by Eq. (17). From Eq. (23) follows a simple exponential relaxation to the steady state; the size distribution for the dust adsorbed on the carriers, \( n_s(r) \), and that of the free dust, \( n_v(r) \), read

\[
n_v(r) = \frac{N_d(r) B(r)}{A(r) + B(r)}, \quad n'_v(r) = \frac{N_d(r) A(r)}{A(r) + B(r)}
\]

(28)

The coefficients \( \alpha_{frag} \) and \( \alpha_{agg} \) characterize the efficiency of fragmentation and aggregation processes. For \( \alpha_{frag} \gg 1 \) almost all collisions lead to shattering, while
Figure 1: Size distribution of the fraction of the free dust, $n_v(r)/N_d$. $\alpha_{agg} = 500$, $\alpha_{frag} = 10^5$.

Figure 2: Size distribution of the free dust $n_v(r)/N_d$. $\alpha_{agg} = 500$, $\alpha_{frag} = 10^7$. 
for $\alpha_{\text{frag}} \ll 1$ the collisions do not efficiently release the surface dust. Similarly, $\alpha_{\text{agg}} \gg 1$ refers to the case when the major fraction of the dust-carriers collisions cause the dust attachment and $\alpha_{\text{agg}} \ll 1$ correspond to the opposite case.

In Fig. 1 and Fig. 2 we show the dependence of the function $n_v(r)/N_d(r)$ for two sets of parameters, $\alpha_{\text{frag}} = 10^5$, $\alpha_{\text{agg}} = 1$ and $\alpha_{\text{frag}} = 10^9$, $\alpha_{\text{agg}} = 500$. For the first case, depicted in Fig. 1, one can clearly see the depletion in the size distribution for small dust particles, while for larger sizes practically all the dust particles are free. The second case corresponds to the more efficient fragmentation, but also more efficient aggregation. The two competing mechanism lead to a resulting non-monotoneous size distribution.

It is interesting to analyze the particle size distribution for the case of real systems. Motivated by the application to the Saturn rings e.g. [7], we choose the following size distribution, $N_d(r) \sim r^{-3}$ and plot the volume size distribution $n_v(r)$ in Fig. 3. As it follows from our analysis, the interaction of the dust particles with the carriers lead to the depletion of the size distribution at small sizes and noticeable deviations from the initial power law for the particles of intermediate size.

![Graph](image-url)

Figure 3: Size distribution of dust particles in the bulk $n_v(r)$, for the total size distribution of dust, $N_d \sim r^{-3}$. $\alpha_{\text{agg}} = 500$, $\alpha_{\text{frag}} = 10^9$. Dotted line corresponds to the distribution in the case of vanishing adsorption, $n_v = N_d$.

## 5 Conclusion

We study the particle size distribution in a rarified system of macroscopic particles which suffer fragmentative collisions at high impact velocities and aggregative collisions for low velocities. The system addressed in our study is composed or large particles (carriers) and small particles (dust). The dust particles may sit on
the surface of the carriers, kept by the adhesive forces, or move freely in space, colliding with other particles. Collisions of dust particles with carriers may be aggregative. The adhesive interactions, which are responsible for the formation of the dust-carriers aggregates, are described with the use of the JKR theory. For simplicity we assume that particle velocities obey the Maxwellian distribution, with the same kinetic temperature for all species, and neglect the formation of carrier-carrier and dust-dust agglomerates. Under these approximations we develop an analytical theory for the size distribution for the free and bound dust particles. Depending on the system parameters, we reveal a rich behavior of this function. In particular we find that for a power-law size distribution of dust, motivated by application to the planetary rings, a depletion of the size distribution for small particles and significant deviations from the power-law is observed.

References


[3] Eq. (7) may be obtained, equating the initial relative kinetic energy to the elastic energy at maximal compression, \( \int_0^{\xi_0} F_{H}(\xi) d\xi \).


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The direct simulation Monte Carlo of near-continuum flows with condensation process

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Abstract

The general model of neutral cluster formation for the direct simulation Monte Carlo method has been developed. The model takes into account association processes due to triple collisions, monomer-cluster, cluster-cluster collisions and decay of cluster by one monomer evaporation. In present study we considered possibility of partial excitation of cluster vibration degrees of freedom. The model was applied for simulation of near-continuum stationary flow of water molecules from spherical evaporating ice surface into vacuum. The behavior of condensation process in such flow in dependence of main characteristic parameters are discussed.

1 Introduction

The direct simulation Monte Carlo (DSMC) method is the most powerful technique for modelling of near-continuum, transient and free molecular gas flows for which the characteristic Knudsen number \( Kn = \frac{\lambda}{R} > 10^{-5} \div 10^{-4} \) (\( \lambda \) is the characteristic mean free path, \( R \) — the characteristic size). Such flows take place in the fields of aerospace technique, vacuum technologies and very often are accompanied by condensation processes. As an example of flows with condensation may be pointed nozzle plumes expanding in vacuum [1].

The DSMC method gives possibility to simulate flows of free geometry and to take into account different physic-chemical processes [2]. The condensation models for the DSMC technique were developed for the high-temperature flows of laser ablated material [3],[4] and for the free nozzle jets of inert gases [5]. The most complex moment of application of the condensation models is in accuracy of description of energy redistribution between different energy modes of colliding particles during cluster formation process. Usually some simplifications are used. For example, it is supposed that all vibration degrees of freedom of cluster are fully excited. Such approach is applicable for high-temperature flows but doubtful for low-temperature
flows. The first aim of present work is to suggest general model of cluster formation process for DSMC method which gives possibility to takes into account partial excitation of vibration degrees of freedom.

The second aim of this paper is to analyze the influence of condensation processes on gasdynamic picture of flow and to set characteristic parameters which determine behaviour of the flow. As an example of the near-continuum flow with cluster formation process we consider the expansion of water molecules from spherical source into vacuum. Such flows take place in the field of comet physics [6].

2 The model of cluster formation

In this study we develop our model of neutral cluster formation suggested for the case of condensation of laser ablated niobium atoms [3],[4]. In previous work the clusterization substance was atomic and clusters have fully-excited internal degrees of freedom. Here we elaborate general model of formation of molecular clusters with partially excited vibration degrees of freedom.

We consider elastic collision of monomers

\[ M + M \rightarrow M' + M', \]  (1)

monomers recombination by three body collision

\[ M + M + M \rightarrow M'_2 + M', \]  (2)

association of monomer and clusters

\[ M_i + M \rightarrow M'_{i+1}, \]  (3)

association of clusters

\[ M_i + M_j \rightarrow M'_{i+j}, \]  (4)

atom evaporation from a cluster

\[ M_i \rightarrow M'_{i-1} + M'. \]  (5)

Here \( M \) — monomer (for water it is water molecule), \( M_i \) — cluster which consists of number of monomers \( i \), index ‘ relates to the particles after collision (reaction).

In case of three body collision (2) or pair collisions (3), (4) association takes place with some probabilities. These probabilities in general case are functions of energy of relative motion, values of internal energy of colliding particles, configurations of clusters and geometry of collision. For water the values of probabilities are unknown for wide range of temperatures.

For triple collisions (2) the probability \( p_r \) may be determined by approach suggested in [7]:

\[ n_M^3 k_r = N_{tr} \int_0^\infty p_r(E_c) f(\frac{E_c}{k_B T}) d(\frac{E_c}{k_B T}), \]  (6)

where \( n_M \) is the number density of monomers, \( k_r \) — constant of recombination rate, \( N_{tr} \) — the number of triple collisions, \( E_c \) — the full energy of triple collision, \( T \) —
The direct simulation Monte Carlo of near-continuum flows with condensation process

temperature, \( k_B \) — Boltzmann constant, \( f \) - distribution function of full energy. The experimental data about \( k_B \) does not known for water molecules. The approximate approach (so-called simple approach for triple collisions) for determination of \( k_B \) [8] and use of (6) give the values \( p_r > 1 \) for the range of temperatures typical for comet nucleus evaporation. In simulations we set \( p_r = 1 \). For comparison in [5] the value of \( p_r \) was 0.217 for triple collisions of argon atoms and this result was obtained by molecular dynamic simulation. The characteristic life time of triple collision was set to be inversely proportional of average relative velocity of monomers in cell.

The values of probabilities for reactions (3) and (4) are set also equal to unities for water. It is typical assumption for the case when colliding partners in total have around ten atoms or more [9].

A cluster is described by number of monomers \( k \) (for the case of water — \( k \) is the number of water molecules in a cluster), mass \( m_k \), radius \( r_k \), velocity \( \vec{v}_k \), internal energy \( E_{\text{int},k} \), and binding energy \( E_b(k) \).

Cluster radius is defined by modified spherical drop liquid model \([10]\)

\[
r_k = r_w(k - 1)^{1/3} + r_1, r_w = \left( \frac{3m}{4\pi \rho} \right)^{1/3},
\]

where \( r_1 \) — radius of hard sphere (HS) model for monomer, \( m \) — mass of monomer, \( \rho \) — the density of ice.

The internal energy of a cluster is presented as \( E_{\text{int},k} = E_{r,k} + E_{v,k} \), where the rotation internal energy is \( E_{r,k} = \frac{\zeta_r}{2} k_B T \), the vibration internal energy is \( E_{v,k} = Z^e_v k_B T \) (\( \zeta_r \) and \( Z^e_v \) number of rotation and effective vibration degrees of freedom correspondingly). For water molecules and clusters \( \zeta_r = 3 \). For determination of effective vibration degrees of freedom for the case when vibration modes of cluster are not fully excited we use tradition presentation of vibration energy \([2]\)

\[
E_{v,k} = \sum_{i=1}^{Z_v} \left( \frac{k_B \theta_i}{\exp(\theta_i/T) - 1} \right),
\]

where \( \theta_i \) — characteristic temperature of vibration mode \( i \). The number of vibration modes is determined as \( Z_v = 3k_a - 6 \), where \( k_a \) — the number of atoms in a cluster. The characteristic temperatures of vibrations for water dimer and most stable water trimer are brought from \([11]\). For clusters with size larger than trimer we use for \( 3k \) inter-molecular modes the same values as for trimer and for each of other \((Z_v - 3k)\) modes — average value of characteristic vibration temperatures of intra-molecular vibration modes of water trimer.

The binding energy of a water cluster may be presented as \([12]\) \( E_b(k) = Ak + B \), where \( A=-11.388 \text{ kcal/mole} \) and \( B=17.327 \text{ kcal/mole} \).

We employ Larsen-Borgnakke (LB) model \([2]\) for description of energy exchange between reacting particles and theirs vibration-rotation-translation (VRT) degrees of freedom.

For determination of atom evaporation frequency according to process (5) we use next equation from RRKM theory \([13]\):

\[
\nu = \nu_0 k_a \left( \frac{E_{\text{int},k} - \Delta E_b}{E_{\text{int},k}} \right)^{Z^e_v - 1}, \Delta E_b = E_b(k) - E_b(k - 1).
\]
Here $k_s$ – number of surface monomers, $\nu_0 = 10^{13}c^{-1}$ – characteristic frequency of vibration.

3 The problem setting

As an example of model application we are considering the problem of 1D stationary gas expansion in vacuum from spherical evaporating surface in near-continuum and transient flow regimes.

The calculated region in simulation represents a field between a spherical evaporating surface with radius $r$ and external spherical boundary with radius $L >> r$.

The evaporating substance is the ice with temperature $T_w = 166K$ that typical for comet nucleus. It is supposed that only water monomers are evaporated from the surface. The flux of water molecules through the surface is determined by Hertz-Knudsen equation $F_+ = \frac{1}{4}n_w\nu_T$ ($n_w$ is equilibrium density of water vapor corresponds to the temperature $T_w$ and $\nu_T = (\frac{8k_BT_w}{\pi m})$ — the average velocity of water monomers). The initial velocities of evaporating from the surface water molecules are modelled by semi-Maxwellian distribution function.

The evaporating water monomers in considering temperature range have only rotation degrees of freedom and internal energy of these molecules is $E_{\text{int}} = E_{\text{int},r} = \frac{1}{2}k_BT_w$. Such setting is typical for comet problems [6].

The particles which achieve external boundary excluded from simulation (the hypersonic boundary condition). The evaporated monomers were associated in the flow according presented cluster formation model.

For the description of particle motion we employ the DSMC method. The numerical scheme with no time counter (NTC) is realized with the hard-sphere (HS) collision dynamics [2]. The cross-section for particles collisions for HS-model is defined as $\sigma = \pi(r_i + r_j)^2$ ($r_i$, $r_j$ – the radii of particles i and j correspondingly). These radii is determined by (7). The radius of monomer was equal 3.62Å which corresponds temperature $T_w$ [6].

The gasdynamics of flow is determined by Knudsen number $Kn = \lambda_w/r$ ($\lambda_w$ is the mean free path corresponding to $n_w$ and $T_w$), the characteristic rates of reactions (2)-(5) or Damkelers numbers $D_i = r/(\nu_T\tau_i)$ ($\tau_i$ is the characteristic time of process i) and parameters of presented condensation model. Below we present results which correspond to the range of Kn numbers belong to $10^{-4} \div 10^{-2}$ and $D$ numbers belong to $7.1 \times 10^{-3} \div 71$. As D number we consider the number corresponding to the rate of triple collisions with characteristic time between collisions $\tau_{tr} = 1/\nu_{tr}$ ($\nu_{tr}$ — the frequency of triple collisions determined by parameters near the surface).

4 Results

The influence of condensation process on flow gasdynamics depends on condensation degree. We determine this degree as an integral parameter over whole flowfield $\alpha = (\sum_{k=2}^{\infty} kN_k)/(\sum_{k=1}^{\infty} kN_k)$ ($N_k$ — is the number of particles with size k in flowfield). For considering variants $\alpha = 5.5 \times 10^{-4}$ for $Kn = 0.01$, $D = 7.1 \times 10^{-3}$ (Var.1), $\alpha = 0.18$ for $Kn = 0.001$, $D = 0.71$ (Var.2), $\alpha = 0.017$ for $Kn = 0.001$, $D = 0.071$.
The direct simulation Monte Carlo of near-continuum flows with condensation process

Figure 1: The density (a) and velocity (b) of gas mixture. 1 — Kn = 0.01, D = 7.1 \cdot 10^{-3} \text{ (Var.1)}, 2 — Kn = 0.001, D = 0.71 \text{ (Var.2)}, 3 — Kn = 0.001, D = 0.071 \text{ (Var.3)}, 4 — Kn = 0.0001, D = 71 \text{ (Var.4)}, 5(dashed) — without condensation Kn = 0.001 \text{ (Var.5)}. The density is normalized to the equilibrium value corresponded to $n_w$.

(Var.3), $\alpha = 0.41$ for Kn = 0.0001, D = 71 (Var.4). The variant 5 corresponds to the case without condensation and Kn = 0.001. The variants 1 and 3 correspond to the case of week condensation and for them the behaviour of gasdynamic parameters (density, velocity, temperature) is the same as in case without condensation (Fig.1,2). It should be underlined that for the same Knudsen numbers variants 2 and 3 are characterized by different condensation degree and different distributions of gasdynamic parameters.

The presence of condensation changes flow picture. Firstly we can see the more rapid drop in density of gas mixture for variant 2 in comparison with variant 5 without condensation. Such behaviour of density may be explained by energetic effect of condensation. Energy release due to condensation for considering model is provided by triple collisions. The third monomer in (2) takes part of energy released during particles association. Under reactions (3) and (4) the released energy is spreaded through internal degrees of freedom. This energy released leads to the rise of temperature and velocity of gas mixture (Fig.1,2).

The cluster formation process change quantitative but not qualitative view of distributions of gas mixture density and velocity (Fig.1). In opposite to these distributions the shapes of temperature curves are affected more seriously by condensation process. For variants 1,3 (small values of condensation degree) and 5 (without the condensation process) the maximum of temperature is in the source surface. The presence of condensations leads to (1) appearance of temperature maximum in temperature curve, (2) rapid rise of temperature (Fig.2). The temperature maximum travels toward the surface with the rise of Knudsen number.
The temperature of the gas mixture. The definition of curves is the same as in Fig. 1.

The concentration of whole clusters and of clusters with size $k = 30$, velocity of clusters with size $k = 30$ are presented in Fig. 3 for variant 2 ($Kn = 0.001$, $D = 0.71$). For this variant distributions of clusters concentration have the maximum just near the surface. The interplay of two factors — (1) appearance and rise of number of clusters in flowfield and (2) expanding character of the flow — leads to appearance of this maximum. The behaviour of velocity of clusters with size $k = 30$ is the same as of monomers velocity.

The integral size distributions of clusters are shown in Fig. 4a. For the variant 1 ($Kn = 0.001$, $D = 7.1 \times 10^{-3}$) with small condensation degree the maximal size of cluster is less than ten. With the rise of collision (decrease of $Kn$) we can see the increasing of number of clusters. The maximal cluster size for variants 2 and
The direct simulation Monte Carlo of near-continuum flows with condensation process

Figure 4: Integral size distribution (a) and the number of vibration degrees of freedom. Circles — Var.1, triangles — Var.2, squares — Var.4. 1 — Var.4, 2 — Var.2, 3 — $Z_v = 3k - 6$, 4 — $Z_v = 3k_a - 6 - 3k$, 5 — $Z_v = 3k_a - 6$.

4 is exceed 50 monomers. The interesting moment of the presented study is the treatment with partially excited vibrational degrees of freedom of a cluster. The Fig. 4b demonstrates the number of excited vibration degrees of freedom. The curve 1 corresponds to the variant 4 ($Kn = 0.0001, D = 71$), the curve 2 corresponds to the variant 2 ($Kn = 0.001, D = 0.71$). The curve 3 presents the dependence $Z_v = 3k - 6$, the curve corresponds to equation $Z_v = 3k_a - 6 - 3k$ which describes the number of intra-molecular vibration degrees of freedom in a cluster, the curve 5 corresponds to the maximal possible number of vibration degrees of freedom $Z_v = 3k_a - 6$. As we can see the number of effective vibration degrees of freedom is less than number of intra-molecular modes. For considering range of temperatures for water vapor expansion it is possible to use as the approximate assumption the equation $Z_v = 3k - 6$.

5 Conclusions

The cluster formation model for the direct simulation Monte Carlo method is presented. In this study we considered possibility of partial excitation of vibration degrees of freedom of a cluster. Such approach give chance to simulate flows for wide temperature range. As an example of simulation of near-continuum and transient flows with condensation the 1D problem of stationary spherical expansion into vacuum of evaporating from ice surface water molecules was analyzed by the use of suggested model.
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Parallelization of algorithms for the solution of elasto-plastic problem on shared memory multiprocessor computer

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Abstract

Results of applying of the parallel calculations for the solution of 2D elasto-plastic problems with large plastic strains using finite element method are presented. Numerical realization has been implemented on the Massively Parallel Computing System with common memory PrimePower-850. As an example, we consider the problem of cylinder compression from elasto-plastic isotropic and isotropic-strengthened material by flat plates. For the solving of the linear algebraic equation system, which has the banded matrix, the parallel algorithms of the Gauss method was applied. By computing experiments a limiting characteristics of the paralleling efficiency and program productivity was obtained.

The applicability of parallel computations for the solution of elasto-plastic problems with small elastic and large plastic strain by using finite element method is investigated in this work. As an example, we consider the problem of cylinder compression from elasto-plastic isotropic and isotropic-strengthened material by flat plates. The solution is based on a principle of virtual capacity of the speed form [1]:

\[
\int_V (\sigma + \Delta t \dot{\sigma}) \cdot \nabla h \, dV + \int_\Sigma (P + \Delta t \dot{P}) \cdot h d\Sigma = 0.
\] (1)

Constitutive equations are presented at the work [2]. The Coulomb’s law was applied on contact with plates. A lateral surface of the cylinder is free from loadings. By means of finite element approximation the equation (1) is leads to the linear algebraic equation system (LAES)

\[
Az = b,
\] (2)

A, b, z — initial matrix, right part vector and decision vector of the system, respectively. A is asymmetrical banded matrix.
Solving the problem (1) by means of Finite Element Analysis consists of 3 basic stages:
1. making of the matrix,
2. solving of the LAES(2),
3. calculating of deflected mode at the end of loading iteration.

The parallel algorithms for solving every of this stages were developed. They have been implemented on the shared memory multiprocessor computer PrimePower-850 with 7 processor by help of the MPI and OpenMP. Application of OpenMP on shared memory multiprocessor computer in comparison with MPI showed higher computation speedup and efficiency. The same results are presented by the authors of the article [4].

![Figure 1: The speedup of computing time for the different stages](image)

Time results of developed algorithms for the first an third stages of solving the problem showed that with increasing number of processor a paralleling effectiveness is rises (fig 1., fig 2.).

As a speedup the ratio between the computing time on one processor and the computing time on a multiplicity of processor. The results are presented for the case when dimension of grid is 20x20. The parallel algorithms for these stages are based on division of volume of computational work between processors for equal parts.

Dependence of computing time speedup for the different stages on the number of processor is presented at the fig.1. It can be seen, that speedup rises linearly while the number of processor less then 4. That is the parallel algorithms for the 1 and 3 stages, presented in this paper, are effective. If the number of processor more then 4 the linearity is vanishing because of the communication overheads are rising.

As a speedup the ratio between the computing time on one processor and the computing time on a multiplicity of processor. The results are presented for the case when dimension of grid is 20x20. The parallel algorithms for these stages are based on division of volume of computational work between processors for equal parts.

Dependence of computing time speedup for the different stages on the number of
Parallelization of algorithms for the solution of elasto-plastic problem on shared memory multiprocessor computer

Figure 2: The speedup of computing time for the 1 and 3 stages

Figure 3: The speedup of computing time for the first parallel algorithm of Gauss elimination

Two parallel algorithms of the Gauss method were applied to obtain solution of LAES. The first one [3] is based on fragmentation of parent matrix between processor. The second algorithm is based on parallelization of elimination of matrix column. Implementation of the first algorithm show that with increasing number
of processor a computation time is increase due to a significant communication
overheads (fig. 3).

![Graph showing speedup vs. number of processors for different matrix dimensions.]

Figure 4: The speedup of computing time for the second parallel algorithm of Gauss elimination

Solving results of the second parallel algorithm of Gauss elimination showed
that with increasing number of processor a computation time is rises (fig.4). With
increasing matrix dimension a paralleling effectiveness rises due to increasing labo-
rriousness of computations on each processor, while communication overheads are
almost dimensionally stable.

The using of parallel algorithms reduces the computing time that allows to recom-
mending them for the solving of greater elasto-plastic problems.

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Theoretical investigation of phisico-mechanical properties of non-closed nanostructures based on crystal bilayered films

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Abstract

We present an investigation of behavior of non-closed nanostructures generated from crystal bilayered nanofilms Ni-Cu. The simulation was carried out on the basis of molecular dynamics method. Interatomic interaction was described in the framework of the embedded atom method. It was shown that formed non-closed nanostructures under conditions without external influences, make mechanical oscillations. The amplitude and frequency of oscillations depend on the length and thickness of an initial film. Dependences of oscillation parameters of non-closed nanostructures on their geometrical sizes were established. The obtained relations can be useful for designing of nanodevice components with various functional purposes.

1 Introduction

In last years the questions of development, creation and studying of features of behavior of nanostructures which are components of various nanodevices pay a steadfast attention [1, 2, 3, 4]. Among studied nanoscale objects it is possible to allocate the structures received on the basis of superthin multilayered films having a crystal lattice. Properties of such nanostructures depend not only on their chemical compound but also on geometrical sizes. Therefore during development of nanodevices of various functional purposes it is important to pick up the geometrical sizes of components with high accuracy. In last years in Institute of Physics of Semiconductors of the Siberian Branch of the Russian Academy of Sciences (Novosibirsk) the unique technology of formation of various types of nanoscale structures develops successfully [5, 6]. The given technology allows receiving a nanoscale objects with precision-built reproduced geometry. In the main of the technology the so-called "sacrificial layer" besieges on a substrate and then two additional layers from
various materials on top of it. After that using the selective etching deletes the "sacrificial layer". The free edges of a "bifilm" start to upwards and twist due to action of the elastic forces caused by discrepancy of atomic lattice parameters of two layers. Thus spirals, nanotubes and others nanoscale structures of the various shapes having the unique physicomechanical properties [4, 5, 6] can be formed.

Note that experimental researches in the considered area meet quite certain difficulties (small times of characteristic processes, the small sizes of studied objects, technical difficulties of nanostructures synthesis, etc.), and also face with necessity to use a high precision and expensive equipment. Using of computer simulation allows one to reduce essentially time and expenses to carry out of experimental investigations. The results of computer modeling can be used as a basis to forecast the behavior of real investigated objects [6, 7, 8, 9, 10, 11]. Using the method of molecular dynamics is represented to be most effective in the case of necessary directly to take into account the discrecity of atomic structure of nanoscale modeled objects [7, 8, 9, 10]. That will enable directly to investigate the atomic mechanisms responsible for unique physicomechanical properties of modeled nanostructures.

In view of the aforesaid the main goals of the present researches were molecular dynamics study of the behavior of nanostructures generated from two-layered nanoscale films and investigation the influence of geometrical factors of initial films on properties of formed non-closed nanostructures.

2 Performance of computer-aided experiment

As a basis of generated non-closed nanostructures the film consisting of crystal layers of copper and nickel was chosen. The choice of metals is proved by that copper and nickel form a continuous number of solid solutions in interval of all concentration. Equilibrium parameters of atomic lattices of the given metals are very close. So, at temperature $T = 0K$ and pressure $P = 0$ parameter of atomic lattice of copper is equal 0,362 nm and for nickel - 0,352 nm. According to experimental data [11] small distinction of parameters of atomic lattices of $Cu$ and $Ni$ allows one to put on a substrate big enough number of atomic layers of these metals without discontinuity. It enables to receive nanoscale structures of various configuration and properties.

The initial structure of modeled crystal bilayered film is shown in Fig. 1. Along axes Y and Z free surfaces were simulated. So-called periodic boundary conditions simulating repeated recurrence of the modeled fragment lengthways X axis were set. Along axis Z the modeled structure was broken into two layers equal on thickness. One layer was consisted of atoms of nickel and another - from atoms of copper. For acceleration of formation non-closed nanostructures process of etching was not modeled. The orientation of the structure was the following: axes X, Y and Z were corresponded to directions of fcc lattice $[100]$, $[010]$ and $[001]$. To set the interaction the interatomic potential calculated within the limits of embedded atom method [12, 13] was used. The given potential allows one with good accuracy to describe elastic characteristics of a material, surface energy, equilibrium volumes of metals and alloys on their basis. These parameters are important at modeling of non-closed nanostructures formation from crystal bilayered film. Thermodynamic characteristics of chosen metals are resulted in Tab. 1. It is visible that results of
Theoretical investigation of phisico-mechanical properties of non-closed nanostructures based on crystal bilayered films

Table 1: Results of elastic constants calculation (C11, C12, C44, GPa), sublimation energy (E_s, eV), vacancy formation energy (E_v, eV).

<table>
<thead>
<tr>
<th></th>
<th>C11</th>
<th>C12</th>
<th>C44</th>
<th>E_s</th>
<th>E_v</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu calc.</td>
<td>167</td>
<td>126</td>
<td>75</td>
<td>-3.49</td>
<td>1.3</td>
</tr>
<tr>
<td>Cu exp. [13]</td>
<td>170</td>
<td>123</td>
<td>76</td>
<td>-3.45</td>
<td>1.3</td>
</tr>
<tr>
<td>Ni calc.</td>
<td>239</td>
<td>178</td>
<td>108</td>
<td>-4.45</td>
<td>1.6</td>
</tr>
<tr>
<td>Ni exp. [13]</td>
<td>247</td>
<td>147</td>
<td>125</td>
<td>-4.45</td>
<td>1.6</td>
</tr>
</tbody>
</table>

calculation are in the good agreement with experimental data.

Figure 1: Structure and orientation of initial bilayered film.

After formation of an initial two-layer film process of relaxation at temperature T = 300K was modeled. Thus it was investigated two cases. In the first case the parameter of substrate’s atomic lattice was set under the formula a = (a_{Cu} + a_{Ni})/2, where a_{Cu} and a_{Ni} – the equilibrium periods of elements atomic lattices at T = 0K. It corresponded to a situation when both metal layers of an initial film were strained. In the second case the parameter of substrate’s crystal lattice (a) coincided with parameter of atomic lattice of one of layers of a binary film (in the present calculations with lattice parameter of Cu) that corresponded to a situation when layer Ni is strained only.

3 Results of numerical simulation

3.1 Formation of non-closed nanostructures

As shown in [5, 10], according to discrepancy of atomic lattices parameters of both metallic layers of initial structure there are moments of forces under which the heterogeneous film starts to be turned off. If it’s geometrical sizes are those that in a condition when edges of nanostructure are maximally brought together and not closed the film starts to be unbent. Without external resistance the given process repeats, and edges of structure make free harmonious fluctuations.

In the present paper the geometrical sizes of modeled film along directions [010] and [001] were chosen so that in as much as possible compressed condition change of distance between edges of a film corresponded ≈70 %. Such amplitude is reached, for example, in crystal bilayered film with the following geometry: thickness of layers Cu and Ni on 10 nuclear planes, length of 400 lattice parameters. Thus in an initial
film both metal layers were strained. It is necessary to note that use of periodic boundary conditions means modeling infinitely long plate in a direction [100].

The amplitude limitation of film oscillation is connected with probability of irreversible structural changes during oscillation and connection of edges of nanostructure. On fig. 2a the given structure is shown in two extreme positions. The structure of the same size but with one initially intense layer (in our case Ni), is shown on fig. 2b. In this case the distance between edges of film in maximal compressed condition is less than for a case when in an initially both crystal layers are strained. The amplitude of fluctuations for such system makes $\approx 85\%$. Time dependence of distance between edges of non-closed nanostructure for both cases is resulted in fig. 3. It is visible that if in the first case the establishment of a stationary mode occurs for some oscillation than in the second case due to non-uniformly distribution of stresses in modeled structure – essentially greater time is required. It is also confirmed by deviation of fluctuations from a harmonic type.

![Figure 2](image_url)

**Figure 2:** Non-closed nanostructures in two extreme positions: a) Both layers are strained initially b) one layer strained only.

Thus efficiency of transformation of reserved elastic energy into energy of mechanical oscillation is above for a case when equilibrium parameters of atomic lattice of a substrate and one of layers of a bilayered film are close. At the same time a situation when the period of atomic lattice of a substrate is in the range between the periods of components of a crystal bilayered film is characterized by practically instant installation of harmonious oscillation. This variant as a rule is used in experiment at creation of nanoscopic structures [6]. Therefore such way of formation of initial film was chosen in our simulations for the further researches.
Theoretical investigation of phisico-mechanical properties of non-closed nanostructures based on crystal bilayered films

3.2 The influence of initial geometrical parameters on properties of nanostructures

Properties of nanostructures are defined not only by initial and boundary conditions but also their geometrical parameters. To investigate the influence of geometry factor on behavior of nanostructures the bilayered films with thickness of each of layers (copper and nickel) equal to 5, 10, 15, 20 and 25 atomic planes were modeled. For each of modeled samples length of a film was selected so that the amplitude of fluctuations of non-closed nanostructures was about \(\approx 70\%\). Corresponding relations of lengths \((L)\) of bilayered films and their thickness \((h)\) are resulted on fig. 4. It is visible that in an investigated range this dependence is well described by the linear law.

Figure 3: Time dependence of the distance between edges of nanostructures with different initially strained conditions

Figure 4: Dependence of a length on a thickness for the film which oscillated with amplitude \(\approx 70\%\)
It is necessary to note, that at the fixed thickness of a film the amplitude $A_m$ of edges oscillation of non-closed nanostructure also depends on initial length. The increase in length modeled nanostructure at the fixed thickness leads to growth of amplitude of oscillation.

3.3 The influence of crystallographic orientation on properties of nanostructures

To investigate the influence of crystallographic orientations on properties of non-closed nanostructure the initial bilayered film was oriented in relation to axes X, Y and Z in following three ways: 1) [100], [010], [001]; 2) [112], [110], [111]; 3) [001], [110] and [110], correspondently. According to chosen crystallographic orientations, metal layers were put in the first case alone direction [001], in case of 2) alone direction [111] and in (3) – [110]. This difference will be used in the further for identification of investigated variants.

Comparison of parameters of harmonious oscillation of non-closed nanostructures for investigated cases was carried out on bilayered films with thickness of metal layers of copper and nickel on 5 atomic planes. Thus thickness $h$ of heterogeneous films for cases of various crystallographic orientations was defined by interplane distance along corresponding directions [001], [111] and [110]. The length of investigated films $L$ was varied in a wide range, but so that in maximal compressed condition changes of the distance between film free edges (Fig. 1) (amplitude of fluctuations) was no more than 70 % from the initial length.

The results show that amplitude $A_m$ and frequency $\nu$ of fluctuations of non-closed nanostructure edges essentially depends not only from its geometrical sizes (initial length and thickness) but from crystallographic orientation also. On fig. 5a dependences of the resulted amplitude of fluctuations of bilayered films with various orientations on its initial length are shown. According to these results the amplitude of oscillation at the fixed thickness nonlinearly grows with increase of initial length ($L$). The greatest growth is observed for bilayered film with orientation [001], the least – for [110]. Thus the absolute lengths of films with orientations [001] and [110] which make oscillations with amplitude of $\approx 70 \%$ differ more than 1.5 times (68 and 105 nm, correspondently). Curves on fig. 5b correspond to dependences of change of oscillations frequency of modeled nanostructures on their initial length for various crystallographic orientations. It is visible the frequency of oscillations for all cases quickly enough decreases with growth of length of initial film. The analysis shows that for all considered crystallographic orientations frequency of oscillations is well described by dependence $1/L^2$. That is in good correlation with data presented in paper [10]. Thus the curve for the case with crystallographic orientation [110] is located above other dependences, for [001] – below.

One of the important parameter describing the properties of modeled nanostructures is efficiency of energy transformation from reserved elastic into the energy of mechanical fluctuations. According to this aim in the paper structures of all of three crystallographic orientations were considered. The lengths which provide the amplitude of fluctuations $\approx 70 \%$ were chosen. According to curves on fig. 5a for orientation [001] length of such film is equal 68 nm, for [111] – 80 nm, and for
Theoretical investigation of phisico-mechanical properties of non-closed nanostructures based on crystal bilayered films

[001] – 105 nm. On fig. 6 change of kinetic and potential energies for the case of crystallographic orientation [001] is shown. Bold lines correspond to energies values averaged over group of the nearest 1000 instant points. Efficiency of elastic energy transformation reserved in nanostructures into energy of harmonious oscillations was defined as a difference between the maximal and minimal average energy values on peaks during the oscillations ($\Delta E$). According to results of modeling the greatest efficiency of elastic energy transformation corresponds to the orientation [110], and the least – [001]. Mean efficiency of reserved elastic energy transformation for crystallographic orientations [110], [111] and [001] at the considered time interval equal 70, 55 and 20 eV correspondently.

Figure 5: Dependence of reduced amplitude (a) and oscillation frequency (b) on initial length of films with various crystallographic orientation

Figure 6: Time dependence of kinetic (E) and potential (U) energies for film with crystallographic orientation alone [001]. The amplitude of oscillation is about 70%
4 Conclusions

Thus non-closed nanostructures generated on the basis of bilayered crystal films without external influences make harmonious oscillations. At this it was shown that the behavior and kinematic properties of the simulated structures can be varied by changing of geometrical parameters and crystallographic orientation of an initial film. The dependence of the amplitude and frequency of mechanical oscillations on the geometrical sizes (length and thickness) was found. With growing of the length at fixed thickness of nanofilm nonlinear increasing of amplitude and reduction of frequency of oscillations were observed. At simultaneous proportional increase of length and thickness of an initial film the resulted amplitude linearly increased.

The analysis of influence of crystallographic orientation of simulated bilayered films shows, that the greatest growth of amplitude of oscillations at the fixed thickness was observed for bilayered film with the orientation \([001]\), and the least one - for \([110]\). The efficiency of transformation of reserved elastic energy in nanostructures into energy of harmonious oscillations was above for the orientation \([110]\) and less for the orientation \([001]\).

Obtained results shown that the non-closed multilayered nanostructures can be used at development of kinematic components of nanodevices of various functional purposes.

Acknowledgements

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Theoretical investigation of phisico-mechanical properties of non-closed nanostructures based on crystal bilayered films


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Stability analysis and modelling the phase transition in BCC lattice

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Abstract

The stability of body-centered cubic (BCC) lattice is studied in the presented work. The material is considered to consist of particles, interacting by means of Morse potential, having one dimensionless parameter, which determines the behaviour of the material. The stability criterions for BCC lattice were obtained both in terms of this parameter and in terms of the Gruneisen parameter, which is the known macroparameter. The process of destruction of unstable BCC lattice was simulated numerically. The raise of Gruneisen parameter, predicted analytically was verified. The result, that BCC lattice transforms to FCC lattice was obtained numerically.

1 Introduction

A number of metals (such as iron, tantalum, niobium) have body-centered cubic (BCC) lattice. It is a simple lattice (e. g. it is congruous to itself shifted via vector, connecting any of its two nods). Different criterions of stability for this lattice were obtained in [2]–[4]. But all of these criterions were not verified. The purpose of this paper is to obtain a verifiable criterion, verify it and to predict the behavior of a material with BCC lattice, when it loses its stability. The main goal of the investigation is to describe the BCC–FCC transition, taking place in iron.

2 Basic data

The material is considered to be consisting of particles, interacting by pair potential. Morse potential is chosen to describe the interaction between particles, as it was done in [2, 3, 4]. This potential is given by formula

\[ \Pi(r) = D \left[ e^{-2\alpha(r-a)} - 2e^{-\alpha(r-a)} \right] . \] (1)
The force of interatomic interaction is

\[ F(r) = -\Pi'(r) = -2\alpha D \left[ e^{-2\alpha(r-a)} - e^{-\alpha(r-a)} \right], \quad (2) \]

where \( r \) is a distance between interacting particles, \( D \) is a deepness of the potential well, \( \alpha \) is a parameter, determining the width of the potential well, \( a \) is an equilibrium distance between two interacting particles. This potential has one dimensionless parameter \( \alpha a = \aleph \). The potential (1) can be rewritten in terms of this parameter:

\[ \Pi(r) = D \left[ e^{-2\aleph(r/a-1)} - e^{-\aleph(r/a-1)} \right]. \quad (3) \]

Plots of the force for different values of \( \aleph \) are presented at figure 1.

![Graphs of force for different values of \( \aleph \)](image)

**Figure 1:** Graphs of force for different values of \( \aleph \)

The stability of the body-centered cubic (BCC) lattice is studied in the presented work. This lattice is a set of particles, located in the nods of a simple cubic lattice and in the center of symmetry of each cube. The stress tensor for this lattice, as for a simple one, can be written as following [1]:

\[ \tau = \frac{1}{2V_0} \sum_{\beta} \frac{\Pi'(a_{\beta})}{a_{\beta}} a_{\beta} a_{\beta}, \quad (4) \]

where \( V_0 \) is a volume of an elementary cell (such a cell, containing one atom, that all the space can be filled out with it). The equilibrium condition can be written in the following form:

\[ \tau = 0. \quad (5) \]

The stiffness tensor in the equilibrium position can be represented as in [1]

\[ ^4C = \frac{1}{2V_0} \sum_{\beta} \left( \frac{\Pi''(a_{\beta})}{a_{\beta}^2} - \frac{\Pi'(a_{\beta})}{a_{\beta}^3} \right) a_{\beta} a_{\beta} a_{\beta} a_{\beta}. \quad (6) \]
The condition of the positive definiteness of the stiffness tensor was chosen as the stability condition.

3 Dependence of components of stiffness tensor on potential parameters. Stability criterion.

For the pair potential the stiffness tensor has only two independent components. Matrix, corresponding to this tensor in the basis ($\varepsilon_1, \varepsilon_2, \varepsilon_3$) has the form

$$C \sim \begin{bmatrix} C_1 & C_2 & 0 & 0 & 0 \\ C_2 & C_1 & 0 & 0 & 0 \\ 0 & 0 & C_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_2 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$  \hspace{1cm} (7)

where

$$C_1 = \frac{1}{2V_0} \sum_\beta \left( \frac{\Pi''(a_\beta)}{a_\beta^2} - \frac{\Pi'(a_\beta)}{a_\beta^3} \right) \left( a_\beta \cdot \varepsilon_1 \right)^4,$$  \hspace{1cm} (8)

$$C_2 = \frac{1}{2V_0} \sum_\beta \left( \frac{\Pi''(a_\beta)}{a_\beta^2} - \frac{\Pi'(a_\beta)}{a_\beta^3} \right) \left( a_\beta \cdot a_\beta \cdot \varepsilon_1 \cdot \varepsilon_2 \right)^2,$$  \hspace{1cm} (9)

From (7), it follows that the stability condition of positive definiteness of the stiffness tensor has the form:

$$C_1 > C_2 > 0,$$  \hspace{1cm} (10)

The dependence of $C_1$ and $C_2$ on $\mathbf{K}$ is presented at figure 2. As one can see from this figure, there exists the critical value of $\mathbf{K} = \mathbf{K}_*$, such that for $\mathbf{K} < \mathbf{K}_*$ the BCC lattice is stable and for $\mathbf{K} > \mathbf{K}_*$ it is unstable. This critical value can be found numerically: $\mathbf{K}_* \approx 4.5176$. So, the criterion of stability in terms of parameter of potential (3) was obtained:

$$\mathbf{K} < \mathbf{K}_* \approx 4.5176$$  \hspace{1cm} (11)

This criterion is convenient for numerical analysis but it can’t be verified, because there exists a problem of determination of $\mathbf{K}$ for real materials. This leads to necessity in a criterion in terms of some macroscopic parameter.

4 Relation between $\mathbf{K}$ and the Gruneisen parameter. Reformulation of the stability criterion.

In [5] the expression of the Gruneisen parameter for materials with simple lattice was obtained:

$$\Gamma = -\frac{\sum_\beta \left( (d + 2) \Phi' (a_\beta^2) a_\beta^2 + 2\Phi'' (a_\beta^2) a_\beta^4 \right)}{d \sum_\beta \left( d \Phi (a_\beta^2) + 2\Phi' (a_\beta^2) a_\beta^4 \right)},$$  \hspace{1cm} (12)
where

$$\Phi (a_\beta^2) = - \frac{\Pi'(a_\beta)}{a_\beta}. \tag{13}$$

Using (12) and (13), one can obtain dependence of $\Gamma$ on $\kappa$. This dependence $\Gamma(\kappa)$ is presented at fig 3. This dependence is monotonic. It means, that it can be unambiguously inverted. One can find dependence of ratio $C_1/C_2$ on $\Gamma$, graph for which is presented at the fig. 4. So, it is possible to find such a value $\Gamma_*$, that the BCC lattice is stable in view of $\Gamma < \Gamma_*$ and unstable in view of $\Gamma > \Gamma_*$. As it will be shown further in this paper, BCC lattice transforms to face-centered cubic (FCC) lattice when it becomes unstable. The Gruneisen parameter of material with FCC lattice is greater than one for material with BCC lattice and with the same $\alpha$. That’s why the stability condition can be rewrited in the following form:

$$\Gamma < \Gamma_* \cong 1.713 \tag{14}$$

This criterion was succesfully verified for more than 30 materials. Results for some of these materials, which are the closest to the boundary of stability, are presented in table 1. From the table 1 one can see when $\kappa$ is such, that BCC lattice is stable, the material always has BCC lattice, not FCC. It can be explained by the fact, that bonding energy for BCC lattice is higher than for FCC.
Figure 3: Dependence of Gruneisen parameter on $\xi$

<table>
<thead>
<tr>
<th>Metall</th>
<th>$\Gamma$</th>
<th>Lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molybdenum</td>
<td>1.58</td>
<td>BCC</td>
</tr>
<tr>
<td>Iron</td>
<td>1.68</td>
<td>BCC</td>
</tr>
<tr>
<td>Niobium</td>
<td>1.68</td>
<td>BCC</td>
</tr>
<tr>
<td>Tantalum</td>
<td>1.69</td>
<td>BCC</td>
</tr>
<tr>
<td>Nickel</td>
<td>1.91</td>
<td>FCC</td>
</tr>
<tr>
<td>Copper</td>
<td>2.04</td>
<td>FCC</td>
</tr>
</tbody>
</table>

Table 1: Gruneisen parameters for materials with different lattices

5 Numerical modelling

The loss of stability of BCC lattice was simulated in numerical experiment. Besides the interatomic interaction, described by potential (1) with $\xi$, corresponding to unstable lattice, small dissipation was introduced into the model. Particles had random velocities, in the range $0-0.1v_0$ ($v_0$ is the long-wave velocity). Method of central differences was used for integration. The step of integration was equal to 4% of the period of characteristic oscillations of the particles. The motions in the system became unapparent after time, equal to 120 periods of oscillations. The procedure of numerical integration is specified in [1].

The first result obtained was that criterion (11) is correct: the BCC lattice for material, satisfying (11) is stable and vice versa. The problem is to figure out to which lattice the BCC lattice transforms when it loses stability. To solve this problem the coordinational diagram was plotted. Coordinational diagram is a diagram, showing the quantities of atomic pairs with different interatomic distances. For
ideal BCC lattice this diagram looks as at fig. 5: it has several peaks, corresponding to radiuses of coordination spheres. The final coordinational diagram is shown at figure 6. The analysis of these diagrams gives several results. The first parameter analysed was the number of atoms in the first coordinational sphere (the number of the "closest" atoms, which is also called the coordinational number). This quantity was counted for all the atoms. At the beginning the coordinational number is equal to 8 for each atom. The coordinational number distribution after the destruction of the BCC lattice can be seen in the table 2. As one can see, the majority of the atoms has the coordinational number 12 after the structural transition. This coordinational number corresponds to two FCC lattice. The ratios of radiuses of the first three coordinational spheres were counted to find out what the prevalent lattice is. Radius of the n-th coordinational sphere is equal to an absciss of the n-th maximum on a coordinational diagram. This ratios are presented in table 3. As one can see from table 3, the values after the transition are close to the FCC values.
Figure 5: coordinational diagram before destruction of the BCC lattice

Table 3: Ratios of radiuses of coordinational spheres

<table>
<thead>
<tr>
<th></th>
<th>BCC lattice</th>
<th>FCC lattice</th>
<th>Before transition</th>
<th>After transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_2/r_1$</td>
<td>1.15</td>
<td>1.41</td>
<td>1.15</td>
<td>1.41</td>
</tr>
<tr>
<td>$r_3/r_1$</td>
<td>1.64</td>
<td>1.73</td>
<td>1.64</td>
<td>1.73</td>
</tr>
</tbody>
</table>
So, it allows us to expect the BCC to FCC structural transition. The ratio $\frac{r_2}{r_1}$ for the atoms, which have the coordinational number 8 is equal to 1.41. So, the rest of atoms is not BCC. It was noticed, that after the transition the Gruneisen parameter raised: before the transition it was equal to 2.61 and after it became equal to 2.69. It means, that the increase of the Gruneisen parameter, predicted analytically takes place in the numerical experiment. It gives hope to be able to simulate such phenomena as the phase transition from BCC to FCC lattice, which takes place in iron.

6 Concluding remarks

In this paper the stability criterion for body-centered cubic lattice is obtained. This criterion was verified with the numerical simulation. It was also reformulated in terms of Gruneisen parameter. This reformulated criterion was verified by comparison with known experimental results. Both verifications showed the correctness of this criterion. The transition from unstable BCC to FCC lattice was modelled. Analogous modelling can be used to describe this transition, taking place with the raise of temperature in iron. As one can see from table 1, iron is the BCC metall, one of the closest to the instability region. It allows to expect loss of stability of BCC lattice under temperature raise, connected with predicted raise of Gruneisen parameter (it is considered to be temperature independent in classical theories, but many investigations [6], [7] showed, that it is not).
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References


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On numerical methods for investigations of toroidal shells

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Abstract

The stress-deformed state of inflated toroidal shell is investigated. Calculations are realized by Galerkin and by finite element methods. Conditions of the shells creasing are discussed.

1 Introduction

Soft shells topologically equivalent torus are considered. It is supposed, that the internal geometry of non-stressed shell coincides with that of torus which has circular meridional cross section. Meridians and parallels of such torus are chosen as material coordinate lines. Coefficients of material elasticity of the shell are considered as known functions of Lagrange coordinates. Changes of the form of the inflated shell are calculated. These calculations are fulfilled by Galerkin method and finite element method.

2 Variational formulation of the problem

The stressed-deformed state of inflated toroidal shell the part of which is shown on figure 1 will be investigated. On this figure the cross section of the shell by a plane including axis $z$ and forming angle $\hat{\psi}$ with plane $xz$ is shown. Position of any point $M$ of the shell in system $xyz$ we shall specify by means of angle $\hat{\phi}$ and distance $\hat{r}(\hat{\phi},\hat{\psi})$ between the point $M$ and point $O_1$ which, as well as the point $M$, lays in the specified section at distance $O_1O = R$ from the axis $z$. The magnitude $R$ is supposed to be not depending on angle $\hat{\psi}$. Dependence of magnitude $\hat{r}$ from $\hat{\psi}$ arises when the shell is not symmetric with respect to axis $z$.

Let at non-stressed state of the shell radius of its meridional cross sections will be noted by $\rho$; the centers of these circular cross sections form the circle of radius $O_1O = R$ laying in the plane $xy$. 
The cartesian coordinates of the point $M$ are determined by formulas:

\begin{align*}
x &= (R + \hat{r}(\hat{\psi}, \hat{\phi}) \cos \hat{\phi}) \cos \hat{\psi}, \\
y &= (R + \hat{r}(\hat{\psi}, \hat{\phi}) \cos \hat{\phi}) \sin \hat{\psi}, \\
z &= \hat{r}(\hat{\phi}, \hat{\psi}) \sin \hat{\phi}.
\end{align*}

Lagrange coordinates $\alpha$ and $\beta$ of particle $M$ are introduced by means of equalities

\begin{align*}
\hat{\psi} &= \beta + \psi(\alpha, \beta), \quad \hat{\phi} = \alpha + \varphi(\alpha, \beta). \tag{2}
\end{align*}

Let’s enter also magnitude $r(\alpha, \beta)$ by equality

\begin{align*}
\hat{r}(\hat{\psi}, \hat{\phi}) &= \rho + r(\alpha, \beta). \tag{3}
\end{align*}

In equalities (2) and (3) magnitudes $\psi(\alpha, \beta)$, $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$ are considered as required functions.

We assume that to non-stressed state of the shell correspond zero values of these functions $\psi(\alpha, \beta)$, $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$. By virtue of this assumption magnitudes $\alpha$ and $\beta$ get sense of angular coordinates of points on meridional sections of the shell and, respectively of these sections. These magnitudes $\alpha$ and $\beta$ are considered as Lagrange coordinates of particle $M$. The functions $\psi(\alpha, \beta)$, $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$ as it is easy to see are representing displacements of the particle.

Using (2) and (3), we shall transform (1) in the next form

\begin{align*}
x &= (R + (\rho + r(\alpha, \beta)) \cos(\alpha + \varphi(\alpha, \beta))) \cos(\beta + \psi(\alpha, \beta)), \\
y &= (R + (\rho + r(\alpha, \beta)) \cos(\alpha + \varphi(\alpha, \beta))) \sin(\beta + \psi(\alpha, \beta)), \\
z &= (\rho + r(\alpha, \beta)) \sin(\alpha + \varphi(\alpha, \beta)). \tag{4}
\end{align*}
Let's calculate metric coefficients $g_{11}$, $g_{12} = g_{21}$ and $g_{22}$ of the shell. We shall calculate them approximately assuming that displacements $\psi(\alpha, \beta)$, $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$ are small and neglecting the small values of second and higher order.

For example we will use the approximated equalities

\[
\cos(\beta + \psi) = \cos \beta - \psi \sin \beta, \quad \sin(\beta + \psi) = \sin \beta + \psi \cos \beta, \quad (5)
\]

\[
\cos(\alpha + \psi) = \cos \alpha - \psi \sin \alpha, \quad \sin(\alpha + \psi) = \sin \alpha + \psi \cos \alpha. \quad (6)
\]

In result of simple calculation we receive

\[
g_{11} = \left(1 + 2 \frac{\partial \varphi}{\partial \alpha}\right) \rho^2 + 2 \rho r, \quad (7)
\]

\[
g_{12} = g_{21} = (R + \rho \cos \alpha)^2 \frac{\partial \varphi}{\partial \alpha} + \rho \frac{\partial r}{\partial \beta} \sin 2\alpha + \rho^2 \frac{\partial \varphi}{\partial \beta} + \cos 2\alpha, \quad (8)
\]

\[
g_{22} = \left(1 + 2 \frac{\partial \varphi}{\partial \beta}\right) (R + \rho \cos \alpha)^2 (R + \rho \cos \alpha) (r \cos - \rho \varphi \sin \alpha). \quad (9)
\]

In case of non-stressed shell $r \equiv \varphi \equiv \psi \equiv 0$. Thus on the basis of (7), (8) and (9) it is received

\[
g_{11} = g_{11}^0 = \rho^2, \quad g_{12} = g_{12}^0 = g_{21} = g_{21}^0 = 0, \quad g_{22} = g_{22}^0 = (R + \rho \cos \alpha)^2. \quad (10)
\]

Rates of elongations for lines of material coordinates are determined by formulas

\[
\lambda_1 = \sqrt{\frac{g_{11}}{g_{11}^0}}, \lambda_2 = \sqrt{\frac{g_{22}}{g_{22}^0}}. \quad (11)
\]

Variation $\chi$ of angle between these lines is determined by equality

\[
g_{12} = \sqrt{g_{11}^0 g_{22}^0 \lambda_1 \lambda_2 \sin \chi}. \quad (12)
\]

Using (7) – (9) and (10) – (12), we can write down
\[
\lambda_1 = \sqrt{1 + 2 \frac{\partial \varphi}{\partial \alpha} + \frac{2r}{\rho}} = 1 + \frac{\partial \varphi}{\partial \alpha} + \frac{r}{\rho},
\]
\[
\lambda_2 = \sqrt{1 + 2 \frac{\partial \psi}{\partial \beta} + \frac{2r \cos \alpha - \rho \psi \sin \alpha}{R + \rho \cos \alpha}} = 1 + \frac{\partial \psi}{\partial \beta} + \frac{r \cos \alpha - \rho \psi \sin \alpha}{R + \rho \cos \alpha}.
\]

Let’s suppose that the shell thus reinforced by threads which located along its coordinate lines that magnitude \( \chi \) negligible influences on density \( u \) of the shell strain energy. According to chosen calculation accuracy we have

\[
u = k_1 \varepsilon_1^2 + k_2 \varepsilon_2^2,
\]

where

\[
\varepsilon_1 = \lambda_1 - 1, \varepsilon_2 = \lambda_2 - 1
\]

– relative elongations of coordinate lines; \( k_1 \) and \( k_2 \) are the coefficients describing elastic properties of the shell.

Thus potential energy of the whole shell will be equal

\[
U = \rho \int_0^{2\pi} \int_0^{2\pi} \left( k_1 \varepsilon_1^2 + k_2 \varepsilon_2^2 \right) (R + \rho \cos \alpha) d\alpha d\beta.
\]

On the basis of (13), (15) and (16) the following expression of potential energy was received with accuracy of the second order, as concerns of small quantities:

\[
U = \rho \int_0^{2\pi} \int_0^{2\pi} \left( k_1 \left( \frac{\partial \varphi}{\partial \alpha} + \frac{r}{\rho} \right)^2 + k_2 \left( \frac{\partial \psi}{\partial \beta} + \frac{r \cos \alpha - \rho \psi \sin \alpha}{R + \rho \cos \alpha} \right)^2 \right) (R + \rho \cos \alpha) d\alpha d\beta.
\]

To take account of energy of the gas embraced by the shell, we shall calculate the volume limited by it. Designating through \( h \) distance from the point \( O_1 \) meridional section up to any point \( N \) of this section, we can the elementary volume containing this point to present in the form of

\[
dv = h(R + h \cos \hat{\varphi}) d\hat{\varphi} d\hat{\psi} d\hat{\phi},
\]

where \( \hat{\varphi} \) is an angle between the segment \( O_1 N \) and a plane \( xy \), \( d\hat{\psi} \) is an angle formed by two meridional sections between which the point \( N \) is located.

The volume of gas contained in the shell can be calculated under the formula

\[
V = \int_0^{2\pi} d\hat{\psi} \int_0^{2\pi} d\hat{\varphi} \int_0^{\pi} \int_0^{\pi} h(R + h \cos \hat{\varphi}) dh,
\]
\[ V = \int \int \left( \int_0^h (R + h \cos \phi) dh \right) d\psi d\phi. \]  

(20)

From here we have

\[ V = \int_0^{2\pi} \int_0^{2\pi} \left( \frac{\hat{r}^2(\phi, \psi)}{2} R + \frac{\hat{r}^3(\phi, \psi)}{3} \cos \phi \right) d\phi d\psi. \]  

(21)

Let's make in last integral replacement of variables under formulas (2).

With the accepted accuracy from (21) it is received

\[ V = \int_0^{2\pi} \int_0^{2\pi} \left( \left( \frac{\rho^2}{2} R + \frac{\rho^3}{3} \cos \alpha \right) \left( 1 + \frac{\partial \psi}{\partial \beta} + \frac{\partial \phi}{\partial \alpha} \right) + \rho \tau (R + \rho \cos \alpha) - \varphi \frac{\rho^3}{3} \sin \alpha \right) d\alpha d\beta. \]  

(22)

The potential energy of the shell and the volume contained by it are expressed by formulas (17) and (22) through required functions \( \psi(\alpha, \beta) \), \( \varphi(\alpha, \beta) \) and \( \tau(\alpha, \beta) \). To position of equilibrium of the shell there correspond such values of these functions at which the following equality is carried out

\[ \delta U - p \delta V = 0. \]  

(23)

Here \( p \) is given pressure inside of the shell, and \( \delta U \) and \( \delta V \) are such variations of potential energy of the shell and of the volume contained by it, as are compatible with continuity of the shell.

### 3 Research of the shell on the basis of Galerkin method

*Orthotropic homogeneous shells*

Let coefficients \( k_1 \) also \( k_2 \) are known constant magnitudes. In this case the shell will be symmetric with respect to axis \( z \). Therefore \( \psi \equiv 0 \). We shall search \( \varphi \) and \( r \) in the following form

\[ \varphi = A \cos \alpha + B \sin \alpha, \quad r = C \cos \alpha + D \sin \alpha. \]  

(24)

Substituting these values \( \varphi \) and \( r \) in (17) and (22) gives the equations

From (17) and (24) we have
\[ U = \rho \int_0^{2\pi} \int_0^{2\pi} k_1 \left( \left( \frac{D}{\rho} - A \right) \sin \alpha + \left( B + \frac{C}{\rho} \right) \cos \alpha \right)^2 (R + \rho \cos \alpha) \, d\alpha \, d\beta + \]
\[ + \rho \int_0^{2\pi} \int_0^{2\pi} k_2 \frac{C \cos^2 \alpha + (D - \rho A) \cos \alpha \sin \alpha - \rho B \sin^2 \alpha}{R + \rho \cos \alpha} \, d\alpha \, d\beta. \] (25)

From (25) it follows that

\[ U = k_1 U_1 + k_2 U_2, \] (26)

where

\[ U_1 = 4\pi \rho \frac{R}{2} \left( \left( \frac{D}{\rho} - A \right)^2 + \left( B + \frac{C}{\rho} \right)^2 \right), \] (27)

\[ U_2 = \rho (C^2 - (D - \rho A)^2 + \rho^2 B^2 + 2C\rho B) I_4 + \]
\[ + \rho ((D - \rho A)^2 - 2\rho^2 B^2 - 2C\rho B) I_2 + \rho^3 B^2 I_0, \]

\[ I_k = \int_0^{2\pi} \int_0^{2\pi} \frac{\cos^k \alpha}{R + \rho \cos \alpha} \, d\alpha \, d\beta, k = 0, 2, 4. \]

From (22) and (24) we have

\[ V = 2\pi^2 \rho^2 (R + C). \] (28)

In accordance to (23) the following equations must hold

\[ \frac{\partial U}{\partial A} - p \frac{\partial V}{\partial A} = 0, \frac{\partial U}{\partial B} - p \frac{\partial V}{\partial B} = 0, \frac{\partial U}{\partial C} - p \frac{\partial V}{\partial C} = 0, \frac{\partial U}{\partial D} - p \frac{\partial V}{\partial D} = 0. \] (29)

Using the equation (29) and formulas (26), (27) and (28) we receive

\[ \rho A - D = 0, \]
\[ BM + CN = 0, \]
\[ BW + CQ = p\pi^2 \rho^3, \]
\[ \rho A - D = 0. \] (30)

where

\[ M = \rho (4k_1\pi R + 2\rho^2 k_2 (I_4 - 2I_2 + I_0)), \]
\[ N = 2(2k_1\pi R + \rho^2 k_2 (I_4 - I_2)), \]
\[ Q = k_1\pi R + \rho^2 k_2 I_4, \]
\[ W = \rho (k_1\pi R + \rho^2 k_2 (I_4 - 2I_2)). \] (31)
From the equation set (30) we obtain

\[ B = -\frac{p\pi^2\rho^3N}{QM - NW}, \quad C = \frac{p\pi^2\rho^3M}{QM - NW}. \]  

(32)

Equivalence of the first and the last equations (30) allows arbitrary choosing one of magnitudes \( A \) or \( D \). But considerations of symmetry the shell with respect to its equator show that zero values must be given to \( A \) and \( D \).

*The shells reinforced by discretely included threads*

The above described Galerkine method may be made more exact by dint of expansion series of type (24). This method also may be applied in cases when elasticity coefficients of the shell are different for different parts of the shell. In the case when the shell are reinforced by discretely included threads these coefficients may be represented by functions that look as follows

\[ k_1(\alpha) = L \sin^{2n} q_1 \alpha, k_2(\beta) = H \sin^{2m} q_2 \beta, \]  

(33)

where \( L, H, n, m, q_1, q_2 \) are chosen arbitrary.

The typical graphic of functions defined by (33) are shown on Fig.2

![Figure 2](image)

Figure 2:

Peculiarities of such presentation of elasticity coefficients suggest generalization of (24) by using of trigonometric series as forms of required functions \( r, \varphi \) and \( \psi \). If the treads are placed wide apart and are hardly extensible then calculation of strain energy of whole shell may be reduced to integration of the threads energy.

4 Research of the shell on the basis of finite elements method

Minimization of the functional \( U \) was also accomplished by the finite elements method. The realization of this method was fulfilled on bases of triangulation of def-
inal domain of functions $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$ and presentation these functions as linear combinations of form-functions

$$f_1 = 1 + \frac{\gamma - \delta}{s}, f_2 = -\frac{\gamma}{s}, f_3 = \frac{\delta}{s},$$

(34)

$$p_1 = 1 + \frac{\delta - \gamma}{s}, p_2 = \frac{\gamma}{s}, p_3 = -\frac{\delta}{s},$$

(35)

The functions defined by (34) correspond to type 1 element of triangulation as well as functions (35) correspond to the type 2. In these formulas $\alpha$ and $\beta$ are local coordinates shown on Fig. 3 and

$$s = \frac{2\pi}{m},$$

(36)

where $m$ is some integer.

![Figure 3](image)

Distinctive feature of these functions is that $f_i$ and $p_i$ equal 1 in apex i and equal zero in other apexes. Everywhere outside of the elements these functions are zero.

In every element the approximating functions look as follows,

$$\varphi = s(q - 1) + \delta + T_k p_1 + T_{k-m} p_2 + T_{k-1} p_3,$$

$$r = s(n - p) + \gamma + V_k p_1 + V_{k-m} p_2 + V_{k-1} p_3,$$

(37)

where $T_i$ and $V_i$ are nodal values of $\varphi(\alpha, \beta)$ and $r(\alpha, \beta)$ in i-th node and $q$ and $n$ are numbers of column and string which cross each other in this node.

Using such approximations for $\varphi$ and $r$ calculation of $U$ and $V$ by formulas (17) and (22) give us $U$ and $V$ as functions of coefficients $U_i$ and $V_i$. Substituting of these functions in (23) give us a set of linear algebraic equations which we investigated by various methods of linear algebra.
5 On convergence of numerical methods

Almost every realization of discussed here calculations show us that the good exactness of solution can’t be obtained. As one of the causes of that may be considered formation of wrinkles on the shell. But according to basic assumptions of proposed here method the shell must be smooth. And it is not so in most cases that may be thought of. It is enough to look at some axisymmetric shells, to understand why the wrinkles are so typical for toroidal soft shells. So, if the inner pressure in the shell that is shown at Fig. 4 rises then as it is clear the radiuses of inner parallels became smaller what causes the wrinkles along inner parts of meridians.

For mathematical investigation of this phenomenon we borrow from [1], [2], [3] equilibrium equations for axisymmetric shells. In adapted here designations the equations are presented as follows

\[
\frac{d}{dz} (\sigma_{11}(z) x(z)) - \sigma_{22}(z) \frac{dx(z)}{dz} = 0, \tag{38}
\]

\[
\frac{\sigma_{11}(z)}{\rho(z)} \pm \frac{\sigma_{22}(z)}{x(z)} \frac{1}{\sqrt{1 + x'^2(z)}} = p, \tag{39}
\]

where \(x\) and \(z\) are co-ordinates of meridian points in plane \(xz\); \(\sigma_{11}\) and \(\sigma_{22}\) are true stresses normal to its parallels and meridians, respectively; \(\rho(z)\) is radius of curvature of meridian; sign "+" or "-" must be taken for elliptical and for hyperbolic points of the shell respectively.

Suppose that torus is symmetric in respect to plane \(xy\). Then on this plane

\[
\sigma_{11}/dz \big|_{z=0} = 0, x'(0) = 0 \tag{40}
\]

and from (38) follows equality \(\sigma_{11}(0) = \sigma_{22}(0)\).
Because of that from (39) we have

$$\sigma_{11}(0) \left( \frac{1}{\rho(0)} \pm \frac{1}{x(0)} \right) = p.$$ \hspace{1cm} (41)

Since $$\sigma_{11}(0) > 0$$ we see that both of equalities (41) may be true only if

$$\rho(0) < x(0),$$ \hspace{1cm} (42)

if it is not so the shell can not exist in smooth form tough it does exist with wrinkles. For example such obvious case we have if inner parallels of the shell are made of inextensible threads and all of them have the same radiuses.

6 Conclusion

In presented paper developed variational method for investigation of soft elastic toroidal shells that are not acted on by any forces except the forces of inner pressure. The proposed methods for calculation of deformations and stresses often give not nice results. That may be explained by formation wrinkles on the shell what was not anticipated.

References


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To the theory of soft toroidal shells

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Abstract

Axisymmetric problem of calculation of stresses arising in a toroidal soft shell is investigated under assumption, that the form of meridional cross section of the shell and internal pressure in it are given arbitrary. Examples of the shells with various constitutive equations are considered. Methods for examining of non-stressed shell’s geometry are developed.

1 Introduction

Methods for determination of stresses and deformations arising in the toroidal axisymmetric soft shells made of fabrics resisting not bending forces are considered. It is supposed that the form of meridional section of the shell and intensity of external forces applied to it are arbitrary given. On the basis of the general equilibrium equations of soft shells [1] methods of calculation of the stresses arising in the shell are developed. Examples of various constitutive equations of materials of which the shell is made are examined. In these examples shells deformations corresponding to calculated stresses are determined. The obtained results are used as basis for development of methods for calculation of geometrical characteristics of non-stressed shells. The knowledge of these characteristics is necessary for solution of cutting problems.

2 The equilibrium equations of the shell in stress’s terms

We will consider meridional section of torus shown on figure 1. For the description of disposition the section we use Lagrange coordinate $\xi$. The changing of $\xi$ corresponds to moving along the contour of the section.

Let’s use following designations. Through $R(z)$ we shall designate distance from any point $M$ of the shell up to axis of its symmetry. Through $\rho$ we shall designate distance from the beginning of coordinate system $xz$ up to some point $O_1$.
arbitrary chosen axis \(x\). The form of meridional sections we shall consider as given parametrically by functions \(x = x(\xi)\) and \(z = z(\xi)\).

We borrow from [3] the following equilibrium equations for axisymmetric shells:

\[
\frac{d}{dz}(\sigma_{11}(z)R(z)) - \sigma_{22}(z)\frac{ds(z)}{dz}\sin\alpha(z) + \frac{ds(z)}{dz}R(z)q_\tau(z),
\]

\[
\frac{\sigma_{11}(z)}{\rho(z)} \pm \frac{\sigma_{22}(z)}{R(z)} \cos\alpha(z) + q_n(z).
\]

Here: \(\sigma_{11}\) and \(\sigma_{22}\) – true stresses normal to its parallels and meridians, respectively; \(\rho(z)\) - radius of curvature of meridian; \(q_n(z)\) and \(q_\tau(z)\) - intensity of normal and a tangent external forces distributed on the shell; sign "+" must be taken for elliptical points of the shell. Further it is supposed that tangent forces \(q_\tau(z) = 0\).

We will introduce the new required function

\[
R(z(\xi)) = \rho + l(\xi).
\]

Then the equations (1) and (2) look like

\[
\frac{d}{d\xi}(\sigma_{11}(\rho + l)) - \sigma_{22}l' = 0,
\]

\[
\sigma_{11}\frac{z''l' - z'l''}{(z'^2 + l'^2)^{3/2}} \pm \sigma_{22}\frac{z'}{(\rho + l)(z'^2 + l'^2)^{1/2}} + q_n = 0.
\]

This equation set easily solved with respect to \(\sigma_{11}\) and \(\sigma_{22}\) if the form of the shell defined by magnitude \(\rho\) and by functions \(z(\xi)\) and \(l(\xi)\), and pressure inside of the shell which equals \(p = -q_n\) does not depend on coordinates.
3 The hypothesis about existence of torus with circular meridional cross-sections

We shall not write down the exact solution of the equation set (5) but we’ll investigate it approximately for torus of which meridional cross-section differs from circular a little. As a first approximation we shall put

\[ z = r \sin \xi, \ l = r \cos \xi. \]  

(6)

Then the equations (4) and (5) become

\[
\frac{d}{d\xi} \left( \sigma_{11}(\rho + r \cos \xi) \right) + \sigma_{22} r \sin \xi = 0, \]  

(7)

\[
\frac{\sigma_{11}}{r} \pm \frac{\sigma_{22}}{\rho + r \cos \xi} \cos \xi - p = 0. \]  

(8)

Elimination of \( \sigma_{22} \) from (6) and (7) give us the equation

\[
\frac{d\sigma_{11}}{d\xi} + \sigma_{11} \left( \mp 1 - \frac{r \cos \xi}{\rho + r \cos \xi} \right) \sin \xi \pm p r \frac{\sin \xi}{\cos \xi} = 0. \]  

(9)

The general solution of the homogeneous equation corresponding (9) is determined by the formula

\[
\sigma_{11} = C \left( \frac{\cos \xi}{\rho + r \cos \xi} \right)^{\mp 1}, \]  

(10)

where \( C \) is a constant of integration.

According to method of constant variation we shall to consider \( C \) as function of argument \( \xi \). Then from (10) it is received

\[
\frac{d\sigma_{11}}{d\xi} = \frac{C'(\cos \xi)^{\mp 1}}{\rho + r \cos \xi} \pm p r \frac{\sin \xi}{\cos \xi} = 0. \]  

(11)

From here we have

\[
C = \mp \int pr \left( \frac{\rho \sin \xi}{(\cos \xi)^{\mp 1} \cos \xi} + \frac{r \sin \xi}{(\cos \xi)^{\mp 1}} \right) d\xi + D. \]  

(12)

Thus, for elliptic points of the shell to which correspond the top signs, we receive

\[
C = pr \left( \rho \cos \xi + \frac{r \cos 2\xi}{4} \right) + D_1. \]  

(13)
\[ \sigma_{11} = \frac{pr(\rho \cos \xi + \frac{r \cos 2\xi}{4}) + D_1}{(\rho + r \cos \xi) \cos \xi}. \] (14)

For hyperbolic points of the shell to which correspond the bottom signs, we receive

\[ C = \frac{pr \rho - pr^2 \ln|\cos \xi|}{\cos \xi} + D_2, \] (15)

\[ \sigma_{11} = \frac{pr \rho - pr^2 \cos \xi \ln|\cos \xi| + D_2 \cos \xi}{\rho + r \cos \xi}. \] (16)

Let’s note, that \( D_1 \) and \( D_2 \) in (13) - (15) are constants of integration which should be expressed through parameters of problem. To find these constants we shall notice, that to value \( \xi = 0 \) correspond extreme external points of the torus. In these points

\[ \sigma_{11} = \frac{pr(\rho + \frac{r}{4}) + D_1}{(\rho + r)}. \] (17)

To the most internal torus’ points corresponds \( \xi = \pi \). In these points

\[ \sigma_{11} = \frac{pr \rho - D_2}{\rho - r}. \] (18)

As stresses on the biggest and on the smallest torus’ parallels are counterbalanced by the internal pressure acting on its half, we can write down

\[ 2\pi \left( pr \left( \rho + \frac{r}{4} \right) + D_1 \right) + 2\pi (pr \rho - D_2) = \pi(\rho + r)^2 - \pi(\rho - r)^2. \] (19)

From here we have

\[ D_1 - D_2 = -\frac{pr^2}{4}. \] (20)

Substituting value \( \sigma_{11} \) in (8), we find \( \sigma_{22} \). Thus for elliptic points it equals

\[ \sigma_{22} = \frac{3pr}{4} + \frac{pr \tan^2 \xi}{4} + \frac{D_1}{r \cos^2 \xi}. \] (21)

For hyperbolic points it equals

\[ \sigma_{22} = -pr(1 + \ln|\cos \xi|) + \frac{D_2}{r}. \] (22)
Let us suppose that stresses $\sigma_{22}$ in meridian torus cross-section are counterbalanced by stress in this section. In this case we have:

$$\int_0^{2\pi} \sigma_{22} \sqrt{z'^2 + l'^2} \, d\xi = \pi r^2 p.$$  \hfill (23)

Considering distinctions of analytical expressions for $\sigma_{22}$, we shall rewrite this equality in the form of

$$\int_{-\pi/2}^{\pi/2} \left( \frac{3pr}{4} + \frac{pr \tan^2 \xi}{4} + \frac{D_1}{r \cos^2 \xi} \right) \, d\xi = \pi r^2 p.$$  \hfill (24)

This equation may be wrote as follows

$$\left( \frac{pr^2}{4} + D_1 \right) \int_{-\pi/2}^{\pi/2} \frac{d\xi}{\cos^2 \xi} + \pi D_2 = \pi pr^2 \left( \frac{3}{2} - \ln 2 \right).$$  \hfill (25)

The integral in formula (25) is divergent. Because of that the next equation should hold

$$D_1 = -\frac{pr^2}{4}.$$  \hfill (26)

Equalities (20), (25) and (26) are incompatible. It means that the hypothesis about existence of torus with circular meridional cross-sections is not true. But supposition that the shell has such parts on which holds equality $\sigma_{22} = 0$ allows to reach agreement of all conditions analogous to (21), (25) and (26).

### 4 The covered by wrinkles parts of shells

The parts of the shells on which $\sigma_{11} > 0$ and $\sigma_{22} > 0$ may to have arbitrary chosen forms of meridians. To obtain any of such form it is enough that the shell was reinforced by threads that are laid on its parallels and have properly given coefficients of elasticity.

The forms of those parts of the shell at which $\sigma_{22} = 0$ can not be given arbitrary. This form must be found in course of investigation of whole problem concerning the shell.

In this case equations (4) and (5) would look as follows

$$\frac{\partial}{\partial \xi} \left( \sigma_{11}(\rho + 1) \right) = 0, \sigma_{11} \frac{z''l' - z' l''}{[z'^2 + l'^2]^{3/2}} = p.$$  \hfill (27)
From (27) taking account of (3) we have

$$\sigma_{11} = \frac{D_3}{R} \int \frac{z''l' - z'l''}{(z'^2 + l'^2)^{3/2}} = p. \quad (28)$$

where $D_3 = \text{const} > 0$ since $\sigma_{11} > 0$.

Instead of variable $\xi$, the variable we’ll use now $z$. Then from (28) follows

$$\pm \frac{R''}{(1 + R'^2)^{3/2}} = K_1 R, K_1 = \frac{p}{D_3}. \quad (29)$$

The signs “+” and “−” in (29) correspond to hyperbolic and to elliptical parts of the shell respectively.

From (29) follows

$$\frac{d(1 + R'^2)}{(1 + R'^2)^{3/2}} = \mp K_1 d(R^2). \quad (30)$$

Thus

$$\frac{2}{(1 + R'^2)^{1/2}} = \mp K_1 d(R^2) + D_4, D_4 = \text{const} \quad (31)$$

and

$$\pm R' = \sqrt{1 - \left(\frac{G \pm vR^2}{G \pm vR^2}\right)^2}, G = \frac{D_4}{4}, v = \frac{K_1}{4}. \quad (32)$$

From (32) we easily see that parallels laying along common boundaries of hyperbolic and of elliptical parts have radiuses $R^*$ determined by formula

$$R^* = \sqrt{\pm \frac{G}{v}} \quad (33)$$

and that existence of such parallels is possible only if inequality $G < 0$ holds. From (32) also follows that extremal magnitudes of parallel’s radiuses $R^*$ equal

$$R^* = \sqrt{\pm \frac{G \pm 1}{v}} \quad (34)$$

The above obtained formulas for torus that has circular meridional cross-sections are true for parts consisting of elliptical and as well of hyperbolic points. Defect of the formulas is that these parts can not be united in one whole torus. It is because the stresses of the parts are not properly adjusted between themselves. The solution given by (14), (16), (21), (22) and (32) opens possibilities for investigation of any
such torus that is consisting of some parts for which $\sigma_{11} > 0$ and $\sigma_{22} > 0$ and of some parts for which $\sigma_{11} > 0$ and $\sigma_{22} = 0$.

Tori's of such sort may have wide range of various meridional cross-sections, some of them represented on Fig. 2 where by solid and by broken lines are shown elliptical and hyperbolic points respectively.

It is useful to underline that meridional contour may have angular points if along the parallels that contain such points are disposed the reinforcing threads characterized by properly chosen elasticity coefficients.

5 Investigation of geometric parameters of un-stressed shells

After the stresses and the form of the shell are found here arises the question of geometry that is inherent in the shell in its unstressed state. The elasticity coefficient $E(z)$ for those parts of the shell on which equality $\sigma_{22} = 0$ holds must be calculated by formula

$$E(z) = \frac{\sigma_{11}(z)}{\sqrt{1 + R'^2(z)}}.$$  \hspace{1cm} (35)

If the some part of the shell consist of points for which co-ordinate belongs to interval $(z, z + \Delta z)$ and the part is made of band with elasticity coefficient $E_0$ than the length of the band must be

$$L(z) = \frac{E(z)}{E_0} R_z.$$  \hspace{1cm} (36)

For those parts of the shell on which equalities $\sigma_{11} > 0$ and $\sigma_{22} > 0$ are true we have
\[ \varepsilon_i(z) = \frac{\sigma_{ii}(z)}{E_i(z)}, \quad i = 1, 2, \quad (37) \]

\[ \varepsilon_i(z) = \sqrt{\frac{g_{ii}(z)}{g_{ii}^0(z)}} - 1, \quad i = 1, 2, \quad (38) \]

where \( g_{ii}(z) \) and \( g_{ii}^0(z) \) are metrical coefficients of the shell in its stressed and unstressed states respectively.

Let’s for shortness suppose that meridians of considered parts of the shell are arcs of circles defined by (6). In this case

\[ g_{11} = r^2, \quad g_{22} = (\rho + r \cos \xi)^2. \quad (39) \]

Let the meridian of unstressed shell be defined by formulas

\[ x = \rho + (r + f(\xi)) \cos(\xi + \varphi(\xi)), \]
\[ y = (r + f(\xi)) \sin(\xi + \varphi(\xi)), \quad (40) \]

where \( f(\xi) \) and \( \varphi(\xi) \) are required functions which are supposed to be small values of first order. Then with accuracy of this order we have

\[ g_{11}^0 = (1 + 2\varphi')r^2 + 2rf, \quad (41) \]
\[ g_{22}^0 = (\rho + r \cos \xi)^2 + 2(\rho + r \cos \xi)(f \cos \xi - r\varphi \sin \xi). \]

From (38) and (41) follows

\[ \varepsilon_1(z) = -\varphi' - \frac{f}{r}, \quad \varepsilon_2(z) = -\frac{f \cos \xi - r\varphi \sin \xi}{\rho + r \cos \xi}. \quad (42) \]

If elasticity coefficients are known then equations (37) and (42) allows realization of calculation of \( f \) and \( \varphi \) after what the form of unstressed shell may be easily determined.

It may be pointed out that obtained results are useful for investigations of many problems that concern toroidal shells. For example we will outline the problem of defining such functions \( E_1(\xi) \) and \( E_2(\xi) \) that correspond to arbitrary given forms of stressed and unstressed shell.

This problem may be investigated on basis of variational equation

\[ \delta U - p\delta V = 0, \quad (43) \]
where \( p \) - is the pressure inside of the shell, and \( \delta U \) and \( \delta V \) - are such variations of potential strain energy \( U \) of the shell and of the volume \( U \) contained by it, as are compatible with continuity of the shell. The magnitudes \( U \) and \( V \) look like

\[
U = 2\pi \rho \int_{0}^{2\pi} (E_1(\xi)\varepsilon_1^2(\xi) + E_2(\xi)\varepsilon_2^2(\xi))(\rho + r \cos \xi) d\xi. \tag{44}
\]

Let \( h \) be distance from a point \( (x = \rho, z = 0) \) of meridional section up to any point \( N \) of this section. The volume of elementary ring that contain this point equals

\[
dV = 2\pi h(\rho + h \cos(\xi + \varphi(\xi))) dh. \tag{45}
\]

Consequently we have

\[
V = 2\pi \int_{0}^{2\pi} (1 + \varphi'(\xi)) d\xi \int_{0}^{r+f(\xi)} h(\rho + h \cos(\xi + \varphi(\xi))) dh. \tag{46}
\]

6 Conclusion

The results obtained in given work may be used as basis for designing of shells with arbitrary presupposed properties. The principal difficulty that we meet here is that are not found yet criteria of existence of such shells.

References


The Nonlinear Control of a Slewing Flexible Beam
Using the Feedback Linearization Technique

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Abstract

In this investigation a nonlinear control technique named feedback linearization is applied to the problem of vibration and tracking control of a slewing flexible beam system. This problem is representative of many real systems as, for example, the one-link flexible space manipulator (operating in the horizontal plane). Using the lagrangian approach, a nonlinear governing equation of motion for the flexible beam is obtained. The nonlinearity considered here comes from the coupling between the flexible beam deflection and the angular displacement of the actuator, a DC motor. The mathematical model for the DC motor is linear. Only local results are considered here, defined in a neighborhood of a specified set of states (in the origin of the coordinate system) and, therefore, this approach guarantees stability locally. In the approach presented, state transformations and nonlinear feedback are utilized to develop a new controllable system equivalent to the original nonlinear one. A linear control law can then be applied. A brief investigation on the stability of the system’s zero dynamics is also developed.

1 Introduction

Real systems with flexible components and which operates in situations of large angular displacements and velocities need a robust controller in order to guarantee precision and stability. Systems presenting such control problems can be found in many applications in industry and space as, for example, in satellite and spacecraft attitude control [8], [10] and electromagnetic suspension system [9]. It is fact that conventional linear controllers are not sufficiently robust to control strong nonlinear systems.

The basic idea of the feedback linearization technique is to find a way of transforming original nonlinear system models into equivalent models of a simpler form. This linearization is achieved by exact state transformation and feedback, rather
The Nonlinear Control of a Slewing Flexible Beam Using the Feedback Linearization Technique

than by linear approximations of the dynamics [\textsuperscript{7}]. The feedback linearization technique is not applicable to any nonlinear system and the access to the complete state is necessary. It also requires an exact model of the nonlinear system. Even with these limitations this technique is a concept of paramount importance in nonlinear control theory [\textsuperscript{7}].

2 Geometric and mathematical model

The geometric model of the dynamic system investigated in this work is illustrated in Figure 1.

![Figure 1: The flexible beam in slewing motion (XY - inertial axes, xy - moving axes and \(\upsilon(x,t)\) - beam deflection)](image)

The governing equations of motion for this system is given by [\textsuperscript{1}]:

\[
\begin{align*}
L_m \dot{i}_a + R_a i_a + K_b N_g \dot{\theta} &= U \\
(I_{\text{shaft}} + I_{\text{motor}} N_g^2) \ddot{\theta} + C_m N_g^2 \dot{\theta} - N_g K_t i_a &= 0 \\
\ddot{q}_j + \mu \dot{q}_j + \omega_j^2 q_j + \alpha_j \dot{q}_j - \dot{\theta} \ddot{q}_j &= 0
\end{align*}
\]

plus the boundary conditions \(\phi''(L,t) = 0\) and \(\phi'''(L,t) = 0\).

In the set of governing equations given by Equations (1), the first two equations are related to the DC motor (electric equation and mechanical equation, respectively) and the last one is related to the flexible beam-like structure. In Equations (1), \(L_m\) represents the armature inductance, \(R_a\) represents the armature resistance, \(K_b\) represents back e.m.f. constant, \(N_g\) represents the gear ratio, \(I_{\text{shaft}}\) represents the inertia of the connecting motor-beam shaft, \(I_{\text{motor}}\) represents the inertia of the motor, \(C_m\) represents the motor internal damping, \(K_t\) represents the torque constant, \(\mu\) represents the beam structural damping, \(\omega_j\) represents the natural frequency of mode \(j\) (of the beam) and \(\alpha_j\) represents the modal inertia of the mode \(j\).

In these equations, \(i_a\) represents the electric current in the DC motor, \(\theta\) represents the angular displacement of the motor axle (also known as the slewing angle) and \(q_j\) represents the time component of each one of the vibration modes of the
flexible structure. In the analysis developed here, the flexible structure is geometrically modeled assuming linear curvature and the Euler-Bernoulli assumptions for a slender beam are considered. Only the first flexural mode of the beam is considered. The last equation in the set (1) is a discretized equation.

Considering only the first flexural mode of the beam, Equations (1) can be written in state space form as:

\[
\begin{align*}
\dot{x}_1 &= -c_1 x_1 - c_2 x_3 + c_3 U \\
\dot{x}_2 &= x_3 \\
\dot{x}_3 &= -c_3 x_3 + c_4 x_1 \\
\dot{x}_4 &= x_5 \\
\dot{x}_5 &= -\omega_1^2 x_4 - \mu x_5 + \alpha_1 c_3 x_3 - \alpha_1 c_4 x_1 + x_2^2 x_4
\end{align*}
\]

where

\[
c_1 = \frac{R_a}{L_m}, \quad c_2 = \frac{x_a N_a}{L_m}, \quad c_3 = \frac{C_m N_g}{I_{shaft} + I_{motor} N_g}, \quad c_4 = \frac{K_t N_g}{I_{shaft} + I_{motor} N_g} \quad \text{and} \quad c_5 = \frac{1}{L_m}.
\]

In Equations (2), the states under consideration are: \(x_1 = i_a, \quad x_2 = \theta, \quad x_3 = \dot{\theta}, \quad x_4 = q_1 \quad \text{and} \quad x_5 = \dot{q}_1.\)

3 The feedback linearization technique

The feedback linearization control technique is based on the canceling of the nonlinearities present in the system nonlinear dynamics and the imposition of a desired linear dynamics. This technique can be applied to a class of nonlinear systems described by the so-called companion form, or controllability canonical form. A system is said to be in companion form if its dynamics is represented by [6], [3]:

\[
\dot{x} = f(x) + g(x)u
\]

where \(u\) is the scalar control input, \(x\) is the scalar output of interest, \(x\) is the state vector, and \(f(x)\) and \(g(x)\) are nonlinear functions of the states.

For the system investigated in this work, the companion form as given by Equation (3) is given by:

\[
\begin{align*}
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\dot{x}_3 \\
\dot{x}_4 \\
\dot{x}_5 
\end{bmatrix}
&= \begin{bmatrix}
-c_1 x_1 - c_2 x_3 + c_3 U \\
\quad x_3 \\
-c_3 x_3 + c_4 x_1 \\
\quad x_5 \\
-\omega_1^2 x_4 - \mu x_5 + \alpha_1 c_3 x_3 - \alpha_1 c_4 x_1 + x_2^2 x_4
\end{bmatrix}
+ \begin{bmatrix}
c_5 \\
0 \\
0 \\
0 \\
0
\end{bmatrix} U
\end{align*}
\]

The vector fields \(f\) and \(g\) are therefore given by:

\[
f(x) = \begin{bmatrix}
-c_1 x_1 - c_2 x_3 + c_3 U \\
\quad x_3 \\
-c_3 x_3 + c_4 x_1 \\
\quad x_5 \\
-\omega_1^2 x_4 - \mu x_5 + \alpha_1 c_3 x_3 - \alpha_1 c_4 x_1 + x_2^2 x_4
\end{bmatrix}
= \begin{bmatrix}
f_1 \\
f_2 \\
f_3 \\
f_4 \\
f_5
\end{bmatrix}
\]

\[
g(x) = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}.
\]
\[ g(x) = \begin{pmatrix} c_5 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \end{pmatrix} \]  

(6)

In order to verify whether a nonlinear system (as the one given by the set of Equations (12)) is input-state linearizable or not, one must check the controllability condition and the involutivity condition for this set of equations. Both conditions must be satisfied [6].

### 3.1 The controllability matrix

The controllability matrix, \( C \), for a system of same dimension (5) as the one under investigation is given by [6]:

\[ C = \begin{bmatrix} g & adf \cdot g & adf^2 \cdot g & adf^3 \cdot g & adf^4 \cdot g \end{bmatrix} \]  

(7)

where each column is represented by a Lie bracket, as defined in Sub-Section 3.3 afterward. In [2], it was shown that this matrix is of rank 5 in the neighborhood of the origin.

### 3.2 The involutivity condition

The other condition to be verified is that the distribution:

\[ \Delta = \text{span} \{ g, \ adf \cdot g, \ ..., \ adf^{n-2} \cdot g \} \]  

(8)

be involutive near the origin, \( x_0 \). This condition is a result of the Frobenius Theorem and guarantees the existence of a diffeomorphic transformation [6].

The existence of a diffeomorphic transformation implies the existence of a 1-to-1 mapping from a nonlinear vector field to a linear vector field and vice-versa. In other words, if a Lie bracket is formed by two vectors (from a determined set, as the distribution presented in (9), for example) the vector field resulting from this operation can be expressed as a linear combination of the original set of vector fields [3].

In this work, since there are five states, one must verify the involutivity of:

\[ \Delta = \text{span} \{ g, \ adf \cdot g, \ ..., \ adf^2 \cdot g, \ adf^3 \cdot g \} \]  

(9)

In [2] it was proven that this distribution is involutive.

### 3.3 Defining the Lie brackets

The Lie bracket of the vector fields \( f \) and \( g \) is a third vector field commonly written as \( adf \cdot g \) and defined by [6]:

\[ adf \cdot g = [f, g] = \nabla g \cdot f - \nabla f \cdot g \]  

(10)
They are necessary, as stated forward, in order to determine the new set of state variables.

Repeated Lie brackets can be defined recursively by:

\[ a d_f^0 g = g \]  \hspace{1cm} (11)
\[ a d_f^i g = [f, a d_f^{i-1} g] = \nabla a d_f^{i-1} g f - \nabla f a d_f^{i-1} g \quad \text{for } i=1,2,... \]  \hspace{1cm} (12)

For the case investigated here one has \( n = 5 \) (five states). Therefore, applying (11) and (12) results:

\[ g = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \]  \hspace{1cm} (13)
\[ a d_f g = \begin{pmatrix} c_5 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \]  \hspace{1cm} (14)
\[ a d_f^2 g = \begin{pmatrix} c_6 \\ c_4 c_5 \\ -c_7 \\ -\alpha_1 c_4 c_5 \\ 2x_3 x_4 c_5 + c_8 \end{pmatrix} \]  \hspace{1cm} (15)

where:
\[ c_6 = c_7^2 c_5 - c_2 c_4 c_5 \]
\[ c_7 = c_1 c_4 c_5 + c_3 c_4 c_5 \]
\[ c_8 = \alpha_1 c_4 c_5 (\mu + c_1 + c_3) \]
\[ a d_f^3 g = \begin{pmatrix} c_9 \\ c_7 \\ -c_{10} \\ 2x_3 x_4 c_{11} + 2x_1 x_4 c_5^2 c_5 + 2x_3 x_5 c_4 c_5 + \alpha_1 x_3^2 c_4 c_5 + c_{12} \end{pmatrix} \]  \hspace{1cm} (16)

where:
\[ c_9 = c_1 c_6 - c_2 c_7 \]
\[ c_{10} = c_4 c_6 + c_3 c_7 \]
\[ c_{11} = c_7 + c_4 c_5 \mu - c_3 c_4 c_5 \]
\[ c_{12} = \alpha_1 (c_{10} - c_4 c_5 \omega_1^2) + c_8 \mu \]
The Nonlinear Control of a Slewing Flexible Beam Using the Feedback Linearization Technique

\[ \text{ad}_f^4g = \begin{cases} 
  c_{23} \\
  c_{10} \\
  -c_{24} \\
  2x_3x_4c_{22} - 4x_1x_4c_3^2c_5 - 4x_3x_5c_4c_5 - \alpha_1x_3^2c_4c_5 - c_{12} \\
  2x_1x_4c_{19} - 2x_3x_4c_{20} + 2x_3x_5c_{21} + 4x_1x_5c_3^2c_5 - 4x_3^2x_4c_4c_5 + x_3^2c_{17} - c_{18} 
\end{cases} \] (17)

where:
\[
\begin{align*}
  c_{13} &= c_4c_{11} - c_1c_3^2c_5 \\
  c_{14} &= c_3c_{11} + c_2c_3^2c_5 + c_4c_5\omega_1^2 \\
  c_{15} &= c_{11} - c_3c_4c_5 - c_4c_5\mu \\
  c_{16} &= c_{10} + c_{11}\mu \\
  c_{17} &= c_8 + \alpha_1c_4c_5\mu \\
  c_{18} &= c_8\omega_1^2 - c_12\mu - \alpha_1(c_4c_9 + c_3c_{10}) \\
  c_{19} &= c_{13} + c_3^2c_5\mu \\
  c_{20} &= c_{14} + c_4c_5\omega_1^2 - c_{16} \\
  c_{21} &= c_{15} + c_4c_5\mu \\
  c_{22} &= c_3c_4c_5 - c_{11} \\
  c_{23} &= c_1c_9 - c_2c_{10} \\
  c_{24} &= c_4c_9 + c_3c_{10}
\end{align*}
\]

4 Determination of the new set of state variables

The basic idea here is to simplify the form of the original nonlinear system’s dynamics by choosing a different state representation. In this sense, feedback linearization techniques can be viewed as ways of transforming original system models into equivalent models of a simpler form. In the case investigated here one needs five new states.

Let the first new state \( z_1 \) be given by:
\[
z_1 = x_2 + x_4 \tag{18}
\]

For the determination of the other four states, one must check the relative degree associated with this new state. The relative degree is defined as the integer \( r \) such that:
\[
\nabla z_1 \text{ad}_f^i g = 0, \quad \forall x \in U_0, \ 0 \leq i \leq r - 2 
\tag{19}
\]
\[
\nabla z_1 \text{ad}_f^{i-1} g \neq 0, \quad \forall x \in U_0 
\tag{20}
\]

where \( U_0 \) is a neighborhood of the origin.

Performing these calculations, one obtains:
\[
\nabla z_1 \text{ad}_f^0 g = \nabla z_1 g = 0 \tag{21}
\]
\[
\nabla z_1 \text{ad}_f^1 g = 0 \tag{22}
\]
\[
\nabla z_1 \text{ad}_f^2 g = c_4c_5 - \alpha_1c_4c_5 \neq 0 \tag{23}
\]
It shows that the new system presents, for this choice of $z_1$, relative degree 3 anywhere.

The next states $z_2$ and $z_3$ are then given by:

$$z_2 = \nabla z_1 f = x_3 + x_5$$

$$z_3 = \nabla z_2 f = (c_4 - \alpha_1 c_4)x_1 + (\alpha c_3 - c_3)x_3 - \omega_1^2 c_4 - \mu x_5 + x_3^2 x_4$$

The last two states, $z_4$ and $z_5$, can be chosen with some freedom but must be such that:

$$\nabla z_4 g = 0$$

$$\nabla z_5 g = 0$$

Then, the state $z_4$ is given by:

$$\nabla z_4 g = \begin{bmatrix} \frac{\partial z_4}{\partial x_1} & \frac{\partial z_4}{\partial x_2} & \frac{\partial z_4}{\partial x_3} & \frac{\partial z_4}{\partial x_4} & \frac{\partial z_4}{\partial x_5} \end{bmatrix} \begin{bmatrix} c_5 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

The only restriction for $z_4$ is that it can not be a function of the state $x_1$. Let, then:

$$z_4 = x_4$$

Making similar calculations, it can be also shown that $z_5$ can not be a function of the state $x_1$ and, then, let:

$$z_5 = x_5$$

Therefore, the new states are given by:

$$z = \begin{bmatrix} x_2 + x_4 \\ x_3 + x_5 \\ (c_4 - \alpha_1 c_4)x_1 + (\alpha c_3 - c_3)x_3 - \omega_1^2 c_4 - \mu x_5 + x_3^2 x_4 \\ x_4 \\ x_5 \end{bmatrix}$$

The Jacobian matrix of the transformation given by Equation (28) is given by:

$$J = \frac{\partial z}{\partial x} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ c_4 - \alpha_1 c_4 & 0 & \alpha_1 c_3 - c_3 + 2x_3 x_4 & -\omega_1^2 + x_3^2 & -\mu \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The determinant of the Jacobian matrix is given by:

$$\det(J) = c_4 - \alpha_1 c_4$$

which is always different to zero anywhere. Since this matrix is nonsingular one can prove that there really exists a region $U_0$ near the origin where the proposed transformation can be applied [4].
5 Determination of the inverse transformation

According to Equations (28):
\[
\begin{align*}
  z_1 &= x_2 + x_4 \\
  z_2 &= x_3 + x_5 \\
  z_3 &= (c_4 - \alpha_1 c_4)x_1 + (\alpha c_3 - c_3)x_3 - \omega_1^2 x_4 - \mu x_5 + x_3^2 x_4 \\
  z_4 &= x_4 \\
  z_5 &= x_5
\end{align*}
\] (29)

From the last two equations of (29) one has:
\[
\begin{align*}
  x_4 &= z_4 \\
  x_5 &= z_5
\end{align*}
\] (30) (31)

Substituting (30) in the first equation of (29) and solving for \( x_2 \) results:
\[
  x_2 = z_1 - z_4
\] (32)

Substituting (31) in the second equation of (29) and solving for \( x_3 \) results:
\[
  x_3 = z_2 - z_5
\] (33)

Substituting (30), (31) and (33) in the third equation of (29) and solving for \( x_1 \) results:
\[
  x_1 = \left( \frac{c_3 - \alpha_1 c_3}{c_4 - \alpha_1 c_4} \right) z_2 + \left( \frac{1}{c_4 - \alpha_1 c_4} \right) z_3 + \left( \frac{\omega_1^2}{c_4 - \alpha_1 c_4} \right) z_4 + \left( \frac{\alpha_1 c_3 - c_3 + \mu}{c_4 - \alpha_1 c_4} \right) z_5 - \left( \frac{1}{c_4 - \alpha_1 c_4} \right) (z_2^2 - 2z_2 z_5 + z_5^2) z_4
\] (34)

Therefore, the inverse transformation is given by Equations (34), (32), (33), (30) and (31).

Making the first time derivative of Equations (29) results:
\[
\begin{align*}
  \dot{z}_1 &= \dot{x}_2 + \dot{x}_4 \\
  \dot{z}_2 &= \dot{x}_3 + \dot{x}_5 \\
  \dot{z}_3 &= (c_4 - \alpha_1 c_4)\dot{x}_1 + (\alpha c_3 - c_3)\dot{x}_3 - \omega_1^2 \dot{x}_4 - \mu \dot{x}_5 + 2x_3 \dot{x}_3 x_4 + x_3^2 \dot{x}_4 \\
  \dot{z}_4 &= \dot{x}_4 \\
  \dot{z}_5 &= \dot{x}_5
\end{align*}
\] (35)

Using the original set of governing equations as given by Equations (2) one obtains:
\[
\begin{align*}
  \dot{z}_1 &= x_3 + x_5 \\
  \dot{z}_2 &= (c_4 - \alpha_1 c_4)x_1 + (\alpha_1 c_3 - c_3)x_3 - \omega_1^2 x_4 - \mu x_5 + x_3^2 x_4 \\
  \dot{z}_3 &= (c_4 c_5 - \alpha_1 c_4 c_5) U + (\alpha_1 c_3 c_4 - c_3 c_4 + \alpha_1 c_1 c_4 - c_1 c_4 + \mu \alpha_1 c_4) x_1 + (c_3^2 - \alpha_1 c_3^2 + \alpha_1 c_1 c_4 - c_2 c_4 - \mu \alpha_1 c_3) x_3 + (\mu \omega_1^2) x_4 + (\mu^2 - \omega_1^2) x_5 + 2c_4 x_1 x_3 x_4 - (2c_3 + \mu)x_3^2 x_4 + x_3^2 x_5
\end{align*}
\] (36) (37) (38)
\[ \dot{z}_4 = x_5 \]  
\[ \dot{z}_5 = -\omega_1^2 x_4 - \mu x_5 + \alpha_1 c_3 x_3 - \alpha_1 c_4 x_1 + x_3^2 x_4 \]  

Finally, using the inverse transformation, Equations (36) to (40) results:

\[ \dot{z}_1 = z_2 \]  
\[ \dot{z}_2 = z_3 \]  
\[ \dot{z}_3 = b_1 l + b_2 z_2 + b_3 z_3 + b_4 z_4 + b_5 z_5 + b_6 z_2^2 z_4 + b_7 z_2 z_4 z_5 + b_8 z_4 z_5^2 + z_2^2 z_5 - 2z_2 z_5^2 + z_2^2 + b_9 z_2 z_3 z_4 - b_9 z_3 z_5 z_4 + b_10 z_2 z_4^2 - b_{10} z_5 z_2^2 - b_9 z_2^2 z_4^2 z_5 - 3b_9 z_2^2 z_4 z_5^2 + b_9 z_4^2 z_5^3 \]  
\[ \dot{z}_4 = z_5 \]  
\[ \dot{z}_5 = b_{11} z_3 + b_{12} z_4 + b_{13} z_5 + b_{14} z_2^2 z_4 - 2b_{14} z_2 z_4 z_5 + b_{14} z_4 z_5^2 \]  

where:

\[ b_1 = c_4 c_5 - \alpha_1 c_4 c_5 \]  
\[ b_2 = (1 - \alpha_1)(c_2^2 - c_2 c_4) - c_3^2 (1 - \alpha_1) (c_3 - c_1) \]  
\[ b_3 = \frac{\mu \alpha_1 - (1 - \alpha_1)(c_1 + c_3)}{1 - \alpha_1} \]  
\[ b_4 = \frac{\mu \alpha_1 - \omega_1^2 (1 - \alpha_1)(c_1 + c_3) + \mu \omega_1^2 (1 - \alpha_1)}{1 - \alpha_1} \]  
\[ b_5 = \frac{(2\alpha_1^2 - \alpha_1 - 1)\mu c_3 + (\alpha_1 - 1)\mu c_1 + (c_1 c_3 + c_2 c_4)(\alpha_1 - 1)^2 - \omega_1^2 (1 - \alpha_1) + \mu^2}{1 - \alpha_1} \]  
\[ b_6 = \frac{(1 - \alpha_1)(c_1 + c_3) - \mu}{1 - \alpha_1} \]  
\[ b_7 = \frac{4\mu - 2(1 - \alpha_1)(c_1 + c_3)}{1 - \alpha_1} \]  
\[ b_8 = \frac{(1 - \alpha_1)(c_1 + c_3) - 3\mu}{1 - \alpha_1} \]  
\[ b_9 = \frac{2}{1 - \alpha_1} \]  
\[ b_{10} = \frac{2\omega_1^2}{1 - \alpha_1} \]  
\[ b_{11} = \frac{-\alpha_1}{1 - \alpha_1} \]  
\[ b_{12} = \frac{-\omega_1^2}{1 - \alpha_1} \]  
\[ b_{13} = \frac{-\mu}{1 - \alpha_1} \]
Making in Equation (43) the nonlinear control law equal to:

\[
U = -\frac{1}{b_7}(b_8z_2^2z_4 + b_7z_2z_4z_5 + b_8z_4z_5^2 + z_2^2z_5 - 2z_2z_5^2 + z_5^3 + \\
b_9z_2z_3z_4 - b_9z_3z_5z_4 + b_{10}z_2z_4^2 - b_{10}z_5z_4^2 - b_9z_2z_4^2 + \\
3b_9z_2^2z_4z_5 - 3b_9z_2z_4^2z_5^2 + b_9z_2^2z_5^3 - v)
\]

results:

\[
\begin{align*}
\dot{z}_1 &= z_2 \\
\dot{z}_2 &= z_3 \\
\dot{z}_3 &= b_2z_2 + b_3z_3 + b_4z_4 + b_5z_5 + v \\
\dot{z}_4 &= z_5 \\
\dot{z}_5 &= b_{11}z_3 + b_{12}z_4 + b_{13}z_5 + b_{14}z_2z_4z_5 + 2b_{14}z_2z_4z_5 + b_{14}z_4z_5^2
\end{align*}
\]

where v represents the linear control law.

### 6 Study of the zero dynamics

The dynamics which are made unobservable by the linearizing state feedback are called zero dynamics [4], [?]. Let the linear control law in the new coordinates be given by:

\[
v = -K_1z_1 - K_2z_2 - b_4z_4 - b_5z_5
\]

Let

\[
z_1 = z_2 = z_3 = 0
\]

Under these conditions one has:

\[
\begin{align*}
\dot{z}_4 &= z_5 \\
\dot{z}_5 &= b_{11}z_3 + b_{12}z_4 + b_{13}z_5 + b_{14}z_2z_4z_5
\end{align*}
\]

Equations (54) and (55) represents the governing equations of the zero dynamics. The next step is to verify the stability of this new system. In the neighborhood of the initial conditions \(z_4 = z_5 = 0\), for example, the eigenvalues of the Jacobian matrix for the system composed by Equations (54) and (55) are given by:

\[
\lambda = -\mu \pm \sqrt{\mu^2 - 4\omega_1^2(1 - \alpha_1)}
\]

The damping coefficient \(\mu\) is always > 0 and the expression

\[
\mu^2 - 4\omega_1^2(1 - \alpha_1)<0
\]

for a typical dynamic system is always < 0, which means that the zero dynamics is always stable.
7 Conclusions

Feedback linearization has been briefly presented and step by step applied to the tracking and vibration control of a flexible one-link manipulator. A state transformation and a linearizing feedback is developed in this work generating a new system of governing equations of motion. This new system proved to be partially linearized. The zero dynamics associated to this new set of equations is proved to be stable in the neighborhood of the origin.

References


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Application of method of special series for numerical and analytical research of nonlinear partial differential equations

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Abstract

Different constructions of special series with coefficients calculated recurrently are presented. This approach is used for the representation of solutions of a wide class of nonlinear equations of mathematical physics, in particular, for solutions of initial-boundary value problems.

1 Introduction

The most perspective direction of obtaining approximate solutions of nonlinear partial differential equations is combining numerical and analytical methods. Numerical methods are especially laborious in multidimensional case. Therefore, the development of different analytical methods started to construct solutions in a closed form and methods which allow one to find a solution with arbitrary preassigned precision, for example, in the form of series or asymptotic expansions.

The method of separation of variables is effective for linear equations [1]. Nevertheless, for general nonlinear equations this method allows one to obtain only restricted classes of solutions. Although using this method, which in this case may be called a generalized separation of variables method, interesting results for nonlinear problems were obtained concerning nonstationary dissipative structures [2, 3]. Methods of theory of dimensions, which lead to self-similar solutions [4], group methods [5, 6], methods of differential relations [7], method of degenerate hodograph [8, 9], and others turn out to be also effective for nonlinear equations. Investigating real processes, testing and comparing different numerical methods particular solutions obtained by this way are useful. However, as a rule exact solutions describe a class of physical processes restricted enough and to solve actual problems it is hardly to well manage with the obtained set of exact solutions.

The method of special series, whose development has been stimulated by the work of A.F. Sidorov [10], is included into another group of analytical approaches. The
main idea is to expand a solution in a power series with respect to one or several functions chosen in a special way [11, 12] (in the sequel, we call these functions basic). Such a choice, in contrast to the methods of Galerkin type, allows one to find solutions with a check accuracy because the used approaches leads to a chain of finite systems of differential equations, which are, as a rule, linear even for nonlinear equations to be solved, that allows one to obtain new results: in a number of cases it is possible to prove the global convergence even in nonrestricted domains [13, 14], where numerical methods meet essential difficulties. In constructing like this one only the first term of the series may be found as a solution of a nonlinear differential equation. In contrast to Taylor power series, which locally converge for equations of Kovalevskaya type [15] under assumption of analyticity of the problem initial conditions, the constructed special series may converge for wider classes of equations and systems. This special series may be also used for representation of solution of Kovalevskaya type equations but with nonanalytical initial conditions [16].

The approaches more closed to the special series method of obtaining solutions of partial differential equations are related with characteristic expansions investigated in the works of R. Courant [17], G.F. Duff [18], D. Ludwig [19], V.M. Babich [20, 21], A.A. Dorodnitsyn [22]. Further, the developed method of characteristic series for hyperbolic nonlinear equations allows one to solve a number of problems of mathematical physics, which cannot be solved earlier.

Similar ideas to represent solutions of nonlinear ordinary differential equations as a power series with respect to functions defined sequentially from another equations was considered by, for example, A.M. Lyapunov [23]. In this case series with recurrently computed coefficients are also obtained. Thus, in 1892 Lyapunov presented the general solution of an ordinary differential equations system

\[ \dot{x}_s = \lambda_s x_s + \sum_{m_1 + \cdots + m_n \geq 2} q^{(m_1, \ldots, m_n)}_s x_1^{m_1} \cdots x_n^{m_n}, \]

\[ x_s(0) = x_{s0}, \quad q^{(m_1, \ldots, m_n)}_s = \text{const}, \quad s = 1, n, \]

in the form of a convergent series

\[ x_s = u_s + \sum_{m_1 + \cdots + m_n \geq 2} \kappa^{(m_1, \ldots, m_n)}_s u_1^{m_1} \cdots u_n^{m_n}, \]

where \( u_s \) is a solution of the corresponding linear system

\[ u_s = \alpha_s \exp(\lambda_s t), \quad \alpha_s, \kappa^{(m_1, \ldots, m_n)}_s = \text{const}. \]

The convergence of this series is proved for any \( t \geq 0 \) under the assumption that \( \lambda_s < 0 \) and \( m_1 \lambda_1 + \cdots + m_n \lambda_n - \lambda_s \neq 0 \). In this example, the coefficients \( \kappa^{(m_1, \ldots, m_n)}_s \) are found recurrently and functions \( u_s \) are basic according to the terminology accepted in this paper.

Thus, a characteristic feature of special series is, in the formal point of view, that the form of the construction independent from the type of the equation to be solved (as a rule, the type of the equation is closely related with investigation of the convergence of the series).
Another direction in the method of special series is constructions of series on account of specific properties of investigated equations. For example, with the help of such special (consistent) series a class of solutions of the equation of the velocity potential described stationary gas flows was constructed in an axisymmetrical case [14] and the domain of convergence of this series was investigated. Also the logarithmic series [26] and [27] may be classified as a consistent series. In 1975, obvious poorness of the power series used separately was demonstrated for the problem of contiguity of double waves to the rest domain when it turns out that in the solution both the powers of characteristic variable and powers of its logarithms appear while a solution in the form of the power series does not exist.

The next stage of development of the method of special series is the constructions of series for which a known exact solution of the investigated equation suggested to be a zero term of the series. Further, taking into account specific features of initial equation and the chosen exact solution the basic functions have been constructed, which provide a recurrent calculation of the next coefficients of the series. In a certain sense, a “linearization” on the exact solution of the initial problem has been carried out. However, in this case new classes of solutions, which may depend on arbitrary functions, are obtained [28, 29]. At present, this direction is intensively developed.

Another field of application of special series is connected with the possibility of using them to solve initial-boundary value problems. In case zero boundary conditions are given, for a wide class of nonlinear equations it is possible to construct series converging to a solution of the problem and exactly satisfying the boundary condition [13] including two-dimensional complex domains [33].

Thus, the considered different constructions of special series turn out to be convenient apparatus for constructive investigation of the structure of solutions of nonlinear partial differential equations and allow one to prove theorems of the existence of solutions of initial-boundary value problems.

## 2 Method of special series

Before describing constructions of special series we pay attention to requirements which have to be satisfied with the series when solving differential equations and to difficulties which have to be overcome for effective application of the series. The basic requirements formulated by Sidorov [31] for such “useful” series are the following:

- the series have to converge in sufficiently large domains;
- the series have to converge fast (several first terms of the series are desirable to correctly represent a basic features of the solution);
- the coefficients of the series have to be computed with using non-expensive and effective algorithms;
- the construction of the series has to be applicable to a wide class of equations.
Taylor series (for equations of the Kovalevslaya type) and Fourier series (especially for linear equations of mathematical physics) are the most famous and applicable for representation of solutions of equations. However, as a rule Taylor series converge only locally and rather slowly, in a number of cases, and applying Fourier series for nonlinear equations leads to infinite systems of nonlinear equations for the coefficients; it is necessary to truncate these systems and obtain approximate values of Fourier coefficients.

To fulfill the requirements formulated above it is generally desirable to find the series coefficients not by successive differentiation (as for Taylor series) but by integration of simple recursive systems of ordinary differential equations. The constructions of series presented below satisfy the requirements to some extent.

Let us describe certain possible approaches to construct special series on the example of the following equation:

$$\frac{\partial u}{\partial t} = F(t, u, \ldots, \frac{\partial^{k_1 + \cdots + k_m} u}{\partial x_1^{k_1} \cdots \partial x_q^{k_m}}, \ldots),$$

(1)

where $F$ is a polynomial in $u$ and the corresponding partial derivatives with respect to $x_s$ and the coefficients are continuous and bounded functions for $t \geq 0$.

Consider the ring $K_t$ whose elements are multiple series in powers of functions $P_1(x), \ldots, P_m(x)$

$$u(x, t) = \sum_{|n|=0}^{\infty} g_n(t) \prod_{i=1}^{m} P_i^n(x),$$

(2)

which absolutely converge in some domain, where $\mathbf{x} = (x_1, \ldots, x_q)$, $\mathbf{n} = (n_1, \ldots, n_m)$, and $|\mathbf{n}| = n_1 + \cdots + n_m$.

Assume that the functions $P_1(x), \ldots, P_m(x)$ satisfy differential relations of the following form:

$$\frac{\partial P_i}{\partial x_s} = \sum_{j=1}^{m} a_{ij}s P_j + W_{is}(P_1, \ldots, P_m).$$

(3)

Here $a_{ij} = \text{const}$, $i = 1, m$, $s = 1, q$, and the functions $W_{is}(P_1, \ldots, P_m)$ are analytical with the conditions $W_{is}(0, \ldots, 0) = 0$, $\partial W_{is}(P_1, \ldots, P_m)/\partial P_j = 0$, $i, j = 1, m$, for $P_1 = P_2 = \cdots = P_m = 0$. Relations (3) imply that the ring $K_t$ is invariant with respect to the operation of differentiation with respect to $x_i$.

The following assertion is valid.

**Assertion.** For a suitable recurrence construction of the coefficients $g_n(t)$, the multiple series (2) is a formal solution of equation (1).

This assertion is proved in [32] and is verified by substituting series (2) into equation (1), differentiation, and multiplication of the series with taking into account relations (3). Then, equating expressions with the same powers of $P_1^n(x), \ldots, P_m^n(x)$ the series coefficients $g_n(t)$ are found from a sequence of ordinary differential equations. The equation for the free term $g_0(t)$ of the series may be nonlinear. Note that the recurrence of obtaining the coefficient of the series is achieved by a special
form of the linear part of system (3). The following numerical function setting an order of calculation of coefficients $g_n(t)$:

$$c(n) = \sum_{j=1}^{m-1} (m-2+j)n_{j+1} + \frac{1}{m} \prod_{i=0}^{m-1} \left( \sum_{j=1}^{m} n_{j+i} \right)$$  \hspace{1cm} (4)$$

Coefficient $g_{l_1}(t)$ is calculated before coefficient $g_{l_2}(t)$, if the inequality $c(l_1) < c(l_2)$ is carried out.

For double $(m = 2)$ special series and $q = 1$ (the case of one spatial variable $x$) this is proved in [24], where a solution of the initial equation is found in the form of a double series

$$u(x, t) = \sum_{m,n=0}^{\infty} a_{mn}(t)P^m(x)Q^n(x).$$

It was shown that if the basic functions $P(x)$ and $Q(x)$ satisfy the system of ordinary differential equation

$$P' = a_1P + b_1Q + c_1P^2 + d_1PQ + e_1Q^2 + \ldots = p(P, Q),$$ $$Q' = b_2Q + c_2P^2 + d_2PQ + e_2Q^2 + \ldots = q(P, Q),$$

then for $m + n = N$ ($N = 1, 2, \ldots$) the coefficients $a_{mn}(t)$ are found from a sequence of ordinary differential equations, whose right-hand sides nonlinearly include the coefficients $a_{mn}(t)$ for calculated previously $m + n < N$.

A more complicated example of basic functions for $m = 5$ and $q = 2$ which satisfy relations (3) is the system of functions

$$P_1(x_1, x_2) = \sin \left( \frac{\pi}{x_1^2 + x_2^2} \right), \quad P_2(x_1, x_2) = \cos \left( \frac{\pi}{x_1^2 + x_2^2} \right),$$ $$P_3(x_1, x_2) = \frac{x_1}{x_1^2 + x_2^2}, \quad P_4(x_1, x_2) = \frac{x_2}{x_1^2 + x_2^2}, \quad P_5(x_1, x_2) = \frac{1}{x_1^2 + x_2^2},$$

which is used in [33] to describe nonlinear oscillations of a film with the fixed boundary in the domain $x_1^2 + x_2^2 \geq \pi$.

The above considered constructions of series are more convenient for solving Cauchy problems when it is not necessary to satisfy boundary conditions. In [34] it is considered the question on the possibility of representing solutions of equation (1) by series with a more general than (2) structure

$$u(x, t) = \sum_{k \geq 0} u_k(t)P^k(x, t),$$  \hspace{1cm} (5)$$

or

$$u(x, t) = \sum_{m+n \geq 0} u_{mn}(t)P^m(x, t)Q^n(x, t)$$  \hspace{1cm} (6)$$
with functions $P$ and $Q$ including a functional arbitrariness. In [34] it is shown that if the basic function $P$ in (5) satisfies the differential equations
\[
\frac{\partial P}{\partial x} = \sum_{k=1}^{\infty} g_k(t) P^k, \quad \frac{\partial P}{\partial t} = \sum_{k=1}^{\infty} h_k(t) P^k,
\]
then the coefficients of series (5) are found recurrently representing solution of equation (1). To find the coefficients of series (5) the following chain of ordinary differential equation is obtained:
\[
u_0' = F(t, u_0, \ldots, 0, \ldots),
\]
\[
u_k' = F_k(t, u_k, \ldots, u_0) \quad k = 1, 2, \ldots.
\]
where the right-hand sides $F_k$ include only $u_j$ with $j \leq k$ and the coefficients $u_k$ may be contained only linearly. Note that the first term of the series $u_0$ is determined from the nonlinear differential equation (8), and all the subsequent coefficients $u_k$ are found as solutions of linear ordinary differential equations.

The simplest examples of basic functions $P$ including an arbitrary function $f(t)$ are presented in [34], where the case when series (7) are finite is considered. In particular, the basic functions may have the form
\[
P = (e^{bx} + f(t))^{-1}
\]
for case (5) and
\[
P = (c\chi bx + f(t))^{-1}, \quad Q = shbx(c\chi bx + f(t))^{-1}
\]
for case (6), where $b = \text{const}$. In what follows, the series in the powers of basic functions $P$ of type (10) are applied for initial-boundary value Cauchy problems in semibounded domains.

General scheme of the application of series (5) and (6). Let for the case of one spatial variable $x$ the initial conditions for equation (1) be representable in the form of a power series with respect to basic function $P$
\[
u(x, 0) = \sum_{k \geq 0} \varphi_k P^k(x, 0),
\]
where series (11) converges, for example, in a semibounded domain. Then, substituting series (5) into equation (1), equating expressions with the same powers of $P$, taking into account differential relations (7), we obtain a sequence of ordinary differential equations of the form (8) and (9) to calculate the coefficients $u_k(t)$ of the series. The constants $\varphi_k$ in (11) set initial conditions for these equations. The following problem is to investigate the convergence of the constructed in such a way formal solution of equation (1).

For the first time convergence of special series with functional arbitrariness was proved in [35]. In particular, it was shown that a solution of the Korteweg–de Vries (KdV) equation is representable in the form of series (5), (10) and converges in the semibounded domain for $x \leq 0, \ t \geq 0$.

To describe the field of application of special series of the form (5), (6) Sidorov proposed [34, 31] the hypothesis that functional arbitrariness contained in basic functions may be used.
• to prove and to accelerate the convergence of special series,
• to satisfy a given boundary condition,
• to obtain exact solutions.

At present, there is no complete answer to the first and third questions. There is a number of model equations for which it is shown that choosing the arbitrary function the special series possible both to be made convergent in the whole domain (to obtain a global solution of the Cauchy problem) and to be made nonconvergent [14]. There are obtained the positive answer to the second question [36].

The convergence of special series is established for a wide class of nonlinear equations and systems which occur in continua media mechanics [12, 13, 14, 25, 26].

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Application of method of special series for numerical and analytical research


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Effect of Statistical Distribution of Grain Properties on Development of Free Surface Roughness

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Abstract

Microforming is an important technology to fabricate very small metal components, which are required in many industrial products. In particular, microtube is commonly used and required for micro components, for example micro nozzle, painless needle, micro exchanger and micro reactor. However, it is not easy to scale down the conventional process to micro-scale. It is increasingly difficult to fabricate a micro tool with high accuracy, and to insert a plug and a mandrel into a microtube. Dieless drawing process without tools and dies was applied to fabricate the microtubes by authors. However, surface smoothing by sliding with die cannot be expected in the dieless drawing process. Roughening phenomenon on free surface is the overwhelmingly dominant factor in case of the dieless drawing process. Thus, the prediction of surface roughness evolution on the free surfaces is an important, particularly, in the case of the deformation at large strain in dieless drawing process. In this study, the roughness evolution on the free surfaces is calculated by mesoscopic FE (finite element) analysis considering grains located near the free surface. Roughening phenomenon occurred due to inhomogeneity on the basis of the grain orientation in the material. In this model, each grain has different material properties on the basis of the grain orientation. Furthermore, strain rate sensitivity and strain hardening sensitivity of the grains was assumed in this model. Particularly, the effect of statistical distribution of grain properties on development of the free surface roughness was investigated.

1 Introduction

Fabrication and application of micro electro-mechanical system (MEMS) for mechanical sensors and actuators have attracted attention in this decade. Microforming is an important technology to fabricate very small metal components, which are
required in many industrial products [1]. Recently, the demand of miniaturization comes from technical applications such as electronic devices, medical equipment, sensor technology and optoelectronics. These kinds of micro devices are mainly made of silicon or glass and these devices are fabricated by semiconductor manufacturing technology. However, the semiconductor manufacturing has many issues such as limitation of applicable materials and manufacturing device with high cost. Recently, the development of a novel micro metal forming technology with high productivity, which a large number of smallest metallic parts can be produced, is needed. In scaling down the dimensions of conventional metal forming technology, various influential factors must be considered. So far, many studies on micro forming have been conducted from the aspects of materials, working processes, and processing machines [2-4].

On the other hand, in the miniaturization of sheet metal forming technology, the proportion of surface roughness of the material to total thickness becomes larger with decreasing sheet thickness, which must be considered as non-uniformity of the thickness. Particularly, the surface roughness on the free surface, which the materials come in non-contact with tools, increases during the deformation. That is to say, on the micro-scale region, the surface roughness of the material is thought to be the important process factor related to formability in micro scale. It is well-known that grain size and crystal structure affect the roughness evolution and the formability of the material [5-7]. However, it is not clarified that the effect of mechanical properties of materials such as strain hardening sensitivity and strain rate sensitivity on roughening evolution.

In this study, finite element (FE) simulation considering grain was performed for the prediction of the evolution of the surface roughness with plastic deformation. Particularly, the effect of statistical distribution of grain properties on development of free surface roughness was investigated.

2 Roughness evolution on free surface

When forming a sheet metal, the free surface of the sheet becomes rough with increasing plastic strain. This is well-known as "roughening phenomenon on free surface" and has a great effect not only on the surface quality of a product, but also on the forming limit. Therefore, the surface roughening is one of the important problems in sheet metal forming. In particular, in micro materials such as thin sheets and foils used in micro forming. In micro-scale, the forming limit of the thin sheets and foils decrease because the surface roughness and asperities of the micro materials is regarded as the variation of the thickness of the micro materials. Because, the surface roughness gradually increases with increasing plastic strain, and a localized necking begins to develop from the deepest trough of surface asperities.

Roughening phenomenon on the free surface in polycrystalline metal during plastic deformation is closely related to the inhomogeneous deformation in the respective grain at the surface [8]. It is known that the inhomogeneous deformation is caused by the difference in crystal orientation of each grain at the surface. Many experimental studies have been carried out that the roughening phenomenon on free surface are greatly influenced by the grain size and crystal structure. These two parameters
have been shown by Yamaguchi et al. [5-8] that the roughness on free surface of material increases approximately in proportion to the magnitude of the equivalent plastic strain and to the grain size. The following equation was obtained experimentally and is given as [5]

\[ R = c d_g \varepsilon_{eq} + R_0 \]  

(1)

where \( R \), the surface roughness exiting at the equivalent strain \( \varepsilon_{eq} \); \( R_0 \) the initial surface roughness of the undeformed material; \( d_g \) the average grain diameter of the undeformed sheet; \( c \), crystal structure index. The Eq. (1) is in large disagreement with the experimental results at large plastic strain. Yamaguchi et al. carried out a deep drawing experiment with rubber tools to investigate the free surface roughening behavior [5]. The results showed that surface roughness did not increase linearly for \( \varepsilon_{eq} \geq 0.6 \), and the rate of surface roughness decreased with the increase in \( \varepsilon_{eq} \). Additionally, we investigated the roughening phenomenon on free surface during multi-pass dieless drawing process for microtubes [4]. The results showed that the surface roughness of the microtubes decreases gradually and converges to a value at large plastic strain. These phenomena can be explained by Eq. (2) considering the ratio of change in surface area \( S_0/S_1 \) expressed by Osakada et al [6].

\[ R = c d_g \frac{S_0}{S_1} \varepsilon_{eq} + R_0 \]  

(2)

\( S_0/S_1 \) represents \( \exp(-\varepsilon_{eq}/2) \) in the case of tensile deformation. Previous reports point that the roughening phenomenon on free surface is only depending on grain size \( d_g \), crystallographic factor \( c \) and equivalent strain \( \varepsilon_{eq} \).

3 FE Simulation

3.1 FE model

For the simulation of surface roughening behavior, an FE simulation considering crystal grains is performed [9]. The roughening phenomenon on the free surface during plastic deformation is modeled using Marc/Mentat ver.2005. A simple model of a sheet used for the simulation is shown in Figure 1. One of the parts of the material assuming plane strain tensile deformation is modeled. In this model, crystal grains are assumed to be square, 25\( \mu \)m in side length as shown in Figure 2. A square group of 4 \( \times \) 4 elements is given the same material properties. The crystal grains are modeled in neighborhood free surface because internal crystal grain in the material does not influence the roughness behavior on the free surface [10]. The length of the layer from the free surface which the crystal grains are considered is 125\( \mu \)m in this model. The sheet is deformed at 5\( \mu \)m/s to the X-direction.

3.2 Material model of crystal grains

For the prediction of the roughening phenomenon on the free surface with plastic deformation, it is essential to take into consideration the inhomogeneity of material.
The flow stress of crystal grains included in a material differs from grain to grain. That is to say that the spread of crystallographic grain orientations is simulated by ascribing different material properties to each grain, with statistical distribution chosen at random. In this paper, each grain is treated as rigid-plastic, with strain hardening sensitivity as shown in Eq. (3).

\[ \sigma = \alpha K \epsilon^n \]  

K value is the average strength coefficient of grains. In other words, this means that K value is homogeneous strength coefficient macroscopically. However, the material is inhomogeneity microscopically, because the crystal grains differ from grain to grain due to crystal orientation. So, Crystal grain with individual strength coefficient for each grain must be assigned. In this model, strength coefficient ratio \( \alpha \)-value was considered for each grain. In addition, the distribution of strength coefficient ratio depends on microscopic properties of materials. In this model, the three types of statistical distribution of strength coefficient ratio(\( \alpha \)-value) were defined as shown in Figure 2, which are assumed by changing arbitrarily the crystal orientation to the tensile direction. Three conditions of statistical distribution, where the minimum and maximum value are from 0.8 to 1.2, 0.6 to 1.4 and 0.4 to 1.6. In these models, average strength coefficient ratio(\( \alpha \)-value) were 1.0. This means that these materials with Type 1, 2 and 3 are equivalent macroscopically. Figure 3 shows a example model of statistical distribution of the \( \alpha \)-value of each crystal grain. Strain hardening sensitivity index (n-value) of each crystal grain is not varied on the basis of flow stress of single crystal [8, 11]. Additionally, note that crystal rotation and grain sliding is not considered and modeled in this model, because the
problem becomes complex and excessive computational resources needed.

Figure 2: Probability distribution used for strength coefficient ratio

4 Results and Discussion

4.1 Effect of variation in strength coefficient ratio of grain

The effect of variation in the strength coefficient ratio $\alpha$ on roughness evolution on the free surface was investigated. Figure 4 shows the relationship between arithmetical mean roughness $Ra$ and equivalent strain $\varepsilon_{eq}$ for the model with probability distribution of Type 1. The rate of increasing in surface roughness $Ra$ increases with increasing in the range of variation in strength coefficient ratio $\alpha$. On the contrary, The rate of increasing in surface roughness $Ra$ decreases with decreasing in the range of variation in strength coefficient ratio $\alpha$. The rate of increasing in the surface roughness for the model with $0.4 \leq \alpha \leq 1.6$, 3 times bigger than the one for the model with $0.8 \leq \alpha \leq 1.2$. This means that the rate of increasing in surface roughness is large because the variation in strength coefficient ratio $\alpha$ in case of the large difference in crystal orientation of each grain.
Effect of Statistical Distribution of Grain Properties on Development of Free Surface Roughness

Figure 3: FE models of sheet considering crystal grains used

Figure 4: Effect of strength coefficient ratio on roughness evolution on free surface
4.2 Effect of probability distribution of strength coefficient ratio of grain

Effect of probability distribution of strength coefficient ratio of grains on roughness evolution on the free surface was investigated. Figure 5 shows the relationship between arithmetical mean roughness $Ra$ and equivalent strain $\epsilon_{eq}$ for the model with probability distribution. Types 1, 2 and 3 of probability distribution with variation in strength coefficient $\alpha$ of grains from 0.6 to 1.4 as shown in Figure 2 were used in the simulation. It is found that the rate of increasing surface roughness was depends on the probability distribution of grains. The rate of increasing surface roughness of Types 1 and 2 probability distributions shows a similar tendency up to equivalent strain $\epsilon_{eq}$ of 0.5. The rate of increasing surface roughness of Type 2 were less than one of Types 1 and 3. Therefore, in case of uniform distribution of strength coefficient ratio of grains as Type 2, the rate of increasing surface roughness becomes decreasing. Thus, if materials have same grain size, the rate of increasing surface roughness can be changed depending on probability distribution on grains. However, it is found that the effect of variation in strength coefficient ratio of grains has greater effect on roughness evolution on free surface as shown in Section 4.1 compared with the effect of probability distribution of strength coefficient ratio.

![Figure 5: Effect of probability distribution of strength coefficient ratio of grains on roughness evolution on free surface](image)

5 Conclusion

In this paper, FE simulation considering grain was performed to predict the evolution of the surface roughness with plastic deformation. We focus on the effect of statistical distribution of the strength coefficient of grains on roughening phenomenon on the
free surface of materials. As a results, the rate of increasing in the surface roughness increases with increasing in the range of variation in the strength coefficient ratio of grains. Furthermore, the rate of increasing surface roughness can be changed depending on probability distribution on grains. In addition, the effect of variation in the strength coefficient ratio of grains has greater effect on roughness evolution on the free surface compared with the effect of probability distribution of strength coefficient ratio.

Finally, for the prediction of the roughness evolution on the free surface, to clarify the statistical distribution of the strength coefficient ratio of the grains due to inhomogeneity in materials is important. In the future, it should be considered essential to obtain the statistical grain properties quantitatively.

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Nonlinear highly elastic-plastic model of continuum with volume changing under deformation

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Abstract

The phenomenological model of structurally heterogeneous media capable to carry significant nonlinear elastic and plastic deformations accompanied with appreciable volume change is developed. Nanocomposites on a basis of polyolefine matrix and lamellar silicate filler belong to these systems.

The computational scheme of this model consists of two elements connected in tandem: elastic and plastic. It is assumed that only the elastic element answers for the volume change. The elastic potential for compressible continuum is written down as the sum of two parts responsible for the shape and volume changes separately. The plastic element behavior is defined by the classic plastic flow theory.

The given approach was used for description and comparison of mechanical properties between pure polyethylene and polyethylene/clay nanocomposite. Numerical dependences between stresses, relative volume change and deformation of material were constructed. The results obtained in modeling have provided an explanation how the process of elastic-plastic deformation in such "compressible" systems develops.

The phenomenological model of mechanical behavior of polymer/clay nanocomposites is evolved. The material is considered as a nonlinear elastic-plastic medium changing its volume as a result of damage accumulation. These systems represent a mix of thin silicate nano-scale lamellas arbitrarily located in polymeric matrix. Particles can form separate packs from several parallel located lamellae (intercalated filler) or to be distributed on material volume chaotically (exfoliated filler) [1].

It is experimentally established that such nanocomposite systems can change essentially their volume under deformation due to accumulation of internal defects. A relative volume change can reach 20-25% at ultimate deformations 700-800%. This approach allows modeling mechanical behavior of such materials with good accuracy.

To obtain the constitutive equations, the differential approach based on interpretation of the mechanical behavior of material with the help of symbolical circuits
Figure 1: The symbolic circuit of elastic - plastic model

and the additive decomposition of the rate of deformation tensor in elastic and plastic parts is used [2]. Constitutitional equations are written down without objective derivatives from the stress tensor. Therefore a question on a choice, in what kind of them to write down, does not arise. The given technique is able to describe not only hardening of a material at plastic flow, but also its softening (descending branch of a stress-strain curve). Mathematical expressions used in the model can be essentially nonlinear.

The computational scheme of this model consists of two elements connected in tandem: elastic and plastic (by analogy to Prandtl model). It is shown on fig. 1. Here point \( A \) defines the general mechanical behavior of a material, \( B \) — connects elastic and plastic elements, \( C \) — is fixed. The tensors of rate of deformation for elastic and plastic elements can be calculated under the following formulas

\[
D_A = D, \quad D_B = D_A - D_1 = D_2, \quad D_C = 0,
\]

where \( D \) — rate of deformation tensor of the whole system and only this one can be expressed through a deformation gradient \( F \) of continuum. According to the tandem circuit stress tensors in elements should be identical and equal to total medium stress tensor \( T \).

The conventional equations of the nonlinear theory of elasticity for compressible medium are used for the description of mechanical properties of the elastic element. The elastic potential for the "compressible" medium is written down as the sum of two summands \( w^* \) and \( w^+ \). If the volume of a body does not vary \( (V = V_0 = \text{const}) \) that \( w^+ = 0 \), at all-round hydrostatic expansion \( w^* = 0 \). For maintenance of this condition a new "normalized on volume" variable is entered

\[
\alpha_i = \frac{\lambda_i}{J^{1/3}} = \frac{\lambda_i}{(\lambda_1\lambda_2\lambda_3)^{1/3}}, \\
w = w^* (\alpha_1, \alpha_2, \alpha_3) + w^+ (J),
\]

where \( J = \lambda_1\lambda_2\lambda_3 \) - relative change of volume, \( \lambda_i \) - stretch ratios. The idea of normalization of independent variables is frequently applied to the description of elastic behavior of compressible media [3].

Function \( w^* \) for the "compressible" elastic environment is set as power-mode potential

\[
w^*_N = C_N \left(\alpha_1^N + \alpha_2^N + \alpha_3^N - 3\right) = C_N \left(J^{-N/3}\text{tr} (V^N) 3\right),
\]

where \( V \) — left stretch tensor, \( N \) can be as the whole, and fractional number. Modeling calculations were carried out for value \( N = 2 \).
Assuming, that the dependence between average stress and volumetric deformation is linear, volumetric function \( w^+ \) is taken in the following kind
\[
w^+ = \frac{K}{2} (J - 1)^2 = \frac{K}{2} (\lambda_1 \lambda_2 \lambda_3 - 1)^2, \tag{4}\]
where \( K \) — elastic bulk modulus.

Deformation of a nonlinear elastic element is set with the help of the evolutionary equation (5) through a material derivative from Cauchy-Green tensor \( B_1 = V_1^2 \).
\[
\frac{DB_1}{Dt} = \dot{B}_1 + B_1 W_R - W_R B_1 = 2V_1 D_1 V_1, \tag{5}\]
where \( W_R = \dot{R} R^T \) — medium spin tensor, \( R \) — rotation tensor in the left polar decomposition \( F = VR \) of the deformation gradient of the medium.

Mechanical properties of a plastic element are defined by analogy to basic equations of plastic flow by Prandtl - Reuss [4]. The dependence between stress tensor deviator \( T_2 \) and rate of plastic deformation tensor \( D_2 \) is taken in the following kind
\[
D_2 = \sqrt{\frac{D_2 \cdot D_2}{\text{dev} \ T_2 \cdot \text{dev} \ T_2}} \text{dev} \ T_2. \tag{6}\]

As in the right part of this formula stress deviator \( T_2 \) stands, for tensor \( D_2 \) the condition
\[
\text{dev} \ D_2 = D_2 \tag{7}\]
should satisfy. The spherical part of stress deviator \( T_2 \) by definition is equal to zero, so it should be equal to zero and trace \( D_2 \). Otherwise there is a contradiction. Thus, with the help of expression (7) it is postulated, that all plastic deformations arising in a material occur for the account shape distortion. Change of volume is provoked only by elastic deformations. It, by the way, is completely be coordinated to base positions of the classical theory of plasticity.

Expression (6) contains uncertainty. For its disclosing one more dependence between \( D_2 \) and \( \text{dev} \ D \) (that can be measured in experiment) has been entered. Considered, that they are connected by a proportional ratio
\[
D^{(2)}_{\text{int}} = \sqrt{D_2 \cdot D_2} \equiv \sqrt{\text{dev} D_2 \cdot \text{dev} D_2} = \kappa \sqrt{\text{dev} D \cdot \text{dev} D} = \kappa D_{\text{int}} \tag{8}\]
where \( \kappa \) — non-negative parameter. If \( \kappa = 0 \) the material behaves as only elastic, at \( 0 < \kappa < 0 \) — as elastic - plastic with hardening, a case when \( \kappa = 1 \) corresponds to ideal plasticity and, at last, at \( \kappa > 1 \) true stress - strain curve becomes descending, i.e. a material softening is observed. It is visible from the formula (8), that this parameter connects the expressions similar classical intensities of stress tensor and tensor of small deformations (to within constant multiplication factor). Therefore \( D^{(2)}_{\text{int}} \) and \( D_{\text{int}} \) also have been named as intensities of tensors \( D_2 \) and \( D \). In model parameter \( \kappa \) is set through yield function \( \Phi_2 \) as
\[
\kappa = \begin{cases} 
0, & \Phi_2 (V) < q_2, \\
\sigma (q_2), & \Phi_2 (V) = q_2, 
\end{cases} \tag{9}\]
where \( q_2 = \max \Phi_2(V) \), \( V \) — left stretch tensor from polar decomposition of deformation gradient \( F = VR \).

It is considered, that \( \Phi_2 \) only from tensor \( V \) (dependences on other parameters of medium state were not examined). In this case it is a hyper-surface of plasticity in space of the deformations. Thus, plastic deformation occurs only in case when \( \Phi_2 \) has the maximal value for all previous history. In the model the parameter \( \Phi_2 \) has been taken as

\[
\Phi_2 = \sqrt{\text{dev} V \cdot \text{dev} V} = \left(1/\sqrt{3}\right) \sqrt{(\lambda_1 - \lambda_2)^2 + (\lambda_2 - \lambda_3)^2 + (\lambda_3 - \lambda_1)^2}. \tag{10}
\]

For uniaxial stretch of a compressible material one can receive from (10)

\[
\lambda_1 = \lambda, \lambda_2 = \lambda_3 = \sqrt{J/\lambda} \Rightarrow \Phi_2 = \sqrt{2/3 \left(\lambda - \sqrt{J/\lambda}\right)}. \tag{11}
\]

Thus, it is necessary to know dependence \( \zeta(q_2) \) for the description of plastic behavior of a material. This information was received from the analysis of experimental data.

Experimental curves of uniaxial loading for pure polythene and polymer/clay nano-composite its basis have been theoretically investigated with the help of the given approach. Works on synthesis and an experimental research of mechanical properties such composite materials have been executed in the Institute of Petrochemical Synthesis RAS (Moscow) \[5\]. These experiments also have shown that rather significant dilatation is observed under deformation. Most likely, it is connected with development of internal damage accumulation.

The experimental data represented dependences of true (\( \sigma \)) and nominal (\( \sigma^0 \)) tensile stresses on stretch ratio (\( \lambda \)), i.e. from their comparison it is possible to receive the information on change of a specimen volume. Polyethylene of high density (PE) was used as a matrix. Sodium montmorillonite (\( \lambda \)), modified by superficial active substances was taken as a filler. The examined composite contained 2% in mass of the filler in intercalated state. The average size of particles was about 80 nm in diameter and few 1-10 nm thin.

Modeling dependences of true (\( \sigma \)) and nominal (\( \sigma^0 \)) tensile stresses on specimen main stretch ratio (\( \lambda \)), are shown in fig. 2. Modeling curves practically coincide with experimental ones (distinction is no more than one percent). It is necessary to note, that on an interval \( 1.5 < \lambda < 5.5 \) the necking-down and propagation in the specimen was observed. So the greatest real interest represent initial (\( \lambda < 1.5 \)) and final (\( \lambda > 5.5 \)) parts of plots.

Deformation dependences of parameter \( \kappa(\lambda) \), describing a ratio between plastic and total medium deviators of rate of deformations tensors are shown in fig. 3. Fig. 4 shows how the bulk module of material \( K \) changes at sample stretching.

Parameters \( \kappa \) and \( K \) allow to understand, how plastic flow is developing in the medium examined. Also they help to estimate the volume change that develops in the material, which can be caused in polymers both by development of internal damage accumulation, and by other structural reorganizations (crystallization, reorientation of an arrangement of nano particles and polymeric molecules at deformation, etc.) Thus, the given model could be used in investigation the internal structural transformations occurring in so specific polymeric materials.
Nonlinear highly elastic-plastic model of continuum with volume changing under deformation

Figure 2: Modeling dependences of true (solid lines) and nominal stresses (dashed lines)

Figure 3: Modeling dependences of parameter $\kappa$ on specimen stretch ratio

Figure 4: Modeling dependences of bulk modulus $K$ on specimen stretch ratio
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References


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Experimental and theoretical research of elastic-viscous-plastic properties of polymeric composites with clay lamellar nanofiller

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Abstract

A method of constructing the system of constitutive equations for incompressible nonlinear dissipative materials capable of working under finite deformations was developed. This method was applied to develop models describing the behaviour of polyethylene. Suggested models simulated with a good accuracy the viscoplastic properties of polyethylene under cyclic deformation with time interval of stress relaxation.

A method of constructing the system of constitutive equations for incompressible nonlinear dissipative materials capable of working under finite deformations was developed. To construct the constitutive equations, a phenomenological scheme for the mechanical behaviour of the material was used. The points on this scheme are connected by elastic, viscous, plastic elements. The material properties of each of the scheme elements are described by the known equations of the nonlinear elasticity theory, the theory of nonlinear viscous fluids and the theory of plastic flow under finite deformations. To complete the system of constitutive equations it is suggested to use a proportional relation between the strain rate tensor of the material and the strain rate tensors of plastic elements.

In the model we do not use the concept of deformation gradients for internal points in the scheme for the mechanical behaviour of the material. Therefore it is impossible to use multiplicative decomposition of the deformation gradient of the material into the product of deformation gradients of scheme elements. Instead, for creation of the mathematical model the hypothesis about additive decomposition of the rate of deformation tensor of the medium into the rate of deformation tensors of the elements is used.

The mathematical model describing the mechanical behavior of the polyethylene is schematically represented in fig. 1. The system of constitutive equations is constructed in correspondence with following rules:
1. To each point of the scheme the rate of deformation tensor of this point is assigned, which plays the role of a tensor parameter necessary for construction of the mathematical model.

2. The Cauchy stress tensor and the rate of deformation tensors are assigned to the elastic, viscous and plastic elements of the scheme.

3. It is assumed that the rate of deformation tensor of the left point of the scheme coincides with the rate of deformation tensor $D$ of the medium, and the rate of deformation tensor of the right point of the scheme is equal to zero.

4. The rate of deformation tensor of elastic, viscous and plastic elements is calculated as the difference between the rate of deformation tensors of the left and right points of these elements.

5. The material is assumed to be incompressible. The trace of any rate of deformation tensor in the model is equal to zero.

6. The Cauchy stress tensor $T$ of the medium is equal to the sum of the Cauchy stress tensors of elastic elements connected with the left point of the scheme.

7. The sum of the Cauchy stress tensors of elastic, viscous and plastic elements connected on the left with any inner point of the scheme is equal to the sum of the Cauchy stress tensors of elastic, viscous and plastic elements connected on the right with this point of the scheme.

Our investigation focuses on the study of isothermal processes. To describe the properties of elements shown in the scheme, the known formulas from continuum mechanics are used. For calculation of the Cauchy stress tensors $T_i$ of elastic elements, we take the mass density of free energy $f$, which is the function of stretch ratios of all elastic elements 

$$f = f(\theta, \ldots, \lambda_1^{(i)}, \lambda_2^{(i)}, \lambda_3^{(i)}, \ldots),$$

where $\lambda_1^{(i)}, \lambda_2^{(i)}, \lambda_3^{(i)}$ are the stretch ratios for the $i$-th elastic element. This means that the deviator of the Cauchy stress tensor of the $i$-th elastic element should be calculated by the formula of the nonlinear elasticity theory 

$$\text{dev} T_i = \text{dev} \left( \rho \sum_{k=1}^{3} \lambda_k^{(i)} \frac{\partial f}{\partial \lambda_k^{(i)}} n_k^{(i)} \otimes n_k^{(i)} \right),$$

$$\text{dev}(\cdot) = (\cdot) - \frac{1}{3} \text{tr}(\cdot),$$
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Figure 2: Comparison of theoretical (solid line) and experimental data (dashed line) for polyethylene under cyclic deformation with 10 minutes of stress relaxation at maximum and minimum values of material stretches on each cycle

where $\rho$ is the mass density of the material, and $n_1^{(i)}$, $n_2^{(i)}$, $n_3^{(i)}$ form an orthonormal triple of eigenvectors of the stretch tensor $V_i$ of the elastic element. $V_i = \lambda_1^{(i)} n_1^{(i)} \otimes n + \lambda_2^{(i)} n_2^{(i)} \otimes n_2^{(i)} + \lambda_3^{(i)} n_3^{(i)} \otimes n_3^{(i)}$.

For the $i$-th elastic element, the material time derivative of the stretch tensor $\dot{V}_i$ is calculated by equation:

$$2 V_i D_i V_i = \left( V_i^2 \right)^\cdot - V_i^2 W_R - W_R V_i^2,$$

$$W_R = \dot{R} R^T,$$

where $R$ is the rotation tensor in the polar decomposition $F = VR$ of the deformation gradient of the medium $F$ into the left stretch tensor $V$ and the rotation $R$.

The known equations of the nonlinear elastic theory describing the time variation of stretch ratios of the $i$-th elastic element

$$\dot{\lambda}_k^{(i)} = \lambda_k^{(i)} n_k^{(i)} \otimes n_k^{(i)} \cdot D_i, \quad k = 1, 2, 3$$

and the rate of work in this element

$$T_i \cdot D_i = \rho \sum_{k=1}^3 \frac{\partial f}{\partial \lambda_k^{(i)}} \dot{\lambda}_k^{(i)}$$

are the consequences of equation (1).
The deviator of the Cauchy stress tensor of the $j$-th viscous element is calculated by the formula from the theory of nonlinear viscous fluids

$$\text{dev} \mathbf{T}_j = 2\eta_j \mathbf{D}_j,$$

where the shear viscosity coefficient is the non-negative function of state parameters $\eta_j \geq 0$.

The deviator of the Cauchy stress tensor of the plastic element is calculated by the formula of the plastic flow theory

$$\mathbf{D}_n = \sqrt{\frac{\mathbf{D}_n \cdot \mathbf{D}_n}{\text{dev} \mathbf{T}_n \cdot \text{dev} \mathbf{T}_n}} \text{dev} \mathbf{T}_n,$$ \hspace{1cm} (2)

where $n$ is the number of the plastic element. For modeling the plastic flow process, it is necessary to exclude the ambiguity in expression (2). To this end, it is offered to use the mathematical expression which links the rate of deformation tensor of the plastic element with the rate of deformation tensor of the medium:

The symbol $\kappa_n$ designates the non-negative function of state parameters. When calculating, we assume that plastic flow is possible under the following condition:

$$\max \text{inv}(\mathbf{T}_n) = \text{inv}(\mathbf{T}_n),$$ \hspace{1cm} (3)

where

$$\text{inv}(\mathbf{T}_n) = \sqrt{\text{dev} \mathbf{T}_n \cdot \text{dev} \mathbf{T}_n},$$

i.e., when the invariant of stresses in the appropriate plastic element is equal to the maximum of this invariant in the considered element during the whole deformation history of the medium.

The method of constructing the system of constitutive equations was applied to develop models describing the behaviour of polyethylene (fig. 1). Suggested models simulated with a good accuracy the viscoplastic properties of polyethylene under cyclic deformation with time interval of stress relaxation (fig. 2).

The tensor equations describing those or other properties of material stand behind each element on the circuit. Elements 1 and 3 model the behavior of a rigid nano-structure skeleton formed in polymer by spherulites or some other supramolecular formations in. Deformation of material provokes its destruction. It is well visible on reduction of the initial module of an element 1 at deformation of medium (fig. 3). Except for it the relative positioning of spherulites also varies. The growth of residual deformations in a material indicates this phenomenon (fig. 4). It is interesting to note, that the plastic flow in polythene starts practically from the very beginning of material loading. There are no parts of the load curve where only elastic properties are demonstrated.

Elements 2 and 4 model the flow of a complex viscous liquid inside a material. Most likely, it is an amorphous part of polymer. Such flows can be seen between lamellae inside spherulites (one scale level) and in spaces between spherulites (another scale level).

The conclusion. The suggested mathematical model is capable not only to describe mechanical polythene behavior, but also allows to receive some important information about multi-scale structural processes in material.
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Figure 3: Initial module of the element 1 descending under deformation

Figure 4: Dependence between the residual stretch ratio of material after relaxation and maximal stretch ratio of the specimen attained during the load process
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Tensile strength calculations in simulated cohesive granular assemblies

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Abstract

An intrinsic and essential feature of powders is their ability to resist an applied tensile pressure. This macroscopic resistance has its origin in the attraction due to the van der Waals force existing between individual grains. After the analysis using the Discrete Elements Method, we report some preliminary results obtained from applying progressive leaps of tensile pressure on different granular assemblies, until the breakage of the structure occurs. A continuous and slow isotropic rate stress is also imposed to investigate the breakage. We focus our attention on three related issues: (i) the dependence between the maximum tensile stress resisted and the initial degree of bulk compactness, (ii) the effect of two different procedures to induce the structural stretching until the breakage, and (iii) the adequacy of simplified models commonly used to predict the typical intergranular force in non-cohesive granular materials (Rumpf, 1958). In that respect, since the very loosely cohesive simulated packings present a numerically computable porous distribution, we suggest some conceptual modifications in the existing model: the aim is to find an appropriate theoretical framework within which all those predictions of the interparticle adhesive forces fit, taking into account both the fabrication process and the interparticle parameters. This preliminary study of tensile strength suggests a transition from ductile to fragile behavior as density increases, as well as an important role of the initial connectivity of the contact network.

1 Introduction

Although numerical simulations have been widely used for several decades [1] to investigate microscopic mechanisms and classify mechanical properties of granular systems, studies of cohesive materials are still far less common, and almost exclusively limited to dense materials. Thus, the effects of capillary cohesion in wet sand
or bead packs have been simulated [2, 3], as well as the compaction of metallic powders [4, 5, 6, 7] to states of very high density, or the behavior in shear tests of 2D dense cohesive packs with plastic deformation of contacts [8, 9]. Loose structures formed by particles packed under gravity and stabilized thanks to adhesion have been simulated [10]. The most recent research dealing with simulations of loose cohesive packings study the dynamical compression regimes (collapse under growing loads) [11, 12, 13, 14] or shear flows [15, 16, 17, 18]. However, as far as we know there is a gap in the knowledge of loose structures under tensile mechanical conditions. Experiments with powders have shown that one of the most important tests to characterize any cohesive powder is based on the application of tensile stresses [19, 20, 21, 22].

In a companion study also presented in this book of proceedings, as well as in refs. [27, 28, 29, 30], we have extensively studied by DEM simulations the assembling process, the geometrical structure, the force distributions and force patterns, the elastic moduli and the plastic compaction of a model, two-dimensional (2D) cohesive granular material in loose equilibrium configurations. We now investigate the mechanical response of the same model granular material under isotropic tensile stresses until the breakage of the granular structure. This work is organized as follows. In Section 2 a brief introduction of the numerical model as well as the set of equations to be solved are presented. Section 3 is devoted to describing in detail how we proceeded to apply isotropic tension on the granular structure. Section 4 presents the results of the mechanical response obtained from different sets of configurations, where discussions about the geometrical aspects connected with the material strength are developed. Finally, Section 5 presents our conclusions about these preliminary results as well as some comments pointing to further investigations.

2 Computational method

2.1 System definition

We consider a two-dimensional model material: an assembly of \( N \) disks with diameters \( \{d_i\}_{1 \leq i \leq N} \) uniformly distributed between \( a/2 \) and \( a \). The maximum diameter, \( a \), will be used as unit of length. The mass of grain \( i \) is \( m_i = d_i^2/a^2 \) and its moment of inertia \( I_i = m_i d_i^2/8 \), i.e. disks are regarded as homogeneous bodies and the mass of a disk of maximum diameter \( a \) is the unit of mass.

The disks are enclosed in a rectangular cell, the edges of which are parallel to the axes of coordinates \( x_1 \) and \( x_2 \), with respective lengths \( L_1 \) and \( L_2 \). Periodic boundary conditions are used, thereby avoiding wall effects. Neighboring grains, say \( i \) and \( j \), might interact if they are brought into contact or very close to each other, hence a force \( \vec{F}_{ij} \) and a moment \( \Gamma_{ij} \) exerted by \( i \) onto \( j \) at the contact point. Simulations do not model material deformation in a contact region, but consider overlapping particles, and the contact point is defined as the center of the intersecting surface of the two disks. In the case of an interaction without contact, the force will be normal to the surfaces at the points of nearest approach, and therefore carried by the line of centers. Let \( \vec{r}_i \) denote the position of the center of disk \( i \). \( \vec{r}_{ij} = \vec{r}_j - \vec{r}_i \) is
the vector joining the centers of i and j, and \( h_{ij} = |\vec{r}_{ij}| - (d_i + d_j)/2 \) their overlap distance.

### 2.2 Equations of motion

The degrees of freedom, in addition to the positions \( \vec{r}_i \), are the angles of rotation \( \theta_i \), velocities \( \vec{v}_i \), angular velocities \( \omega_i = \dot{\theta}_i \) of the grains (1 ≤ i ≤ N), the dimensions \( (L_\alpha)_{\alpha=1,2} \) of the cell containing the grains and their time derivatives, through the strain rates:

\[
\dot{\varepsilon}_\alpha = -\frac{\dot{L}_\alpha}{L_\alpha^0},
\]

in which \( L_\alpha^0 \) denotes the initial size for the corresponding compression process. The time evolution of those degrees of freedom is governed by the following equations.

\[
\begin{align*}
\sum_{j=1}^{N} \vec{F}_{ij} &= \sum_{j=1}^{N} \Gamma_{ij}, \\
\sum_{j=1}^{N} \Gamma_{ij} &= \sum_{j=1}^{N} \vec{F}_{ij},
\end{align*}
\]

\[
M \dot{\varepsilon}_\alpha = \sigma_{\alpha\alpha}^I - \sigma_{\alpha\alpha}^M
\]

\[
\sigma_{\alpha\alpha}^M = \frac{1}{A} \sum_{i=1}^{N} \left[ m_i v_{i,\alpha}^2 + \sum_{j \neq i} F_{ij}^{(\alpha)} r_{ij}^{(\alpha)} \right].
\]

In Eqns. 2 and 3, only those disks j interacting with i, that is, in contact or very close to each other, will contribute to the sums on the right-hand side. In Eqn. 4, \( \sigma_{\alpha\alpha}^I \) is the externally imposed stress component and the definition of \( \sigma_{\alpha\alpha}^M \) given by 5 is the measured stress component, resulting from ballistic momentum transport and from the set of intergranular forces \( \vec{F}_{ij} \), \( A = L_1 L_2 \) denotes the cell surface area, and \( M \) is a generalized inertia parameter.

Stresses \( \sigma_{11} \) and \( \sigma_{22} \), rather than strains or cell dimensions, are controlled in our simulation procedure. Note that compressions are counted positively for both stresses and strains. Eqn. 4 entails that the sample will expand (respectively, shrink) along direction \( \alpha \) if the corresponding stress \( \sigma_{\alpha\alpha}^M \) is larger (resp., smaller) than the requested value \( \sigma_{\alpha\alpha}^I \), which should be reached once the system equilibrates. This barostatic method is adapted from the ones initially proposed by [31, 32, 33] for Hamiltonian, molecular systems. The choice of the “generalized mass” \( M \) is rather arbitrary, yet innocuous provided calculations are restricted to small strain rates. In practice we strive to approach mechanical equilibrium states with good accuracy, and choose \( M \) in order to achieve this goal within affordable computation times. We usually attribute to \( M \) a value equal to a fraction of the sum of grain masses (3/10 in most calculations), divided by a linear size \( L \) of the cell. This choice is dimensionally correct and corresponds to the appropriate time scale for strain fluctuations in the case of a thermodynamic system.
2.3 Control parameter

We assume the external pressure as the main control parameter. The adhesive strength $F_0$ in contacts sets a force scale in the material behavior, and hence (in 2D) the reduced pressure, defined as

$$P^* = \frac{P \, a}{F_0},$$

(6)

in which $a$ is a typical grain diameter, is a crucial dimensionless state parameter. The main objective of this piece of research is the study of the process by which, as the structure is stressed, cohesion-dominated loose structures, for which $P^* < 0$, get irreversibly broken as $P^*$ reaches a characteristic value. Such value of $P^*$ generating a tension, denoted here by $P^*_T$, will depend on the previous degree of compactness of the granular assembly, i.e. the past history. Such a feature was experimentally observed in fine powders [22]. In that respect, we say that a granular specimen was \textit{preconsolidated} under $P^*_C$ when its structure was previously compacted under such isotropic pressure.

3 Tensile stress application

From a practical point of view, our interest is to mimic a quasistatic procedure to detect the maximum tensile strength sustained by the granular structure. Hence, two procedures have been used to reach the breakage of the sample under an isotropic tension.

3.1 Step-wise mechanism

A step-wise mechanism consists of applying small enough, isotropic and tensile (negative) leaps of pressure. The simulation program loads a list of values of pressure that will be imposed to the sample. Starting from an initial and well-determined state under mechanical equilibrium, the barostatic procedure described by eqs. 4-5 is switched to imposing a new $P^*$—value. Once the mechanical equilibrium is reached under the new pressure, the internal variables as well as the new configuration are recorded for further analysis. This procedure requires (i) defining the mechanical equilibrium of the structure and (ii) defining a procedure to determine the tensile yield strength. Both requirements are described in the following paragraphs:

3.1.1 Equilibrated states

A typical intergranular force value $F_1 = \max\{F_0, |P|a\}$ to set the tolerance levels is used. Therefore we say that a configuration is deemed \textit{equilibrated} when i) the net force on each disk is less than $10^{-4}F_1$, and the total moment is lower than $10^{-4}F_1a$, ii) the difference between imposed and measured pressure is less than $10^{-4}F_1/a$ and iii) the kinetic energy per grain is less than $5 \cdot 10^{-8}F_1a$. We observed that once samples were equilibrated according to those criteria, then the Coulomb criterion $|T_{ij}| \leq \mu N_{ij}$, as well as the rolling friction condition $K_r|\delta \theta_{ij}| \leq \mu_r N_{ij}^\circ$ were satisfied as
strict inequalities in all contacts, where \( N_{ij}^e \) is the repulsive elastic part of the contact force. When these conditions are fulfilled, no contact is ready to yield in sliding, and with rolling resistance (RR) no contact is ready to yield in rolling either. We found that these criteria allowed us to identify the force-carrying structure clearly enough.

### 3.1.2 Dynamical breakage criterion

Very small and contiguous leaps of stress applied on the granular network produce slight variations in the total kinetic energy. The dissipative (restitution) and frictional (sliding and rolling) mechanisms together with the cohesive bonds existing at intergranular contacts stabilize the structure under any variation of external pressure. However, once the granular network is unable to reach a new mechanical equilibrium, the barostatic procedure cannot match the internal pressure to the external applied stress. Under this situation, the strain rate associated to cell variations (eq. 1) suffers an increase with an order of magnitude of two or three, as fig. 1 shows. This is a well-detectable feature to determine the instant of the onset of breakage. (To express magnitudes associated with time, we use the natural inertial time associated with the characteristic force \( F_0 \), given by \( T_0 = (m a / F_0)^{1/2} \), where \( m \) is the mass of a disk of diameter \( a \)). We have checked that this dynamical criterion is quite robust and characteristic of all studied samples. However, this procedure has two pitfalls. On the one hand, this is a costly computational procedure, since the mechanical equilibrium (described above) must be fulfilled. On the other hand, the accuracy to determine the real tensile yield strength of the structure is subjected to the size of the leap of imposed stresses. In other words, we have to reach a compromise between the computational time and the accuracy of the measurement.
3.2 Uniform stretching mechanism

This is a time-dependent mechanism consisting of imposing a uniform but low enough stress rate, i.e. we set the value of the first time-derivative of the normal components of the stress tensor: \( \dot{\sigma}_{xx} \). In principle, in a process in which we are imposing a progressive change of the stress tensor components, the structure does not have time to reach the mechanical equilibrium. However, it will depend on the strictness of the equilibrium criteria. For such reason, we impose a variation of the stresses as small as the limit of the criterion defined previously: \( \dot{\sigma}_{xx} T_0 = 10^{-4} F_0/a \).

This progressive and slow increase minimizes any undesirable dynamical effect due to the rapidity of the process [29]. This procedure resembles that used by anyone who wants to break some object by stretching. At the beginning the object puts up resistance, and that is why one naturally performs a progressive increase of the applied strength until the breakage of the object. In fig. 2 we show the evolution of the instantaneous isotropic stress using eq. 5 along time. This plot clearly shows the limit of the maximum tensile stress held by the sample under different preconsolidations. Once the structure fails, the instantaneous calculated stresses fall to zero. The maximum value of the stress as well as the configuration are recorded, since they are taken as the feature which is characterizing the breakage point. It can be noticed that samples which are more weakly consolidated reach the breakage point sooner than the more highly preconsolidated ones. Moreover, the looser samples produce more fluctuating stresses close to the breakage.
Figure 3: Reduced tensile strength ($P_T^*$) as a function of the reduced preconsolidation stress ($P_C^*$). To apply the isotropic tension, two procedures are presented: the step-wise mechanism described in Sec. 3.1 (circles: solid without RR and void with RR) and the continuous stretching mechanism described in Sec. 3.2 (squares). In this last procedure, only samples with RR are presented. In all cases, the granular packing was assembled with 1400 particles.

4 Results

As we commented before, we have observed an important mechanical feature in these cohesive granular networks: the onset of the plastic deformation as well as the breakage strength depend on the initial preconsolidation degree.

4.1 The tensile strength values

Figure 3 shows the comparison between the two previous procedures to calculate the tensile strength. The value of the tensile strength is represented as a function of the preconsolidation pressure. The samples used for these calculations were two set of configurations each one composed of 1400 particles. Configurations with ($\mu_r/a = 10^{-2}\mu$) and without RR ($\mu_r/a = 0$) were used. The value of the friction coefficient was $\mu = 0.5$ (more details about other parameters of the contact law, as well as the assembling procedure can be consulted in our companion study from this book of proceedings).
It is worth mentioning some issues about the results shown in figure 3. On the one hand, it is interesting to note that the procedure described by section 3.2, despite representing a mechanism which is keeping the granular structure out of the mechanical equilibrium, produced a very similar result. The importance of this fact is twofold: (i) the perturbed state of increasing the external pressure by an increment equal to $10^{-4} F_0/a$ is still very close to the “real” equilibrated state and hence useful to be worth analysing, and (ii) the stretching mechanism is computationally much faster than the step-wise mechanism (which may take some days due to the relaxation force, as opposed to the two or three hours required by the stretching procedure). On the other hand, once the level of preconsolidation is above $P^*_C \sim 1$, the samples break at a similar value of $P^*_T$. This behavior can be explained as follows: when a cohesive granular structure is compressed above a certain level (i.e., usually when $P > F_0/a$), any new internal rearrangements will produce a very small increase of the density ($\Phi$) and the network connectivity ($z$) [30]. Under this situation, the mechanical properties of cohesive granular materials approach the properties of non-cohesive ones because the external applied forces dominate over the internal cohesive bonds. This behavior remains true if the interaction between particles does not take into account any contact plastic deformation. On the contrary, if the external pressure during the preconsolidation stage induces plastic deformation in the contacts, the connectivity may growth significantly. In this case, the structure requires much higher values of the tensile strength (in absolute value) to reach the breakage.

From the set of samples used to compared the procedures described in sec. 3, we have found out that preconsolidated states under $P^*_C = 0.178$ and $P^*_C = 0.237$ gave a very similar tensile strength value (see fig. 2). Of course, this is a particular feature of such sample, something that depends on the past history, i.e. the assembling process. However, this peculiarity can be considered as a validation of both tensile application procedures, since both produced the same material response.

### 4.2 The ductile-to-brittle transition

Figure 4 shows the stress-strain diagram obtained from applying the stretching mechanism to our samples prepared with different initial preconsolidated states. Because of the wide range of deformations generated, the horizontal axis is represented using a logarithmic scale. This figure shows that the lower preconsolidation is, the larger deformation is produced before the breakage. Fig. 5 shows some snapshots for the case $P^*_C = 0.042$, where the contact network evolves from its maximum extension to the total breakage. Such an extension becomes narrow as $P^*_C$ increases. This is a classical feature of brittle materials: they are able to hold very high stresses, whilst strains hardly change. Fig. 6 shows the snapshots during the breakage for the case $P^*_C = 13.3$. It is important to notice that at the instant immediately after the maximum tensile strength, the most of the interparticle bonds (above 80%) are under tensile condition. This may suggest that a very important fraction of total particles may loose their contact integrity at the same time. We have not observed this characteristic in ductile structures, where the lost-contact mechanism takes place more progressively. This “synchronous” lost-contact mechanism is one of the principal assumptions held by the theoretical framework developed by Rumpf. However, we have
found a clear disagreement with this theoretical prediction, regardless the degree of preconsolidation, as we shall present in the following section. Due to the specific geometry of loose systems, in which dense zones are weakly connected through thin arms, better connected, solid-like regions tend to move like rigid bodies [30], while fragile junctions progressively break and rearrange. This kind of evolution prevents a collective contact breakage, as it is assumed in the argument supported by the Rumpf formula. This is the main reason why the prediction provided by Rumpf fails with our cohesive granular model.

4.3 Relation between strength and packing geometry

In the absence of cohesion, the distribution of force values is usually normalized by its average, which scales with the applied pressure. This scaling can be made more quantitative on using a general relation between pressure $P$ and the average normal contact force $F_N = \langle N_{ij} \rangle$ and particle diameter $d$, which is known in the literature on powders as the Rumpf formula [23]. However, this formula is often associated to a means of predicting the macroscopic tensile strength of a powder. Let us briefly expose how to obtain its expression. To derive this formula, we define $P = D^{-1} \sum_{\alpha=1}^{D} \sigma_{\alpha \alpha}$ which is nothing more than the standard formula for stresses in an equilibrium configuration given by eq.4, where $D$ is the dimension of the system. For the average pressure, one assumes that elastic deflection between particles is $h_{ij} \ll (d_i + d_j)/2$ and then neglects correlations between particle radii and forces, assuming $\langle N_{ij}(d_i + d_j)/2 \rangle \simeq F_N(d)$. Then, with a simple transformation of the sum,
Figure 5: (Color online) Series of snapshots obtained during the ductile breakage presented by a preconsolidated sample under $P_C^* = 0.042$. Red and green colors represent the normal forces under compression and tension, respectively.
Figure 6: (Color online) Series of snapshots obtained during the brittle breakage presented by a preconsolidated sample under $P_C^* = 13.3$. Colors have the same meaning as in fig. 5. At the instant $1044T_0$, 83.5% of contacts are sustaining tensile forces, and the average elastic normal force is $\langle N_{ij}/F_0 \rangle = -0.297$, which is close to the typical value given by $Pa$. 
one obtains

\[ P = \frac{1}{\pi} \frac{\langle d \rangle}{\langle d^2 \rangle} z \Phi F_N. \]  

(7)

In this expression it is common to introduce two important quantities in granular materials: the coordination number \( z \) and the solid fraction \( \Phi \). The former is the average number of contacts per particle, i.e., \( z = 2N_c/N \), where \( N_c \) and \( N \) are the total contact and particle numbers, respectively. The later quantity is the ratio between the real volume occupied by the particles and the total volume of the confining space. With \( D = 2 \), \( \Phi = 0.25N\pi\langle d^2 \rangle/A \) and using our diameter distribution (\( \langle d \rangle = 3a/4 \) and \( \langle d^2 \rangle = 7a^2/12 \)) we obtain

\[ F_N = \frac{7\pi a}{9} \frac{P}{z \Phi}. \]  

(8)

We found relation 8 to be remarkably accurate in all our simulations, with or without cohesion, with configurations obtained by different assembling methods, thereby checking that the correlations between particle sizes and contact forces could safely be neglected.

Let us return to the definition given by eq.7 characterized by an assembly of non-equal disks. In our previous studies of density correlations [27], we showed that loose configurations can be regarded as dense packings of self-similar blobs of typical size \( \xi \) (about 10 times as large as the average diameter in our case), as in fractal clusters produced by colloid aggregation models. Our estimated value of the pseudo-fractal dimension, with RR, is compatible with the 2D result for ballistic aggregation, even when the coordination number is different [29]. We shall consider a re-scaled problem assuming that the granular packing is formed by a set of pseudo-fractal blobs with a typical length given by \( \xi \). Behind this hypothesis, one may consider such blob either as a solid entity or a hole entity, which are, in principle, equivalent. In few words, the quantity \( \xi \) represents a density correlation length. The relationship between the tensile strength value and the density correlation length from our samples can be well represented by means of a power law, as it is shown in fig. 7.

In the following, we present three different estimations to link the geometrical concept of blob with the tensile strength values. In all of them, we shall adopt the same assumptions to derive eq. 7. The results presented below are obtained from the set of samples with rolling resistance previously shown. The three estimations share the definitions for: \( P \) (mean pressure), \( \xi \) (holes radius) and \( \langle ... \rangle \) (average over the hole size distribution).

### 4.3.1 Estimation A

In this estimation we shall consider the dual problem associated to the particles: we have an assembly of holes, or interstices, formed between particles. The holes diameters are arranged under a size distribution function that we can calculate directly from the configuration using a special software that we have developed:

\[ P = \frac{1}{2\pi} \frac{\langle \xi \rangle}{\langle \xi^2 \rangle} z \Phi F_{N,\xi}. \]  

(9)
where, $F_{N,\xi}$ is the average normal “interacting” force between holes, $z_\xi$ is the hole coordination number (i.e. the average number of holes surrounding one hole) and $\varepsilon$ is the void fraction ($\varepsilon = 1 - \Phi$). Let us apply eq.9 to a state under $P^* = 0$ which was preconsolidated up to $P^*_C = 13.3$. Direct calculations using such a sample provided the results shown in the table 1. The values related to the hole size distribution can be calculated with good accuracy, however we are forced to admit some assumptions concerning the values for $z_\xi$ and for $F_{N,\xi}$. To establish an assumption to estimate the value of $z_\xi$ is a rather uncertain task, so we have resorted to the simplest procedure: the visual inspection of the structure. After this “analogical” procedure, we have observed that $z_\xi$ is within the range $(3 - 8)$. On the other hand, maybe the more uncertain assumption is to admit that $F_{N,\xi} \sim -F_0$. The result, including configurations with and without RR, was $P^*_T = (-0.19, -0.52)$. The numerical result of the tensile strength calculated from the simulation is approximately in the middle of this range, i.e., $P^*_T \simeq -0.3$. In principle,
if one considers that $F_{N,\xi} \sim -F_0$ is not a crude assumption one obtains that $z_\xi \sim 5.5$. This value is close to the maximum number of nearest neighbors of a two-dimensional dense network formed by hard and equal disks, i.e., $z = 6$. It is worth mentioning that we obtained $P_T^* \simeq -0.3$ for the samples with and without RR. This fact can be explained as a result of the relatively high level of initial compaction. Under this situation, the cohesive granular structure is quite brittle and the effect of a small level of RR is negligible. Nevertheless, although we have checked that this estimation works correctly for high consolidations, this is not the case for loose samples. Additionally, this approximation introduces a clear disadvantage: the difficulty to physically justify the meaning of $F_{N,\xi}$.

4.3.2 Estimation B

In this estimation we write the Rumpf’s equation as follows:

$$P = \frac{1}{2\pi} \frac{\langle \xi \rangle}{\langle \xi^2 \rangle} z \Phi F_0, \tag{10}$$

where $F_0$ is the adhesive bond between two particles, and $z$ and $\Phi$ are the coordination number and the solid fraction occupied by the particles. In Fig. 8(a) we show the results. Although the results seem to be logic, we have problems with this estimation because we are mixing two different scales: from the geometrical point of view, we are using $\xi$, i.e., a pseudo-fractal scale, whilst at the same time we are using $z$ and $\Phi$ associated to the scale of the particle. To overcome this pitfall, we resort to the next estimation.

4.3.3 Estimation C

In this estimation we modify the concepts for $z$ and $\Phi$ as follows:

$$P = \frac{1}{2\pi} \frac{\langle \xi \rangle}{\langle \xi^2 \rangle} z_b \Phi_b F_0, \tag{11}$$

where $F_0$ is the adhesive bond between two disks, $z_b$ is the blob coordination number and $\Phi_b$ is the solid fraction occupied by the blobs. In principle, it is very difficult to measure $z_b$, however one can assume as a first approximation some kind of simple algebraic relation between $z$ and $\Phi$, as it is often assumed in non-cohesive ensembles [24, 25]. In any case, taking into account the preliminar character of these estimations, this number is normally within the range $(2 - 6)$ for two-dimensional systems. On the other hand, we can calculate a more precise value of $\Phi_b$ in the following way. Let us consider the solid fraction occupied by the assembly of blobs as:

$$\Phi_b = N_{blobs} \frac{\pi \langle \xi^2 \rangle}{4A}, \tag{12}$$

where $A$ is the sample area and $N_{blobs}$ is the number of blobs presented in the sample. In principle, the last number can be calculated just counting the existing blobs (i.e., the holes). However, we have checked that this would not be a good
Figure 8: Estimations derived from the Rumpf formula to connect the tensile strength with the pseudo-fractal domain given by the length $\xi$. See text for more details.
procedure, since the samples contain a big number of small interstices which are not statistically represented by the blob status. It means that including these interstices in $N_{\text{blobs}}$, the value of eq. 12 may become bigger than 1. On the other hand, we have also:

$$\Phi = N \frac{\pi (d^2)}{4A} = \frac{7\pi}{12} N \frac{\alpha^2}{A},$$

(13)

and combining with eq. 12 we have:

$$\Phi_b = \Phi \frac{12}{7} \frac{\langle \xi^2 \rangle}{\alpha^2} \frac{1}{n_{\text{blobs}}},$$

(14)

where $n_{\text{blobs}}$ is the average number of particles per blob. This number should follow the classical pseudo-fractal growth given by $n_{\text{blobs}} \sim (\xi/\alpha)^{d_f}$ (except for a numeric prefactor of the order of 1) \cite{26}. After a simple manipulation we obtain:

$$P = \frac{6}{7\pi} \Phi z_b \frac{F_0}{\alpha} \left( \frac{\langle \xi \rangle}{\alpha} \right)^{1-d_f}$$

(15)

In Fig. 8(b) we show the results of this estimation. The fractal dimension calculated from the used sample is $d_f = 1.51$. The explanation about the procedure to calculate $d_f$ can be consulted in ref. \cite{29}. Since we know nothing about $z_b$, two limit cases are presented: $z_b = 2$ and $z_b = 6$. Just in order to compare these trends, the hypothetic case $z_b = z$ has been also depicted. From fig. 8(b) one can see that the best approximation is given by the assumption for which $z_b = 2$. In this respect, a more refined investigation of $z_b$ is required. This quantity may be strongly affected by the intermediate process during the relative motion of dense zones moving like rigid solids. We have checked that, during the tensile application and sample elongation, the coordination number does not follow a predictable trend: $z$, and hence $z_b$ are sensitive to the destruction of local interconnected clusters. This may be the reason why eq. 15 disagrees quantitatively with the result presented in fig. 7.

5 Conclusions

Using a simple two-dimensional model of a cohesive granular material, we have simulated a quasistatic-like process of isotropic tension. Two different ways of applying the tensile stresses have been proved. On the one hand, a series of small leaps of stress are imposed on the barostatic mechanism responsible for the control pressure. On the other hand, a faster, and presumably similar in accuracy, method is proposed, which is based on the application of a slowly increasing stress rate. The results of both procedures have been satisfactorily very similar. We have also calculated the tensile strength values required to break granular structure. We have found that, in agreement with the experimental measurements, the tensile strength depends significantly on the preconsolidation pressure. The numerical results proved that there is a limit for the maximum tensile strength (in absolute value), which is determined by the preconsolidation value given by $P_\text{C}^* = 1$. The origin of this behavior is supported by the purely elastic character of the intergranular forces. The geometrical features
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of our pseudo-fractal loose samples are related to the macroscopic tensile stresses. We have used the Rumpf formula to link both sides. The direct application of this formula to our granular material has shown that it is not possible to use it to predict the tensile rupture. Rumpf prediction overestimates the necessary tensile strength, since it does not take into account the complex movement mechanisms taking place during the ductile regime of deformation. To overcome this situation, three estimations based on slight modifications of the Rumpf formula have been presented. In these estimations we have implemented, using different scale arguments, the internal porosity presets in loose samples. Unfortunately, we have found that the geometrical features based on the density heterogeneities are not sufficient to predict the macroscopic tensile stresses. In that respect, we think that dynamical characteristics during the deformation process must be taken into account, as for example the hierarchical formation process of dense zones produced by the “collision” between “lumps” (or blocks) moving like rigid solids. This may visibly affect the process of internal connectivity, and hence affect the total external stress required to break the sample.

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Compaction of fine powders: Discrete Element Method simulations

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Abstract

Discrete Element Method simulations are used to investigate the structure and mechanical properties of a simple two-dimensional model of a cohesive granular material. Intergranular forces involve elasticity, Coulomb friction and a short range attraction akin to the van der Waals force in powders. The effects of rolling resistance at intergranular contacts are also studied. The microstructure of the cohesive packing is shown to depend sensitively on the assembling procedure which is applied to the initially isolated particles of a granular gas. While a direct compression produces a final equilibrated configuration with a similar density to that of cohesionless systems, the formation of large aggregates prior to the application of an external pressure results in loose packings, with a structure similar to that of ballistic aggregation clusters. Specific features of force networks and density heterogeneities due to cohesion, and their change as function of loading and unloading paths, are characterized.

1 Introduction

Although DEM simulations have often been applied to the study of the mechanical properties of cohesionless granular materials in quasi-static conditions (see [1, 2] and many examples in [3, 4, 5, 6]), micro-mechanical modeling of the loose structures formed by cohesive powders is much less common (in spite of a few recent studies, see [5, 7, 8, 9, 10]). Cohesive particle packings can form stable solid structures at very low densities, and are sensitive to stress intensity (as opposed to direction), and larger confinement pressures entailing irreversible compaction. We briefly present here the result of a DEM study of a model cohesive powder, as presented in Section 2, assembled using two different procedures or preparation producing loose, but yet mechanically stable configurations. In Section 3 we analyze the effects of the two most important parameters concerning the preparation and further compaction. In
Section 4 the samples are subjected to stepwise isotropic pressure increases. The resulting data of cycles of applied pressure are presented, where the similarities between our simple model and laboratory experiments on real powders are stressed. Additionally, some aspects of the influence of the micro-mechanical parameters on the initial state and the plastic isotropic consolidation curve is discussed. Finally, in Section 5 we state the conclusion.

2 The model

2.1 Contact law

![Graphical representation of the model for the adhesive elastic contact force as a function of the distance between the surfaces of particles i and j, h_{ij}, or simply h. Each region of the force law is color-coded: blue - distant interaction (or bonds), green - tensile contact forces and red - compressive elastic reaction. This code will be used in the next contact network analyses. (Left) The elastic normal force consists of a repulsive Hookean (red) part \( N_{ij}^e = -K_N h_{ij} \) plus a linearized attractive (blue) part (see second line in Eq. 1). (Center) The elastic tangential force is limited by the Coulomb cone (adhesion shifting its tip to \(-F_0\) on the normal force axis). (Right) Rheological representation of the sliding (up) and rolling (down) mechanisms of friction.

The contact law we implemented is an elaboration of the spring-dashpot model (see for example Luding and Herrmann in Ref. [3]) with the following ingredients: (i) normal and tangential elasticity, involving stiffness constants \( K_N \) and \( K_T \); (ii) a viscous component added to the normal force, related to a constant coefficient of restitution \( e \); (iii) an attractive force given by Eq. 1; (iv) the Coulomb condition involving the repulsive elastic part of the normal force, and optionally (v) resistance to rolling, modeled as in Tordesillas et al. (Ref. [11]). Our model for the van der Waals-like attraction introduces a range \( D_0 \) and a maximum tensile force \( F_0 \) as follows:

\[
N_{ij} = \begin{cases} 
-F_0 + N_{ij}^e & \text{if } h_{ij} \leq 0 \\
-F_0 \left( 1 - \frac{h_{ij}}{D_0} \right) & \text{if } 0 \leq h_{ij} \leq D_0 
\end{cases}
\]
In Fig. 1, the normal and tangential components are depicted. Sliding and rolling frictions are included by means of the Coulomb condition involving the repulsive elastic part of the normal force and momentum, respectively. Resistance to rolling shares the same scheme of implementation as the sliding friction, just substituting the tangential force (T) with the rolling moment (Γ), relative tangential displacement (s) with relative angle of rotation (∆θ), tangential stiffness constant (KT) with rolling stiffness constant (Kr) and friction coefficient (µ) with rolling friction coefficient (µr). These coefficients µr = µl and Kr = KNl2, introduced by the moment opposing rolling in contacts Γ, involve a small length scale l of the order of the size of asperities on the particle surfaces. An important feature of our implementation of sliding and rolling friction is that contacts transmit tangential forces up to µF0 and rolling moments as large as µrF0, since the total normal force can be equal to zero because the attraction F0 may be compensated by elastic repulsion KNh0, where h0 is the spontaneous elastic deflection defined as h0 = F0/KN. This “natural” deflection is produced when an elastic contact sustains only the always-present attractive force F0.

### 2.2 Model parameters

If sets of dimensionless numbers are appropriately chosen, we may express the relative importance of different physical phenomena. Therefore this enables comparisons with real materials. This model naturally leads to a formulation of a set of dimensionless parameters, on the one hand related to the contact model and on the other hand related to the physical conditions.

The contact parameters are the reduced interaction range D0/a, where a is the typical grain diameter, the “asperity” to particle size ratio l/a, which determines the rolling resistance, the friction coefficient µ and the coefficient of restitution e. In this work we have used the following values: l/a = 10−2, µ = 0.5, e = 0.2 and KN = KT = 105F0/a. In this set we also need to include the ratio of elastic to adhesive stiffness h0/D0 whose value here is set at 10−2. The physical meaning of this number is similar to that of the Tabor parameter [12], so such a low value corresponds with the DMT limit [13].

Concerning parameters associated to the physical conditions, we emphasize two non-dimensional quantities. On the one hand, we have the reduced velocity given by

\[ V^* = \frac{V}{(F_0D_0/M)^{1/2}} \]  

which is used to quantify the level of kinetic energy per disk, with mass M, during the preparation stage. Quantity in the denominator is the natural velocity in which a pair of disks with zero initial velocity are attracted to each other due to the adhesive bond. On the other hand, we have also the reduced pressure

\[ P^* = \frac{P}{F_0/a} \]  

that characterizes the mechanical situation exerted on the present model and whose
task is to quantify the effect of an external force $P_a$ compared to the adhesion strength $F_0$.

### 2.3 Packing preparation

We have proved two different ways to prepare the initial states of packings. The first way, which is traditionally employed in many works dealing with simulation of granular media, consists in slightly compressing an initially loose configuration. In this procedure, disks are initially placed in random non-overlapping positions in a periodic cell with zero velocity, until a state of mechanical equilibrium is reached in which inter-particle forces balance the external pressure. The low applied external pressure causes the cell to shrink homogeneously. Thus contacts gradually appear and the configuration rearranges until the system equilibrates at a higher density. We may refer to this procedure as a *direct collapse*, corresponding this process to a fast assembling, where particles do not have sufficient time to form aggregates. The second way to create initial packing starts with numerical samples placed in the same random non-overlapping positions as the first way, except that now they are allowed to form aggregates before imposing an external pressure. *Aggregation* is promoted here attributing random velocities to particles according to a Maxwell distribution, with mean quadratic (dimensionless) velocity $V^*$. Once launched with such random velocities the particles are left to interact and stick to one another within a cell of constant size, forming larger and larger aggregates as Fig. 2 shows.

Figure 2: (Color online) Snapshot of the intermediate stage during the aggregation process, where disks arrange in small aggregates. Red and green lines mean attractive and repulsive contacts, respectively. Yellow color represents those particles without contacts, and the arrows are the velocity field. The size of the arrow is proportional to the velocity of the particle. It can be clearly noted how the particle-cluster and cluster-cluster regimes coexist during the aggregation.
This procedure may be considered as the limit opposed to the previous one in which the external pressure is felt only after connected aggregates have formed.

3 Parameter effects

![Figure 3: Final coordination number (mean number of contacts per particle) versus initial average velocity of the agitation (Eq. 2) of the aggregation process. For the sake of completeness, the effect of using different values of the stiffness constant is also presented. The most correct results are obtained close to the limit of rigid bodies \((K_N > 10^3F_0/a)\), where the coordination number of 2D frictional systems is within 2 and 3 [14]. Soft particles \((K_N \leq 10^3F_0/a)\) overestimate the values of the elastic deflection between particles.

Exploring the effects of few parameters in a wide enough range of their values may become very demanding in computational terms. We have focused our attention on the effect of the initial agitation velocity, which leads to the particle aggregation, and the presence of rolling resistance (RR) at contacts.

Low velocity values produce more tenuous aggregates, as Fig. 3 shows (coordination number ~ 2), since even a small level of RR is able to slow down local rearrangements and stabilize tree-like structures immediately after the collisions between particles or small clusters. A large kinetic energy cannot be absorbed by the RR, and as a result disks are able to rotate, which leads to better connected structures (coordination number ~ 3). In that sense, a large \(V^*\) kills the effects of RR in such cases and packings are similar to those made without RR.

Figure 4 shows the resulting structure after the aggregation process obtained with a large rolling resistance: \(\mu_r/a = 0.5\) in a 5600-disk sample. The most contacts carry very small forces. The network force presented in Fig. 4 use the same conventions...
Figure 4: (Color online) Geometrical aspect of two types of force networks in equilibrium under $P^*=0$ after aggregation stage. Large sample, with 5600 particles, was prepared with large RR ($\mu_r/a = 0.5$) and relatively high initial mean quadratic velocity ($V^* = 10$). Inset: sample with 1400 particles, obtained with low initial mean quadratic velocity ($V^* = 0.1$) and small RR ($\mu_r/a = 0.005$). The last configuration corresponds to the bottom left point on Fig. 3.

as on Fig. 1, except for the blue color corresponding to contacts carrying a total force below tolerance $10^{-4}F_0$ (deflection $h_0$ and no mobilization of tangential force). Note the large number of such interactions and the local compensation of attractions and repulsions in small prestressed clusters. To help visualize unstressed regions, disks only interacting at contacts bearing forces below tolerance are filled in light gray. Such packings with large RR therefore approach the limit in which a simple geometrical rule is adopted to aggregate particles: in the present case one recovers the results of the ballistic aggregation algorithm, stipulating that particles or clusters move on straight-line trajectories and join to form larger, rigid objects as soon as
they touch [15, 16]. Again, this results in isostatic structures with coordination number 2, as we commented before.

We therefore conclude that the connectivity of loose samples with RR assembled by aggregation depends on the initial magnitude of velocity fluctuations and on the level of rolling friction.

Cohesive samples in equilibrium comprise a small number of pairs of particles interacting without contact, i.e. separated by a gap smaller than the range of attraction, $D_0$ (1%). Rattlers (isolated disks) are also virtually absent. Cohesion also enhances the role of sliding friction and rolling friction, because the limiting values for tangential contact forces and rolling moments are both proportional to the elastic repulsive part of the normal force: \(|T| < \mu N^e\) and \(|\Gamma| < \mu_r N^e\). Consequently, the contact between an isolated pair of grains in equilibrium with an elastic deflection $h_0$ transmit no normal force, but are able to sustain tangential force components as large as $\mu F_0$ and rolling moments as large as $\mu_r F_0$. Those values might turn out to be large in comparison to the typical level of inter-granular forces under low external pressure $P^* \ll 1$. Therefore, particles with one contact equilibrate when the deflection of that contact is $h_0$. With RR, such a particle is entirely fixed. Without RR, it is only free to roll without sliding on the perimeter of its interacting partner, because such a contact is able to transmit a tangential force smaller than, or equal to, $\mu K_N h_0 = \mu F_0$. Such a rolling motion is not damped in our model. Therefore, after long time, they should eventually stop after a collision, in a stable position with 2 contacts. This issue leads to an appreciable difference in the microstructure during the assembling procedure between samples created via direct collapse and aggregation. As figure 4 shows, the distribution of admissible pairs of normal and tangential forces is quite different for samples prepared with collapse (left) and

![Figure 5](image-url): Aspect of the contact force patterns (values of normal and tangential forces in equilibrium) under $P^* \ll 1$ without RR. Left pattern corresponds to a sample prepared with direct collapse and the right one was prepared with aggregation formation.
aggregation (right). In these samples RR is not present. The right remarkably cross-shaped pattern is caused by the formation of small triangles of disks during the assembling process, where the ratio \(|T/N| = \sqrt{3} \) is favorably satisfied by many contacts [17]. Without aggregation process, such small structures cannot be formed, which explains the more homogeneously distributed cloud of points in the left pattern. Samples with RR present a transitional pattern between them. The reason is the predominant number of disks with two contacts. It reduces the possibility of finding a large number of small local triangles.

4 Compacting process

Specimens can rearrange in more compact configurations if they are subjected to larger pressure levels. In this work, our numerical samples are isotropically compressed by means of the stress-controlled calculation procedure, where the two principal components of the stress tensor are set at \(P \) (through definition given by 3). To investigate this effect, we repeatedly multiply the current value of reduced pressure, by a constant factor \(\alpha_p = 1.334\) and wait each time for the next equilibrium state. After that, we study the resulting configuration series. The specimens were thus compressed from \(P^* = 0.01\) up to \(P^* = 13.34\), and they were subjected to a similar stepwise unloading process, back to \(P^* = 0.01\). Density and various state parameters were recorded for each equilibrated configuration. The left graph in Fig. 6 shows the global response obtained during this cycle for the different preparation types commented above, through the measurements of the solid fraction as a function of the reduced pressure. Each point in this graph corresponds to configurations in mechanical equilibrium, with RR. For the sake of completeness, we include in this general view the non-cohesive response (triangles). Quite different behaviours in these global responses can be appreciated. Especially remarkable are, on the one hand the large difference introduced by the presence of the adhesion in comparison to the cohesionless case, and on the other hand, the large difference between the initial densities at very low \(P^*\), produced by collapse and aggregation (\(\sim 30\%\)).

Figure 6 also shows experimental measurements using the commercial toner CLC700. This toner is composed by irregular grains of polyester with average particle size of \(7.8 \ \mu m\), grain density \(1120 \ Kg/m^3\), work of adhesion \(\nu = 0.04 \ J/m^2\), Young modulus \(E = 3 \ GPa\), Poisson coefficient \(\nu \sim 0.25\) and Yield strength \(\sigma_Y = 50 \ MPa\). The right-top graph in Fig. 6 corresponds with a process of loading and unloading carried out by means of a piston mechanism (details of the experimental setup can be found in [20]). On the other hand, the right-bottom graph of Fig. 6 corresponds with a single process of loading but starting from a very low consolidated state (see Ref. [19]). In this case, the unloading process was not performed, although the result is quite similar to the numerical ones. It is noticeable the similarity of the behavior between the real response and the simulated one, in spite of the simplifications assumed in the numerical model (two-dimensional, linear elastic contact law, absence of the fluid phase, regular grain geometry).

To finish this section, we shall show some details about the internal microstructure under higher pressures. As we have already presented in Sec. 3, samples prepared via aggregation are bearers of peculiar local patterns of forces. On increasing
Figure 6: (Left) Macroscopical response as a function of the reduced pressure for cohesive samples prepared with direct collapse (circles) and aggregation (squares). The non-cohesive response has been also drawn (triangles) to give a general overview of the studied cases. In all these cases $\mu = 0.5$. (Right-top) Result obtained by X. Jia, where a cylindrical probe containing toner CLC700, was compressed using a piston mechanism. An applied load of 150 N was performed. (Right-bottom) Consolidation curve of the same toner using the SPT (Sevilla Powder Tester) [18]. This experimental result, among many others, can be consulted in Ref. [19]. It can be noted the agreement between the real response and the simulated one, in spite of the simplifications assumed in the numerical model: simulation reproduces correctly both regimes of consolidation: low ($P^* < 1$) and high ($P^* > 1$) pressures. The arrows mark the direction of the load.
Compaction of fine powders: Discrete Element Method simulations

(a) Geometrical distribution of normal force values on the network. Line width corresponds with the value of normal force $N(t)$ (Eq. 1). In this state the solid fraction is 77.5%, the coordination number is 3.26, the maximum normal force ($N_{\text{max}}$) is 60.3 $F_0$, the minimum ($N_{\text{min}}$) is $-0.99 F_0$ and the mean ($\langle N \rangle$) is 12.5 $F_0$. Color code was given in Fig. 1.

(b) Coulomb cone.

Figure 7: (a) Macroscopic and (b) microscopic point of view of a cohesive sample without RR under high consolidation, $P^* = 13.34$. 
the applied pressure, the pre-stressed regions causing the patterns shown in the right graph of the Fig. 5 merge together and large forces tend to organize in locally preferred directions, as “force chains”, which are represented in Fig. 7(a). This fact is also clearly reflected on the destruction of the cross-shaped pattern. Figure 7(b) shows the values of the normal and tangential contact forces (normalized by $F_0$) in a sample without RR prepared via aggregation, in equilibrium under $P^* = 13.3$. In spite of the compressed pattern becomes homogeneous, as the pattern in Fig. 7(b) shows, a very small remaining set of these special contacts, commented in Sec. 3, are still evident: marks of the past history. They are arched by a strong neighbouring network sustained by these force chains plotted in Fig.7(a).

5 Conclusions

The numerical study of a simple two-dimensional model of a cohesive granular material confirms that stable low-density structures can sustain a pressure, due to the attractive forces in the contacts. Such tenuous arrangements appear as the particles are agitated in a container and form open aggregates before an external stress is applied. A small level of rolling resistance in the contacts affects visibly the final result of the assembling procedure, producing special micro features at configurations in equilibrium. Likewise we have seen that the initial velocity of fluctuation attributed to particles can have similar results, deciding the internal pattern of the force distribution and therefore the macroscopic behaviour. Upon increasing the pressure, one observes a gradual collapse of the open structure, with a decrease of the mean pore size, until configurations resemble dense packings of cohesionless grains. This is a plastic, irreversible process, controlled by a dimensionless ratio of applied pressure to cohesion strength. Our numerical results are in good qualitative agreement, not only with the plastic behaviour (normal consolidation curve) of real materials, such as cohesive powders [21, 22, 23, 24], but also with the predicted behaviour of the whole regime of compaction.

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Compaction of fine powders: Discrete Element Method simulations


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Abstract

The problem of dissipation of non-linear elastic waves due to thermoelastic effect in solids is discussed. Based on the photoacoustic thermoelastic experimental data for ceramics it is shown that the dependence of the thermoelastic parameter on strains or stresses should be taken into account for a correct description of the thermoelastic dissipation processes of non-linear elastic waves.

1

Non-linear mechanical properties of materials play an important role when investigating various mechanical and physical processes in solids. One important branch of physics and mechanics in which these properties are essential is related with the problem of non-linear elastic waves. These waves are determined by non-linear elastic, thermoelastic and some other properties of materials. Characteristics of these waves, details of their generation and propagation to a great extent are determined by dispersion and dissipation properties of materials. Dispersion of non-linear elastic waves is determined by linear and non-linear elastic properties of a material. One important and universal mechanism of dissipation of elastic waves is connected with the thermoelastic processes. The influence of dispersion on non-linear waves and solitons is analyzed in details at present [1, 2]. Essentially less attention has been paid to the problem of dissipation of these waves. In the paper [2] it is theoretically shown that heat transfer and thermoelastic interaction caused by the strain-induced heat release is an important reason for their damping both at low and high frequencies.

The main purpose of this article is to analyze in more details the situation with the thermoelastic dissipation based on the obtained by us experimental results. Let
us consider this problem by using as an example the equation for non-linear longitudinal waves in a plate which takes into account the interaction of the longitudinal displacement component with the temperature field. It is shown in the papers [1, 2] that in this case the equation for non-linear elastic waves can be represented in the form

\[
\frac{\partial^2 u}{\partial t^2} - s^2 \left(1 + \beta \frac{\partial u}{\partial x}\right) \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2}{\partial t^2} \left(g_1 \frac{\partial^2 u}{\partial t^2} - g_2 \frac{\partial^2 u}{\partial x^2}\right) = -\frac{\gamma}{\rho} \frac{\partial T}{\partial x}, \tag{1}
\]

where \(u(x, t)\) is the displacement component along \(x\) direction, \(s = \sqrt{E/\rho(1 - \nu^2)}\) is the speed of longitudinal waves in the plate, \(E\) is Young’s modulus, \(\nu\) is the Poisson’s ratio, \(\rho\) is the density of a body, \(\gamma\) is the thermoelastic parameter for a body, \(\beta\) is the coefficient which characterize non-linear elastic properties of a material, \(g_1\) and \(g_2\) are determined by the temporal and spatial dispersion of longitudinal waves in the plate, respectively.

Equation (1) describes the dispersion and dissipation of longitudinal waves in a plate. It includes elastic and thermoelastic properties of a material. This equation describes also some other important problems. One of them is the generation of non-linear elastic waves by laser radiation based on the thermoelastic effect. When using equation (1) it is usually supposed that \(\gamma = E\alpha\) [3], where \(\alpha\) is the coefficient of thermal expansion. This result is valid exactly in linear thermoelastic theory [3]. In general case \(\gamma\) may depend on strain and stresses in a material [5]. Our results obtained by photoacoustic (PA) thermoelastic microscopy of indented ceramics also demonstrated the dependence of the thermoelastic parameter on the stress [5, 6, 7, 8, 9, 10].

To analyze the situation in more details let us consider some of our experimental results obtained by laser thermal wave and thermoelastic PA methods on hot pressed silicon nitride (Norton Ceramic 132) and Al\(_2\)O\(_3\)-SiC-TiC ceramic (CRYSTALOY 2311 EDX). Residual strains and stresses were introduced in ceramics by Vickers indentation. Samples were indented with loads from 49N to 196N. The average indentation diagonal on the sample surface at the load of 49N was about 105\(\mu\)m for hot pressed silicon nitride ceramic and about 90\(\mu\)m for Al\(_2\)O\(_3\)-SiC-TiC ceramics. The main attention during our thermal wave and PA imaging experiments has been paid to the behavior of these signals near the tips of radial cracks were normally residual strains and stresses are concentrated. It is also important that plastically deformed regions near the crack tips in ceramics are small and did not play an important role in our imaging. In all experiments thermal and acoustic waves in samples were generated by the modulated laser radiation focused on a sample surface.

Let us begin with the results obtained by the PA thermoelastic imaging. The PA images were obtained both for hot pressed silicon nitride and Al\(_2\)O\(_3\)-SiC-TiC ceramics [5, 6, 7, 9, 10]. In all cases the PA signal was detected by the piezoelectric transducer attached to the back surface of a sample. All these images in general have a similar structure, therefore we present here only the PA image of silicon nitride ceramic. The typical image of this type is shown in Fig.1. An important peculiarity of these PA images is the presence of regions with large signal amplitude located near the tips of radial cracks. Previously, analogous features have been reported for
Nonlinear thermoelastic waves in stressed materials and photoacoustic imaging of indented areas in brittle and ductile materials

Figure 1: The amplitude of the PA piezoelectric image of a Vickers indentation in Si$_3$N$_4$ ceramic. The indentation load is 98N, the modulation frequency is 114kHz, the image area is 320 × 370µm$^2$.

the images of Vickers indentations obtained by electron-acoustic microscopy [11].

In general case the PA signal can depend on thermal and thermoelastic properties of a material. Therefore to clarify the dependence of thermal parameters of investigated ceramics on residual stress and its effect on the PA piezoelectric signal we have analyzed also thermal wave images of the same regions by the PA gas microphone, photodeflection and photoreflectance methods. In the photodeflection and photoreflectance modes of our microscope the radiation of a He-Ne laser was used for readout. PA gas microphone and photodeflection measurements are sensitive only to thermal parameters of a sample [7]. Typical image obtained, for example, by photodeflection method for the case of the Vickers indented silicon nitride ceramic is shown in Fig. 2. Both amplitude and phase of photodeflection images for this ceramic do not have any particular features near the radial crack tips.

It should be noted that photodeflection images of Al$_2$O$_3$-SiC-TiC composite ceramic in general are similar to the presented images with the exception of some additional speckle structure. However, this speckle structure is not determined by thermal or thermoelastic properties of this ceramic. It appears only due to different optical properties of Al$_2$O$_3$, SiC and TiC grains of this ceramic. In our experiments with silicon nitride and Al$_2$O$_3$-SiC-TiC ceramics we measured the photodeflection images of various Vickers indentations. In the experiments with silicon nitride the detailed PA gas microphone and photoreflectance measurements were additionally made. In these experiments we did not observe any particular features in the vicinity of the radial crack tips in ceramics, too. Thus, our experimental results for ceramics lead to the conclusion that residual stresses do not influence noticeably their thermal properties.

When comparing various thermal wave and PA images it should be noted that the spatial resolution of thermal wave methods depends both on a heating spot size and thermal wavelength. The heating spot size was the same in all the modes, whereas the thermal wave length is inversely proportional to the square root of
Figure 2: The normal photodeflection image of a Vickers indentation in Si₃N₄ ceramic. The indentation load is 98N, the modulation frequency is 7.6kHz, the image area is 315 × 315µm².

the modulation frequency and in silicon nitride ceramics it is, for example, about 10µm at 100kHz. In the PA gas microphone and photodeflection experiments the modulation frequency is normally lower than 10 kHz, which reduces in several times the resolution of these methods compared to that of the PA piezoelectric method. This distinction hampers direct comparison of images obtained by these methods. The problem disappears using the photoreflectance method operating in a very wide range of the modulation frequency.

In our experiments photoreflectance images were obtained at the modulation frequencies up to 140kHz. Therefore they can be compared directly with images obtained by the PA piezoelectric method at the same modulation frequency. These images were presented by us elsewhere [5, 6, 7, 9, 10]. The photoreflection images being sensitive to the modulation of the optical reflectance coefficient by alternative temperature component did not show any particular features near the ends of radial cracks. Thus, the PA gas microphone, photodeflection and photoreflectance measurements of Vickers indentations in silicon nitride and Al₂O₃-SiC-TiC ceramics lead to the conclusion that residual stress does not influence noticeably its thermal parameters.

In the previous studies of the PA effect in stressed materials the PA response has not been investigated at additional external loading. The study of these effects can provide a direct demonstration of the dependence of the PA signal on mechanical stresses. Therefore we have also investigated the PA and thermal wave responses from regions with residual stresses in ceramics under external loading in direct experiments with ceramics. Compressive external loading was applied in our experiments in the direction parallel to the sample surface. The PA and thermal wave images of Vickers indentations were obtained in unloaded and loaded Al₂O₃-SiC-TiC composite ceramic. First of all it should be noted that the laser thermal wave images of Vickers indented areas in this ceramic do not demonstrate any influence of external loading. This result verifies once more the conclusion about the absence of ceramic
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Figure 3: The PA piezoelectric image of Vickers indentation in Al$_2$O$_3$-SiC-TiC ceramic. a - without external load, b - under the external loading of 170MPa. The indentation load is 98N, the modulation frequency is 142kHz, the image area is 480 × 500µm$^2$.

A typical modification of the PA piezoelectric image of the Vickers indented area in Al$_2$O$_3$-SiC-TiC composite ceramic under external loading is presented in Fig.3. From Fig.3 one can see that strong changes of the PA piezoelectric image with the application of external loading take place near the radial crack tips. This result can be considered as one more direct experimental proof of the PA piezoelectric signal dependence on the mechanical stress.

For interpretation of the obtained experimental results we have proposed the theoretical model of the PA effect in stressed materials [7, 8, 10]. It takes into account non-linear elastic and thermoelastic properties of materials. The thermoelastic energy related to the deformation of the body from the initial state to the final one in this model is represented in the form

$$W_T = -\gamma_{ik}(u_{ik} - U_{ik})(T - T_0),$$

(2)

where $\gamma_{ik} = \gamma_0[(1 + \epsilon_0 U_{pp})\delta_{ik} + \epsilon_1 U_{ik}]$, $\gamma_0$ is the thermoelastic coupling for an undeformed body, $\delta_{ik}$ is the Kronecker’s delta function, $\epsilon_0$ and $\epsilon_1$ are the coefficients taking into account the dependence of the thermoelastic coupling on strain, $u_{ik} = \frac{1}{2}(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i})$ is the strain tensor, $U_{ik}$ is the initial strain tensor, and $T_0$ is the thermal parameter’s dependence on stress.
By applying this model the dependence of the PA signal on the stress has been analyzed. It was shown that at modulation frequencies used in our experiments (usually about 100kHz) the main contribution to the PA signal provides thermoelastic effect [7, 8, 10]. The proposed model was used for explanation of the PA signal behavior near the radial crack tips in ceramics [9, 10]. In Fig.4 the experimental and theoretical results are presented for the PA signal behavior near the tip of the radial crack 1 in Fig.3. It is seen that the theoretical form of the PA signal near the tip of the radial crack is in a good agreement with experimental data. Near the radial crack 1 acts almost normal external stress. Similar analysis was done for the tips of cracks 2 and 4 where external stresses have the tangential character. A good agreement between theoretical and experimental results was obtained also for this case. The presented results allow estimating the thermoelastic parameters $\epsilon_0$ and $\epsilon_1$. From the comparison of theoretical and experimental results it is seen that coefficients $\epsilon_0$ and $\epsilon_1$ for ceramics should be at the level $\approx 10$.

The presented experimental and theoretical results demonstrate that one should take into account the dependence of thermoelastic parameter in Eq.(1) on strains or stresses. This dependence is important for consideration of dissipation properties of non-linear elastic waves. The non-linear thermoelastic properties of the material may be also important for analysis of non-linear laser generated elastic waves in
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solids.

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Simulation of accumulative roll-bonding process

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Abstract

A novel intense plastic straining process named accumulative roll—bonding strip by the plain roll has been simulated. The process has been modeled using a program complex LS—DYNA. Finite element model rolling has been created to define a stressedly—deformed state and to improve the process of getting nanostructured materials by intense plastic straining process.

Ultrafine grained metals (UFG) and alloys with the average grain size smaller than 1 µm have got the outstanding mechanical properties, such as high strength, high toughness and superplasticity at low temperatures [1]. Therefore the application of nanostructured materials is one of important key issue in the near future. Severe plastic deformation is the most effective method of producing UFG materials in bulk dimensions. Different kinds of severe plastic deformation process for bulk materials, such as equal-channel angular extrusion/pressing, high-pressure torsion, cyclic extrusion compression and accumulative roll-bonding (ARB) have been developed so far. Among them ARB is a promising process that has a potential for continuous production of large bulk sheet materials for industrial application [2]. At present the ARB technology is being developed at the Institute of Engineering Science, Ekaterinburg.

The considered ARB process is schematically represented at figure 1. The rolled material is cut and put together to be equal the initial thickness, then it rolls again. The reduction of thickness is 50% in every rolling pass. Research indicates that the process may be repeated scores of times (up to 70-80 cycles). Thus the form of a billet doesn’t change and deformation accumulates. If the reduction is 50% per cycle, the thickness of the strip t after n cycles is \( t = t_0 / 2^n \), where \( t_0 \) is the initial thickness of strips. The equivalent plastic strain \( \varepsilon \) is defined as \( \varepsilon = 0.8n \).

The development of technology is accompanied by the preparation and the theoretical research whose purpose is the design of some general dependence for definition of geometrical and kinematic parameters of the deformation center and the calculation energy-power parameters. Generally the traditional techniques for solving of
that kind of problems are based on the analysis of the simplified two-dimensional models of metal plastic deformation process. Practical opportunities of such analytical methods are limited because of the accepted hypotheses and assumptions. However, the solving of practical questions requires the comprehensive and reliable information about stress-strain state of the metal. The consideration of three-dimensional problems of metal forming processing subject to real mechanical properties of metal is possible only by using of modern numerical methods of the analysis.

One of the numerical methods of three-dimensional nonlinear problems of deformed body is the finite element method (FEM). Generally the modern program packages of FEM-analysis have got a large libraries of finite elements, give a wide range of material models and provide an opportunity to use the various iterative "solvers" depending on kind of problems. One of such packages is LS-DYNA (the development of Livermore Software Technologies Corp., USA), it makes possible to speed up the engineering process, the research time of various processes and designs without applying long and expensive procedure of experimental researches. The operating experience of LS-DYNA has shown that the given package allows to adequately simulate of metal forming processes, which are characterized by the greater degrees of plastic deformation and the essential nonlinearity of geometrical and mechanical factors [3].

The FEA-simulating of two-layer strip rolling process has been made at the rolling mill established at the Institute of Engineering Science. The model is constructed by means of ANSYS, and then was solved by means of LS-DYNA.

Strips with the width of $B_0$ equals 30 mm and the height of $h$ equals 2 mm each have been rolled in bowls with a diameter equals 60 mm and the bowl speed $n$ equals 11 rev/min. The process has accepted to pass at constant temperature equals $600^\circ$C. Specimens were made from Steel 45 that allowed to apply the classical
bilinear isotropic elastoplastic model of material behavior under deforming.

It was accepted that the density \( \rho \) was equaled 7850 kg/m\(^3\), Poisson’s ratio \( \nu \) was equaled 0.3, and the yield point \( \sigma_T \) was equaled 320 MPa. There were made the following assumptions:

- the thermal interference between billet, tool and environment were not taken into consideration;
- the bowl material had been accepted absolutely rigid;
- the contact friction was constant and was submitted to Amonton-Coulomb law with friction ratio \( k \) equals 0.3.

The model is formed from three-dimensional solid-state elastoplastic hexahedral elements. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) method had been chosen to minimize the Lagrangian variational principle functional. The conjugate gradient method was used to solve the system of linear equations at each iteration of functional minimum search. Implicit scheme of integration on time area was used, the step size was equaled 1 msec. To control the stability of numerical solution the inspection of system energy balance was carried out. There were controled the external force work, the forming energy, the potential energy of billet elastic deformation, the kinetic energy of billet and the energy dispersion in billet contact with rollers.

The problem definition and simulation has been carried out successfully. Test and verification according to results of known theoretical decisions have been led. On basis of the received data it is proposed to carry out the practical experiment at mill established at the Institute of Engineering Science and to model the process in the future.

**References**


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Continuum of contacts: a way to model granular media?

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Abstract

Granular media are difficult to model, since they present very complex behaviour. We discuss different ways to model granular media, used in the literature, and their advantages and disadvantages. In our opinion, there are several reasons for the complexity of behaviour of granular materials, among them the multiphase nature of the material, the complexity of a point-body of the medium, and, the most important, the easiness of the change of the structure of contacts between grains. We suggest preliminary ideas for the description of the contact structure.

1 Introduction

1.1 Why is it difficult to model granular materials?

There is a big variety of materials used by humanity, and scientists have developed good theoretical models for most of them. Many of these materials are very sophisticated and have complex structure and properties (e.g. magnetic materials), but we know to describe them. However, this is not the case of granular media. There is no good theory able to describe granular materials and predict their behaviour. Why? Here we list some of the difficulties that we meet studying the behaviour of granular media:

- interaction with the ambient fluid is often important
- grain-grain interaction is non-central, non-linear, inelastic
- grain is much more complex than a mass point: it may rotate, deform, be destructed...
- contact properties vary much under loading
• **granular medium changes its structure easily**

The last difficulty is the worst. Indeed, if a contact is complex, but is present permanently, it is possible to investigate its properties and to make an appropriate model. This is not the case of granular materials, which undergo permanent “phase transitions”, changing the type of material under the loading. As a consequence, granular materials

• demonstrate solid-like, liquid-like and more complex behaviour

• do not behave like classical media

• are highly nonlinear, react differently to different types of loads: tension / compression, fast / slow loads, . . .

• have very few properties measured in a reproducible way

### 1.2 Various methods to model granular media

Scientists try to overcome these difficulties in many ways, and construct theories which reflect some specific features of granular materials, listed above. There are three groups of models:

• theoretical microstructural considerations leading to continuum theories

• computational particle methods

• continuum (phenomenological) theories: incremental theories, classical rigid- and elasto- plasticity, nonlinear elasticity with smooth potential, heteromodular theories, anisotropic models, multiphase models, Cosserat-type theories (elastic and plastic), gradient theories

Various models take into account: multiphase nature of medium, complexity of the material particle, and change of the structure of contacts. We are not going now to consider multiphase neither fractured media. We shall limit ourselves to the consideration of dense granular media where the influence of fluid motion can be neglected. Even for this case there is no good model.

### 2 Experiment

Not pretending to give an overview of experimental work, we shall mention the principal difficulties.

• laboratory scale usually differs much from the scale of the real experiment ⇒ due to inhomogeneities and boundary effects laboratory properties of the material may strongly differ from real ones

• the contact structure in the material changes easily ⇒ it is very difficult or impossible to initialize the material in the same way to obtain reproducible experiments and to have the same material as in the field experiment.
To solve the problem with scale difference engineers have developed an art which puts in correspondence laboratory properties to the field properties (see [1]). To have reproducible experiments usually they initialize the soil in four ways: 1) sow the soil “particle by particle” 2) make a sample by “rain” of particles 3) fluidize it and let it settle down 4) reach by a pre-shear protocol a critical state, when shear does not lead to the volumetric deformation (this is a method of initialization if we provide the same porosity of the material, which can be controlled by independent measurement). In the first two ways the anisotropy and “heteromodularity” is stronger. The third way (fluidization) is a very good method, providing reproducible results, but it is applicable only to a certain class of non-coarse granular materials (for the description of the method and its application in testers see [2]). A pre-shear protocol is very complex and does not always provide the desirable result, before subjecting to a loading protocol it is needed to desaggregate the material, i.e. to put the material in the state, so close to the natural one (zero stresses) as possible. To make this step requires real experimental art, and the result is not guaranteed. To reproduce the field conditions, sometimes they freeze a sample of the material and translate it to the laboratory (not clear at all if this thermic treatment leaves structure intact).

Due to these difficulties, there are very few properties which can be measured, and it lacks clear experimental results to verify numerous existing theories.

What can be measured in experiment? There is a limited number of tests. They allow to measure (if the material is initialized in the appropriate way) speed of wave propagation; effective constants; yield stresses. For description of experiments, see [1, 3]. Tatsuoka [1] underlines the inherent anisotropy and nonlinearity of soils even at small strains.

3 Microstructural considerations

3.1 Change of contacts. Theoretical considerations

Considerations on the microstructural level explain us why it is so difficult to have proper theories and experiment. First, we have nonlinearity even for simple monotone loading: due to the presence of dry friction and nonlinearity of elastic grain-grain interaction even in its simplest variant (contact between two Hertzian spheres, see [4] for the equations of 1D medium consisting of such particles). Change of contact properties leads to the nonlinearity of the medium. Even if contacts do not appear or disappear, their properties change a lot with loading. A contact may be analogous to a nonlinear elastic spring; change from elastic to plastic; change its adhesive properties (e.g. if the asperities on the surface of two particles flatten under compression); change its frictional properties, etc. When contacts appear or disappear, the material properties change drastically. The main reason of the nonlinearity of the granular material is the change of the contact structure.
3.2 Complexity of “particles”. Theoretical considerations

Rotation of grains is always present in shear bands (experiment: see [5]). Rotational degrees of freedom of grains are important in shear processes, avalanches, stability of granular systems, flowability. Local (induced) anisotropy of grains is present due to nonlinear behaviour of the soil or to the existence of coupling of rotation and translational degrees of freedom, seen at mesolevel. Several authors (M. Oda, K. Bagi, De Josseling de Jong, A. Suiker, S. Luding, N. Kruyt, I. Vardoulakis,...) try to make a continuum model based on microstructural considerations. Many of them obtain Cosserat-type theories. In [6] it was introduced fabric tensor characterizing contact distribution. All the microstructural theories have a common disadvantage: they can give only ideas to obtain equations of a real material, since there are many simplifications which can be not relevant but crucial.

3.3 Numerical particle dynamics methods

Apart from theoretical, there are three groups of numerical “microstructural” approaches:

1. Molecular dynamics (MD) methods: particles are material points interacting with a certain potential force. They may be united in aggregates. Potential of interaction between particles of the same aggregate may differ from the interaction potential for particle of different aggregates. Suggested in [7] for liquids. Advantages: easy rearrangement of contacts can be taken into account. In the case of two interaction potentials, formation, destruction and deformation of aggregates can be considered, as well as torque interactions between them. Disadvantages: this method is phenomenological, but it is not based on fundamental laws. The choice of interaction potentials is equivalent to the choice of constitutive equations, but it is done without fundamental theoretical base (unlike to continuum theories). There is no technique developed to verify the model comparing it with experiment or theory. The way to introduce inelasticity is also arbitrary and it is not clear which type of materials it may describe and which not.

2. Discrete elements method (DEM): particles are rigid bodies (usually spheres or disks) interacting with forces and torques approximately modelling contact interaction of elastic or viscoelastic nature. It was suggested in [8]. This model is closer to reality than MD. Torque interactions and rotation of particles are taken into account (contrary to the one-potential MD). However, as any microstructural model, DEM is limited to a particular case and usually does not model a real situation. It is not known which simplifications are admissible and which will give the picture strongly different from the reality. (The shape of particles, their variety in size and properties, and the nature of contacts will strongly influence the result.) Pairwise interaction used as a hypothesis for the calculation of forces is another limitation of the model.

3. Contact mechanics method: particles are rigid bodies with dry friction in contact. Forces are determined for a group of contacting bodies, solved numerically by iterations. The author of this method is J.-J. Moreau [9]. For hard particles it is more rigorous and closer to reality than both MD and DEM. However, again one makes simplifications about the shape of particles and type of interaction between
them which limit the result. The result depends on the initial approximation for contact forces (due to non-uniqueness of solution). Perhaps it reflects the fact we discuss below: the dynamic transient process in granular material may be very important to consider, since the static solution can be non-unique.

4 Continuum theories

We have briefly discussed the experimental and microstructural arguments that allow us to realize the difficulties of suggesting a good theory for the description of granular medium. Let us discuss several of the continuum theories.

4.1 Rigid-plastic and elastoplastic theories without rotational degrees of freedom of particle

The theory represented in classical monography by Sokolovski [10] interprets granular material in terms of rigid-plastic theory with Coulomb yield law with cohesion. In this theory we made a supposition that all the material is in the critical state. This is a theoretical contradiction, which leads, of course, also to discrepancies with experiment.

One can find, for instance, in [11] a short overview of plastic theories of granular materials. We shall quote here an extract from this work. Geotechnical and civil engineers usually use the so-called plastic potential model, in which a yield condition (an algebraic inequality satisfied by the stress components) is assumed to hold in conjunction with the stress equilibrium equations and the strain increment or deformation-rate tensor is obtained by differentiation of the plastic potential with respect to the components of stress. If the yield condition and plastic potential are determined from the same function the flow rule is called associated, otherwise it is called non-associated. For associated plasticity, plastic deformation rate is perpendicular to the yield surface. The “plastic potential function” and yield surface coincide. In non-associated plasticity, there are two different functions for yield surface and for the plastic potential.

Such plasticity models are now widely used in soil mechanics, see for example the classic paper by Drucker & Prager [12], or, for a realistic plastic potential based upon careful experimentation, see Lade [13]. Theories in which the equations are given directly, and no plastic potential exists, are called hypoplastic (e.g. [14]).

Another issue is ill- or well- posedness of the model, term used in the following specific way. A set of partial differential equations is linearly ill-posed with respect to initial conditions if, given a solution to the initial value problem, a sinusoidal perturbation of the given solution grows without bound in the limit of vanishingly short wavelengths.

In the case of granular materials there appears to be no consensus as to whether ill-posed equations form an acceptable model. On the one hand, there is reluctance among many researchers to accept ill-posed theories, on the other hand the fact that granular materials do exhibit unstable behaviour gives credence to the possibility that they be modelled in some sense by an ill-posed theory. However, we think that the nature of the ill-posedness is too strong, too all-pervading to be a reflection, say,
of the growth of a single shear-band. In the authors opinion, a more likely hypothesis is that the models are mathematically ill-posed due to a missing or incorrect physical law or attribute or due to the various physical laws being combined in an inconsistent way [11].

**Coaxial flow rule** is the flow rule which implies the coaxiality of stress and strain tensors (their principal axes coincide). This has to be so for isotropic classical media. However, experimental data say that this is not fulfilled for granular materials, where shear stress usually leads to the dilation or compression of the medium. For this reason, various variants of double-shearing model (non-coaxial flow rule) were developed [15], [16].

There is no theory which is both correct theoretically and describes essential features of granular materials. Coaxial flow rule is more correct theoretically, double shearing is closer to the practice but violates the material objectivity for classical isotropic materials. This problem may be solved in terms of the reduced Cosserat plastic model [11].

Though geoscientists and engineers (e.g. see [1]) insist that soils show a strongly nonlinear behaviour, and in some domains it can be possible to model it by a nonlinear theory with smooth potential, there is no universal theory which would be applicable for a wide class of soils.

**Incremental theories** are empirical theories trying to generalize experimental curves. They give us dependence of the increment of the strain depending on the increment of the stress. However, these theories have a strong defect. Usually they are written only for a certain type of deformation, for instance, for the triaxial test. An attempt to generalize directly the corresponding constitutive equations leads to the violation of the material objectivity principle, and, therefore, is not allowed. In fact, incremental theories are an inaccurate attempt to make linearization of a nonlinear elastoplastic material near a certain nonlinear state. The most popular incremental theory is probably the Cam clay model (series of models suggested in Cambridge: Schofield, Wroth and Roscoe, Burland, 1968). Soil is taken to be frictional with logarithmic compression, yield surface with the plastic potential surface. Increments of strains are represented as a sum of elastic and plastic parts. Elastic constants depend on the porosity and the principal stresses, e.g. the elastic part is nonlinear. The plastic part is also nonlinear in a similar way (see [3]).

### 4.2 Elastic Cosserat-type theories

There are several works taking into account rotation of particles in granular media, e.g. [17] (reduced Cosserat continuum, couple stresses are zero), [18], and other authors (full Cosserat continuum). In works by E.F. Grekova, G.C. Herman, M.A. Kulesh (e.g. [19–21]) the wave propagation in the elastic reduced Cosserat medium is considered. Its main differences in comparison with the classical elastic medium are: 1) strong coupling of shear and rotational waves, and in the anisotropic case also of compressional and rotational waves; 2) existence of a special band of frequencies where some waves do not propagate (the energy is trapped by rotation); 3) strong dispersion and apparent attenuation.

The model of weakly anisotropic reduced Cosserat continuum allows to introduce
“local anisotropy”, widely discussed in literature: for long waves the medium looks isotropic, and for short waves the anisotropy and rotational-translational coupling play role. “Induced anisotropy” may appear also as a result of nonlinear stress state. Of course, if these models or their generalization to elastoplastic case can be applied to granular materials, their applicability is very limited due to the linearity and the fact that the breaking of contacts is not really taken into account.

4.3 Heteromodular theories. Granular material does not present a classical behaviour: model experiment

There were several works by various authors ([22,23] and others) on the problem of a granular medium under the action of a vertical point force. It was observed that in experiments the stress distribution in such a medium is very different from the solution of the Flamant problem\(^1\). For instance, according to [22], the stress distribution in statics for the free lateral walls looks parabolic-like. Therefore the authors of [22] doubt that a granular material could be modelled in terms of continuum mechanics. However, we do not agree with this.

M.A.S. Quintanilla and J.M. Valverde (University of Seville) in collaboration with us made the same experiment with various lateral boundary conditions and obtained that the character of the stress distribution changes from the “diffusive-like” (free lateral walls, Fig. 2a) to “elastic-like” when one first confines the walls (Fig. 2b), and then applies the lateral compression (Fig. 2c).

**Figure 1.** Experiment with one photoelastic block. Experiment is in a good agreement with the analytical solution for the Flamant problem. Different colours correspond to different values of the stress.

**How to explain this model experiment?** If the medium would be linear, the results of the experiment after subtracting the stress caused by boundary conditions only (as done in Fig. 2) would be the same for different static boundary conditions. This is not the case. What could be possible sources of nonlinearity? The results of the experiment made by us with the photoelastic blocks lubricated by olive oil, are practically the same, i.e. the friction between the blocks is not large and does not play the role. Thus we make the following conclusions:

- The contact properties in this medium do not change. **The reason of this behaviour is the possibility of formation and destruction of the contacts between grains.**
- This medium does not resist to tension, but does resist to compression (for the free lateral walls).

---

\(^1\)Flamant problem is the problem of classical linear elastic half-space under the action of a vertical point load [24]. The stress tensor has only the radial component, the lines of equivalent stress are circles touching the surface of the half-space in the point of the loading. A big photoelastic block follows well this solution in the experiment (Fig. 1).
• The result of each experiment depends on the dynamical history of loading. For the case of classical elastic medium, the final stress distribution has only compressive component, but during the transient dynamic process the tensile stresses appear.

Figure 2. Experiment with “granular medium” made of photoelastic blocks: a) free lateral walls b) constrained lateral walls with zero compression c) lateral compression

The grains are rectangular photoelastic blocks of 9 mm height, and varying widths (16, 12, 10.66, 8, 5.33 and 4 mm) of polycarbonate elastomer, \( E = 3.15 \times 10^5 \) Pa, \( \nu = 0.36 \) (the same material as in Fig. 1). The system is placed between two crossed circular polarizers allowing us to visualize the stressed regions when the material is loaded. The punch is applied on top of the structure, its apex consisting of an 8-mm diameter steel sphere, \( F \approx 100 \)N. On the photos we see the difference between stress states, caused by the boundary conditions and the point load, on the one hand, and by the boundary conditions only, on the other hand. White colour corresponds to zero.

Heteromodular theories can be a possible way to treat the change of the contact structure described above. Heteromodular (bimodular, bilinear) elastic medium is a medium which has different ability to resist to the tension and compression. First works in this direction were made by Ambartsumyan [25].

To give an intuitive idea on the heteromodular media we cite for the illustration purpose its equations in 1D case. The equation of the longitudinal vibrations of a heteromodular bar is [25]:

\[
\sigma = \frac{1}{1 + a} E(\zeta - a|\zeta|), \quad \zeta = u'.
\] (1)

Here \( u(x, t) \) is the longitudinal displacement, prime is the derivative with respect to the longitudinal co-ordinate \( x \), \( \zeta \) is deformation, and \( a = \text{const}, \ 0 \leq a \leq 1 \). For the classical elasticity we have \( a = 0 \); for the cohesionless medium, \( a = 1 \).

For the cohesionless medium

• The theory is physically nonlinear and the equation of motion is strongly nonlinear even for small stresses and strains

• The elastic potential is not positive definite, therefore the solution of static problem can be non-unique; thus it is necessary to consider the dynamic transient process even for the quasi-static loading;

• Solutions can be discontinuous, it is possible to have even discontinuous displacements.
We have suggested a generalization for the 3D cohesionless medium of the last equation to take into account that tensile wave cannot propagate. The (isotropic) constitutive equation for 3D case can be formulated as follows. The strain tensor $\varepsilon$ can be represented in the following form:

$$\varepsilon = \zeta e_i, \quad e_i = -\nu I + (1 + \nu) e_{(i)} \otimes e_{(i)},$$  \hspace{1cm} (2)

where the stress tensor

$$\tau = \sum_{i=1}^{3} \sigma_i e_{(i)} \otimes e_{(i)},$$  \hspace{1cm} (3)

$I$ is the identity tensor, $e_{(i)}$ is $i$-th eigenvector of tensor $\varepsilon$; $\nu$ is the Poisson ratio for the compressed medium. Using the law of the balance of force $\nabla \cdot \tau = \rho (\ddot{u} - g)$ (here $g$ is the gravity acceleration) and the approximation of the plane stress state, we obtain the dynamic equations in displacements for 2D isotropic granular plate. They have different structure depending on the signs of deformations $\zeta_i$.

In domains where both deformations $\zeta_i$ ($i = 1, 2$) are negative, one obtains classical equations

$$c_2^2 \Delta u + (c_1^2 - c_2^2) \nabla \nabla \cdot u = \ddot{u} - g,$$  \hspace{1cm} (4)

where $c_1^2 = E/(1 - \nu^2 \rho)$, $c_2^2 = E/(2(1 + \nu) \rho)$. The corresponding statical equations are elliptic.

In domains where one of the deformations $\zeta_i$ (say, $\zeta_1$) is negative and another one is non-negative

$$c_b^2 \nabla \cdot (\zeta_1 e_{(1)} \otimes e_{(1)}) = \ddot{u} - g,$$  \hspace{1cm} (5)

where $c_b^2 = E/\rho$. The corresponding statical equations in this case are parabolic.

In domains where both deformations $\zeta_1$ and $\zeta_2$ are non-negative, the dynamical equations are $\ddot{u} - g = 0$. In the last case the statical problem loses meaning. We show that depending on the signs of deformations there may be domains with elliptic- and parabolic-like static equations, something that we qualitatively see in the model experiment discussed above.

One of the statically admissible solutions of the problem in terms of the cohesionless heteromodular theory, which looks more similar to the result of the experiment with free lateral walls than the solution in terms of classical elasticity, is shown in Fig. 3 (here the gravity is not taken into account).

For a cohesive medium its elastic moduli differ, but their ratio is finite. Even for such a medium, where the moduli differ very little, already for 1D case the solutions become highly nonlinear [26].
5  Change of the contact structure. Continuum of contacts.

In this section we shall give preliminary ideas for the development of a new type of models. Some of them may be wrong. The main difficulty is the easiness of the change of the structure of contacts. Granular material is almost permanently undergoing “phase transitions”. We separate two stages of the deformation: 1) when the structure of contacts is not changed (though the contact properties may change) and 2) when contacts appear or disappear. The first stage in reversible systems may be well described in terms of nonlinear elasticity. The second stage needs more considerations. We have to introduce the continuum of contacts and to write down the fundamental balance laws: the law of balance of energy, the second law of thermodynamics (if we have irreversibility), and, in future, the laws of balance of momentum and moment of momentum for the contact. For the time being, we shall consider only reversible systems.

5.1 Definitions and balance of energy

Definition 1. If we have a system (continuous or discrete) of point-bodies, we say that there is a contact between two of them, if an infinitesimal variation of the relative position and rotation of these point-bodies (provided all other positions and rotations to be “mathematically” fixed) affects any forces or couples in the system. (E.g. two particles glued to each other are in contact; two remote charged particles are in contact.)

Definition 2. The contact is critical if there is a possible infinitesimal change of the relative position or rotation of the point-bodies in contact, which does not affect any forces or couples in the system. We distinguish “translationally critical contacts” (dangerous for the stability) and “rotationally critical contacts” (allowing to store the energy by means of the free rotation).

Let $F$ be the set of all forces and torques in the system, and $q_{12}$ the set of co-ordinates determining the relative position of point-bodies 1 and 2. Then if these point-bodies are not in contact, $\partial F/\partial q_{12} = 0$, and if the contact is critical, this will be true for the subset of the relative co-ordinates that do not influence forces and torques in the system. When we look for the concrete expression of the internal energy $U$, we will have to find on which combinations of strain tensors and characteristics of the system of contact it may depend. This will require, probably, the application of a formalism similar to the one developed by P.A. Zhilin for the shell theory.

Each point of the continuum is described by the inertial properties and a set of contacts, a certain vector family (a “hedgehog”, whose spines are unit vectors $n$ pointing out the directions of contacts of a given point-body). We introduce measures of numbers of critical $c_{cr}$ and non-critical $c$ contacts as corresponding parts of the surface of this unit sphere. $c_{cr}$ corresponds to the easy change of the material structure and strong heteromodularity, $c$ to the classical elastic behaviour; $4\pi - (c + c_{cr})$ — to the weak resitence and easy destruction (for close range interactions).
Definition 3. We introduce contact tensors for non-critical and critical contacts:

\[
\begin{align*}
    c &= \int H d\Omega, \\
    c_c &= \int H n d\Omega, \\
    C &= \int H n n d\Omega, \\
    C_i &= \int H \otimes_i n d\Omega;
\end{align*}
\]

\(H\) is the characteristic function (0 if contact is absent, 1 if present). We introduce analogous tensors for critical contacts: \(c_{cr}, c_{cr}^c, C_{cr}, C_{cr i}\). These tensors describe completely the contact structure in a point of a medium. The magnitude \(c + c_{cr} \in [0; 4\pi]\) (for close range interactions), introduced for the continuum, is analogous to the coordination number in discrete systems. Tensor \(C + C_{cr}\) is similar to the fabric tensor; \(c = \text{tr} C\) (the same for critical contacts). All contact tensors are materially objective.

It is not obvious that we should use contact tensors and some functions from them for the description of the system of the contact. For practical purposes, perhaps, it would be better to choose another system of characteristics, vanishing rapidly enough with the rank of the tensor.

When a contact appears or disappears, there is some energy which is liberated, stored or consumed. Separating the part \(U_{\text{def}}\) of the internal energy corresponding to the deformation without breaking or making the contacts, we write down the balance of energy:

\[
\dot{U} = \dot{U}_{\text{def}} + f \cdot \dot{c} + F^T \cdot \dot{C} + F_i^T(\cdot) \dot{C}_i + f_{cr} \cdot \dot{c}_{cr} + F_{cr}^T \cdot \dot{C}_{cr} + F_{cr i}^T(\cdot) \dot{C}_{cr i}.
\]

\(f, F\) are “energetic structural forces”, they are related to the energetic cost of the change of structure. Probably, for applications it is sufficient to take into account terms with \(i \leq 2\). We have the constitutive equations for the energetic structural forces: \(f = \partial U / \partial c\), \(F = \partial U / \partial C\), and the same for critical contacts.

Definition 4. Tensors of critical directions \(D\) (of any rank) in each point are those tensors on which the energetic forces do not work, e.g. \(F^T \cdot D = 0\) (we can define it separately for critical and non-critical contacts, or for all contacts in total). Their physical meaning: “this change of structure costs nothing”.

If for any reason we know in advance tensors of critical directions in our continuum, we may apply the formalism developed for gyrocontinua and find out from which combination of strain and contact tensors the energy of deformation may depend. This will help to determine the concrete form of \(U\).

5.2 An illustration

To close the system of governing equations we need the law of change of the contact tensors, a condition of making and breaking the contact. What kind of a condition may we have?

A purely geometrical condition (for instance, contact appears when the distance between particles is less than a given length) is fair for non-cohesive media or any other medium where the surface energy of contacts may be neglected. Indeed, in these media jump into the contact and pull-off do not have “energetic cost”. This condition is applied in all methods of particle dynamics known to the authors. The corresponding part of the internal energy equals zero, and the energetic structural forces have to be zero.
In some cohesive media, apparently, energetic and force conditions also play role. For instance, it may be stated that the contact endures a certain limit force. In some cohesive media the surface energy which appears or disappears when the system of contacts changes, may be very important (like it is supposed in contact models by Johnson–Kendall–Robertson [27]). We can consider a simple model of jump-in – pull-off energetic condition: two potential wells and a barrier between them (Fig. 5.2). Which well is deeper, depends on the concrete situation. For such a model, both states (presence and absence of the contact) are, probably, stable (if we do not talk about critical contacts), but to make the transition from one state to another we need some energy. This energy can be obtained, for instance, from the kinetic energy when two particles collide, possibly, from the heat, or from the deformation energy. The difference between the wells can be “given back” to the same sources or stored in some other way. Both particles in fact are changing (or may change) when the contact appears or disappears.

Now let us write down the integral characteristics of the system of contacts. We shall consider the simplest case, when the normals of the contacts are fixed, the (geometrical) neighbours are fixed, and the only thing that may happen is jump into the contact and pull-off. This is something analogous to the model experiment described before, but with cohesion. In this case (\( \dot{n} = 0 \)) we have \( \dot{C} = \int \dot{H} n \ldots n \, d\Omega \). \( \dot{H} = 0 \), if the contact neither appears nor disappears; \( \dot{H} = \delta(t) \), if the contact appears, and \( \dot{H} = -\delta(t) \), if it breaks. First let us consider the case when the energetic “jump-in – pull-off” condition is equal for all possible contacts, i.e. does not depend on \( n \).

\[
\dot{U} = \dot{U}_{\text{def}} + \Delta \int \dot{H} d\Omega = \dot{U}_{\text{def}} + \Delta \dot{c} \tag{6}
\]

Here \( \Delta \) is the difference between energetic levels of both wells (there is a contact and there is no contact). Now, let \( \Delta = \Delta(n) \) (for instance, the condition changes depending on the neighbours). Now let us make a possibly prohibited thing. Suppose that we may expand the function \( \Delta \) in the way analogous to the multipole expansion: \( \Delta = \Delta(n) = \Delta_0 + \Delta_1 \cdot n + \Delta_2 \cdot n \cdot n + \cdots + \Delta_k \cdot \ldots \cdot n \ldots n \). This can be true if the function \( \Delta \) is nice enough (we shall not discuss now the necessary and sufficient
requirements for such functions). Then
\[
\dot{U} = \dot{U}_{\text{def}} + \int \dot{H} \Delta_0 \, d\Omega + \int \dot{H} \Delta_1 \cdot n \, d\Omega + \int \dot{H} \Delta_2 \cdot nn \, d\Omega + \ldots \\
+ \int \dot{H} \Delta_k \cdot \ldots \cdot n \ldots n \, d\Omega + \ldots = \dot{U}_{\text{def}} + \Delta_0 \int \dot{H} \, d\Omega + \Lambda_1 \cdot \int \dot{H} n \, d\Omega \\
+ \ldots + \Delta_k \cdot \ldots \cdot \int \dot{H} n \ldots n \, d\Omega + \ldots = \dot{U}_{\text{def}} + \Delta_0 \hat{c} + \ldots + \Delta_k \cdot \ldots \cdot \dot{C}_k + \ldots
\]

The last equality is true when \( \dot{n} = 0 \). Note that if \( C_k \) vanishes very rapidly with \( k \), we can write down formally the expansion of \( \Delta \) in \( n \) even when this series diverges, since the series of the corresponding products will converge. We see that we obtain the expression for the “energetic structural forces” defined above: at least for the considered particular case with fixed directions of possible contacts they correspond to the derivatives (with respect to the normal \( n \)) of the difference between potential wells of jump-in – pull-off transition. However, the contact tensors and their material derivatives may not vanish rapidly enough, or the function \( \Delta(n) \) may be not possible to expand in \( n \). In this case, probably, we should look for another functions instead of contact tensors, describing the fabric in a given point. This may be also useful if we wish to consider only several first members of the series. We suppose that the expansion (of \( H \) as well as of \( \Delta \)) in spheric harmonics can be useful here, analogously to [28,29]. Then instead of a system of contact tensors we will consider another set of functions characterizing the contact distribution in a point of the medium.

All discussed above concerns only the law of the balance of energy in the jump-in – pull-off transition. We need the laws of dynamics for contact tensors to close the system: \( \dot{C} = \mathcal{L}(F, \text{stress and strain tensors}) \). In existing theories this step is done in an implicit way: the contact disappears, when the stress or strain overcomes a certain limit (heteromodular theories, particle dynamics methods); the medium flows, when stress reaches the yield surface (plasticity); crack propagates if it is energetically favorable. . . Probably, this dynamic law should be written in a way similar to the balance laws for the nucleus of a new phase. This is the direction of the future work.

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Super-elastic collisions of thermal activated nanoclusters

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Abstract

Impact processes of nanoclusters subject to thermal fluctuations are investigated, theoretically. In the former half of the paper, we discuss the basis of quasi-static theory. In the latter part, we carry out the molecular dynamics simulation of collisions between two identical nanoclusters, and report some statistical properties of impacts of nanoclusters.

1 Introduction

The initial kinetic energy of colliding bodies is distributed into the internal degrees of freedom in an inelastic collision. Such a collision is characterized by the restitution coefficient \( e \equiv V' / V \), where \( V \) and \( V' \) are, respectively, the relative colliding speed and the relative rebound speed. Although it is believed that the restitution coefficient \( e \) satisfies \( e < 1 \) for impacts of macroscopic bodies, the anomalous impact with \( e > 1 \) is possible in some special situations for small bodies. Indeed, the prohibition of \( e > 1 \) is originated from the second law of thermodynamics[1, 2], but some terms which disappear in the thermodynamic limit play important roles in the description of small systems. It should be noted that the restitution coefficient projected into the normal direction of the collision can easily exceed unity in the case of oblique collisions.[3, 4]

The low-speed collisions for macroscopic bodies are believed to be described by the quasi-static theory, which is consistent with some experimental results.[5, 6, 7] However, it is not obvious whether the quasi-static theory is applicable to the impact of nanoclusters. Indeed, we expect that the effects of cohesive force among atoms cannot be ignored for such small systems. Awasthi et al.[8] reported that the dependence of the restitution coefficient \( e \) on the impact speed for nanoclusters, which contain adhesions, differs from the prediction from the quasi-static theory based on their molecular dynamics simulation (MDS). In a recent paper, Brilliantov et al. extend the quasi-static theory to the theory of cohesive collisions.[9]
The physics of nanoclusters is one of hot subjects. The MDS is a standard tool to investigate collisions of nanoclusters such as fulleren. Some of such studies focus on fragmentations and coalescences after binary collisions of nanoclusters[10, 11, 12]. The other studies discuss the collisions of a cluster with a substrate[8], the erosion process on a diamond surface[13], and the fragmentation pattern of clusters[14]. So far, we do not know any paper to investigate the effects of thermal fluctuations on collisions of nanoclusters except for our preliminary report.[15]

In this paper, we perform the MDS of colliding clusters to investigate the effect of thermal fluctuations. This is the extension of our previous work.[15] In the first part, we review what model is adequate to describe the collision of nanoclusters. In the next section, we introduce the generalized Langevin equation and the fluctuation-dissipation relation in the first kind. In section 3, we calculate the velocity autocorrelation function (VACF) of a lattice model to apply it to a system of a nanocluster. Then, we justify the quasi-static theory to describe the collisions of nanoclusters. In the second part, we show the detailed results of our numerical simulations. In section 4, we introduce our numerical model of the MDS. In section 5, we explain the results of our simulation, which consist of four subsections. In the first subsection, we check the relaxation of VACF in our model. In the next subsection, we demonstrate sequential snapshots of collisions between two identical nanoclusters. In section 5.3, we compare our numerical result of the impact speed dependence of the restitution coefficient with the quasi-static theory of cohesive or noncohesive collisions. In section 5.4, we show the frequency distribution functions of the restitution coefficient and their dependence on cohesive force between atoms. We also show the probabilities to appear four categories in our simulation when the cohesive parameter is finite. In section 6, we discuss and summarize our results.

2 The Langevin equation

It is well known that we can formally rewrite the Newtonian equation of motion as the generalized Langevin equation for the ‘slow’ variable. When we consider the motion of colliding a pair of small clusters, it is natural to adopt the relative velocity $v$ between the center of mass of each cluster as the ‘slow’ variable[16]. We should note that the center of mass is characterized by the total mass of one cluster, while each element of the cluster can be characterized by the mass for the element. Thus, the effective mass of the center of mass is much larger than the mass of the element. Thus, the generalized Langevin equation is given by

$$\frac{dv}{dt} = -\int_{-\infty}^{t} dt' \gamma(t-t')v(t') + \theta(t) + \frac{F(t)}{M},$$

where $\gamma(t)$, $\theta(t)$, $M$, and $F(t)$ are the memory kernel, the fluctuating force from the fast oscillations, the reduced mass of two clusters, and the systematic force acting on the centers of mass, respectively. The fluctuation force $\theta(t)$ is believed to be unimportant for the impact problem of two clusters. The systematic force $F(t)$ may be approximated by the Hertzian contact force. From the fluctuation-dissipation
relation in the first kind, the Laplace transform \(\hat{\gamma}(\omega) \equiv \int_0^\infty dt \gamma(t) e^{-i\omega t}\) satisfies
\[
(i\omega + \hat{\gamma}(\omega))^{-1} = \frac{M}{T} \int_{-\infty}^{\infty} dt \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle e^{-i\omega t},
\]
(2)
where \(T\) is the temperature, and the Boltzmann constant is set to be unity[17]. We should note that \(\hat{\gamma}(\omega)\) can be defined as the usual Fourier transform if we assume \(\gamma(t) = \gamma(-t)\) for \(t < 0\). If the integration of the velocity autocorrelation function (VACF), i.e. \(\int_0^\infty dt \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle\) is finite, \(\hat{\gamma}(\omega \rightarrow 0)\) is finite. In this case, the generalized Langevin equation can be approximated by the Langevin equation with the white noise satisfying \(\langle \hat{\theta}_i(t) \cdot \hat{\theta}_j(t') \rangle = 2T \gamma \delta_{i,j} \delta(t - t')\) where \(\hat{\theta}_i(t)\) is the \(i\)-th component of \(\hat{\theta}(t)\). It is obvious that this Langevin equation is an irreversible equation. Thus, the behavior of VACF is the most important to characterize the macroscopic dissipation.

3 The relaxation of the correlation function

As discussed in the previous section, the relaxation of VACF plays a key role for the equilibration process of a system. Let us consider the relaxation of VACF in a nanocluster which consists of a regular lattice with equal-mass atoms. When the atoms are confined in attractive potential, the excitation from the ground state is characterized by the harmonic oscillation in a simple cubic lattice. In this section, we demonstrate that VACF of a uniform system in the simple cubic lattice exhibits the slow relaxation proportional to \(1/\sqrt{t}\). The analysis presented here is the straightforward extension of the one-dimensional cases.[16]

Let us consider an infinitely large simple cubic lattice system in which the mass points with mass \(m\) connecting with the linear spring whose spring constant is \(k\). The position of each lattice point can be specified by a set of integer \(\mathbf{n} = (n_x, n_y, n_z)\) in this system. Introducing the characteristic angular frequency \(\omega_0 \equiv \sqrt{k/m}\), the equation of motion of the deviation from the equilibrium position \(\mathbf{r}_n(t)\) obeys
\[
\ddot{\mathbf{r}}_n(t) = -\omega_0^2 (6\mathbf{r}_n(t) - \sum_{i=1}^6 \mathbf{r}_{n+\mathbf{e}_i}(t)),
\]
(3)
where \(\mathbf{e}_1 = (1, 0, 0), \mathbf{e}_2 = (-1, 0, 0), \mathbf{e}_3 = (0, 1, 0), \mathbf{e}_4 = (0, -1, 0), \mathbf{e}_5 = (0, 0, 1)\) and \(\mathbf{e}_6 = (0, 0, -1)\).

Let us introduce the lattice Fourier transform and the inverse Fourier transform as
\[
\hat{\mathbf{r}}_k(t) \equiv \sum_n e^{-ik \cdot n} \mathbf{r}_n(t), \quad \mathbf{r}_n(t) = \frac{1}{(2\pi)^3} \int dk e^{ik \cdot n} \hat{\mathbf{r}}_k(t),
\]
(4)
where \(\sum_n = \sum_{n_x=-\infty}^{\infty} \sum_{n_y=-\infty}^{\infty} \sum_{n_z=-\infty}^{\infty}\) and \(\int dk = \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \int_{-\pi}^{\pi}\). Thus, the equation of motion in the Fourier space is given by
\[
\ddot{\hat{\mathbf{r}}}_k(t) = -4\omega_0^2 \sum_{i=1}^6 \sin^2 \left(\frac{k_i}{2}\right) \hat{\mathbf{r}}(t),
\]
(5)
Furthermore, introducing the Laplace transform \( \tilde{r}_k(z) \equiv \int_0^\infty dt e^{-zt} \hat{r}_k(t) \), we obtain

\[
\tilde{r}_k(z) = \frac{z \hat{r}_k(0) + \hat{r}_k(0)}{z^2 + 4\omega_0^2 \sum_{i=1}^3 \sin^2 \left( \frac{k_i}{2} \right)}. \tag{6}
\]

Let us consider the motion of the mass point at the center of the mass in the system. From the relation \( \mathbf{r}_0(t) = \int \frac{dk}{(2\pi)^3} \hat{r}_k(t) \), we reach

\[
\tilde{r}_0(z) = \frac{1}{(2\pi)^3} \int dk \frac{z \hat{r}_k(0) + \hat{r}_k(0)}{z^2 + 4\omega_0^2 \sum_{i=1}^3 \sin^2 \left( \frac{k_i}{2} \right)}, \tag{7}
\]

where we have used \( \tilde{r}_n(z) \equiv \int_0^\infty dt e^{-zt} \hat{r}_n(t) \).

Here, VACF at the center of the mass is defined by

\[
\phi(t) \equiv \langle \hat{r}_0(0) \cdot \hat{r}_0(t) \rangle,
\]

where \( \langle \cdots \rangle \) represents the ensemble average over the different initial conditions. We assume that the initial condition satisfies

\[
\langle \hat{r}_m(0) \cdot \hat{r}_n(0) \rangle = \delta_{m,n} \frac{3T}{m} \delta_{m,n}, \quad \langle \hat{r}_n(0) \cdot \hat{r}_0(0) \rangle = 0. \tag{9}
\]

Then, the Laplace transform of \( \tilde{\phi}(z) \equiv \int_0^\infty e^{-zt} \phi(t) = z \langle \hat{r}_0(z) \cdot \hat{r}_0(0) \rangle \) of \( \phi(t) \) satisfies

\[
\tilde{\phi}(z) = \frac{1}{(2\pi)^3} \int \frac{zk \hat{r}_k(0) + \hat{r}_k(0)}{z^2 + 4\omega_0^2 \sum_{i=1}^3 \sin^2 \left( \frac{k_i}{2} \right)}
\]

\[
= \frac{3Tz}{(2\pi)^3m} \int \frac{dk}{z^2 + 4\omega_0^2 \sum_{i=1}^3 \sin^2 \left( \frac{k_i}{2} \right)}, \tag{10}
\]

where we have used \( \langle \hat{r}_k(0) \cdot \hat{r}_0(0) \rangle = 3T/m \). From the inverse Laplace transform of \( \tilde{\phi}(z) \) we obtain the expression

\[
\phi(t) = \frac{3T}{m} \int \frac{dk}{(2\pi)^3} \cos \left[ 2\omega_0 t \sum_{i=1}^3 \sin^2 \left( \frac{k_i}{2} \right) \right]. \tag{11}
\]

Since the direct integration of (11) is difficult and we are not interested in the detailed properties of the lattice, we may introduce the approximation \( \sum_{i=1}^3 \sin^2 \frac{k_i}{2} \approx \sum_{i=1}^3 k_i^2 / 4 = k^2 / 4 \approx \sin^2 \frac{k}{2} \), where \( k \equiv \sqrt{\sum_{i=1}^3 k_i^2} \). Once we adopt such an approximation, we obtain

\[
\phi(t) \approx \frac{3T}{2\pi^2 m} \int_0^\pi dk k^2 \cos \left[ 2\omega_0 t \sin \frac{k}{2} \right]. \tag{12}
\]

From the numerical integration of this expression, it is clearly to find \( \phi(t) \sim 1/\sqrt{t} \) (see Fig. 1). Indeed, when we put \( \tau = 2\omega_0 t \sin k/2 \), there is the relation \( k^2 dk = 4dk - 4d\tau / (\omega_0 t) + O(k^4 dk) \). If we ignore the terms of \( k^4 dk \), we obtain the approximate relation \( I(t) \equiv \int_0^\pi dk k^2 \cos[2\omega_0 t \sin k/2] \approx 4\pi J_0(2\omega_0 t) - 4 \sin(2\omega_0 t) / (\omega_0 t) \). From the asymptotic form of the Bessel function, we obtain \( I(t) \approx \sqrt{\pi / (\omega_0 t)} \cos(2\omega_0 t - \pi/4) \) for \( \omega_0 t > 1 \). This result is essentially the same as that for one-dimensional case.
\( \phi(t) \propto J_0(2\omega_0 t) \). This time dependence of VACF can be observed in the direct simulation of nanoclusters in which each cluster is a 13 layer of the spherical cut of face-centered cubic (FCC) lattice, i.e. 682 Lennard-Jones atoms (Fig.3). The setup of our simulation will be explained in the latter part.

In spite of this extremely slow relaxation under the absence of \( \hat{\gamma}(0) \), we can approximately define the friction constant in the Langevin equation to describe the low frequency behaviors. Actually, if we adopt the approximation \( \phi(t) \simeq \alpha \cos(\omega_0 t)/\sqrt{\omega_0 \vert t \vert} \) with a constant \( \alpha \) for large \( t \), substituting this into (2) we obtain

\[
(\omega + \hat{\gamma}(\omega))^{-1} = \alpha \frac{m}{T} \left\{ \frac{1}{\sqrt{2\omega_0 - \omega}} + \frac{1}{\sqrt{2\omega_0 + \omega}} \right\} \simeq \frac{\sqrt{2} \alpha m}{T \omega_0} (1 + \frac{1}{4} \left( \frac{\omega}{2\omega_0} \right)^2 + \cdots )
\]

for \( \omega \ll \omega_0 \). Thus, we may approximate \( \gamma(t) = \int_{-\infty}^{\infty} d\omega / 2\pi e^{i\omega t} \hat{\gamma}(\omega) \) by

\[
\gamma(t) \simeq \Omega \delta(t) - \frac{d\delta(t)}{dt}
\]

where \( \delta(t) \) is Dirac’s delta function and \( \Omega \equiv T / \sqrt{\omega_0} / (\sqrt{2} \alpha m) \). Thus, the memory term can be approximated by

\[
\int_{-\infty}^{t} dt' \gamma(t') v(t') \simeq \Omega v(t) + \frac{dv}{dt} - \delta(0) v(t)
\]

where the last term can be absorbed in the initial condition. Finally, we obtain the effective Langevin equation for the low frequency behavior at \( t \neq 0 \) as

\[
\frac{dv}{dt} = -\frac{\Omega}{2} v + \frac{\theta}{2} + \frac{F}{2M}
\]

which does not have any essential difference from the conventional Langevin equation. This may justify to use the quasi-static theory even when we consider a collision between nanoclusters of a uniform lattice system. Indeed, once we accept
to use the Langevin equation, it is straightforward to derive the quasi-static theory of macroscopic collisions.\[5, 6, 7\]

It should be noted that the motion of the atom at the center of mass can be described by the equation of motion for a harmonic oscillator. In order to use eq.(1), we need to introduce some tricks, such as the mass difference, the contact with the other atoms and the nonlinearity. However, this argument may be instructive to understand the basis of the Langevin equation from the mechanical point of view.

4 Our numerical model

Let us introduce our numerical model. Our model consists of two identical clusters. Each of them is the spherical cut from a 13 layered face-centered cubic (FCC) lattice and consisted of 682 “atoms”. When we simulate larger size of nanoclusters, the system is fluidized in the vicinity of surface, while the data for the smaller systems strongly depend on the specific orientation of impacts. The details of system size dependence of the simulation will be reported elsewhere.

The clusters have facets because of the small number of “atoms” (Fig. 3). All the “atoms” in each cluster are bounded by the Lennard-Jones potential $U(r_{ij})$ as

$$U(r_{ij}) = 4\epsilon \left\{ \left( \frac{\sigma}{r_{ij}} \right)^{12} - a \left( \frac{\sigma}{r_{ij}} \right)^{6} \right\},$$

where $r_{ij}$ is the distance between two “atoms”, $i$ and $j$. The coupling coefficient of the attractive term $a$ is treated as a cohesive parameter between atoms on the surfaces of one cluster and those on the surface of another, while the potential act on the atoms within the same cluster satisfies $a = 1.0$. Here, we will consider collisions for the control parameters $a = 0$ and $a = 0.2$ between different clusters.\[8\]. In eq.(17), $\epsilon$ is the energy constant and $\sigma$ is the lattice constant. When we regard the “atom” as argon, the values of the constants become $\epsilon = 1.65 \times 10^{-21}$J and $\sigma = 3.4$Å, respectively. \[18\] Henceforth, we label the upper and the lower clusters as cluster $C_u$ and cluster $C_l$, respectively. To reduce computational costs, we introduce the cut-off length $\sigma_c$ of the Lennard-Jones interaction as $\sigma_c = 2.5\sigma$.

The procedure of our simulation is as follows. The initial velocities of the “atoms” in both $C_u$ and $C_l$ satisfy the Maxwell-Boltzmann distribution at the initial temperature $T$. The initial temperature is set to be $T = 0.01\epsilon$ or $T = 0.02\epsilon$ in most of our simulations. Sample average is taken over different sets of initial velocities governed by the Maxwell-Boltzmann velocity distribution for “atoms”.

To equilibrate the clusters, we adopt the velocity scaling method \[19, 20\] for 2000 steps in the initial stage of simulations. We have checked the equilibration of the total energy in the initial relaxation process. After the equilibration, we give translational velocities to $C_u$ and $C_l$ at the relative separation $\sigma_c$ between two clusters to make them collide against each other, where the initial colliding speed is achieved by the acceleration $g = 0.01\epsilon/(m\sigma)$ from a stationary state. The relative speed of impact ranges from $V = 0.02\sqrt{\epsilon/m}$ to $V = 0.07\sqrt{\epsilon/m}$, which are less than the thermal velocity for one “atom” defined by $\sqrt{T/m}$, where $m$ is the mass of the “atom”.
Numerical integration of the equation of motion for each atom is carried out by the second order symplectic integrator with the time step $dt = 1.0 \times 10^{-2}\sigma/\sqrt{\epsilon/m}$.

The rate of energy conservation, $|E(t) - E_0|/|E_0|$, is kept within $10^{-5}$, where $E_0$ is the initial energy of the system and $E(t)$ is the energy at time $t$.

We let the angle around $z-$axis, $\theta^z$, be $\theta^z = 0$ when the two clusters are located in mirror-symmetric positions with respect to $z = 0$. In most of our simulation, we adopt the data at $\theta^z = 0$. From our impact simulation for $\theta^z_i = \pi i/18$ ($i = 1, ..., 9$) at $T = 0.02\epsilon$ we have confirmed that the initial orientation does not crucially affect the restitution coefficient.

5 The results of our numerical simulation

5.1 The relaxation of velocity autocorrelation function

At first, we have carried out the contact simulation for two identical nanoclusters contacting each other. From our simulation, we verify that the Hertzian contact theory can be used without introduction of any fitting parameters[15]. The details will be reported elsewhere. Another purpose of the contact simulation is to check whether eq.(12) can be used in our system. For this purpose, we make the two identical clusters contact each other under the mirror symmetric configuration, and equilibrate them at $T = 0.03\epsilon$. After the equilibration, we leave those clusters, and record the time evolution of the velocity of 14 atoms near the center of mass of the upper cluster, and collect 50 samples with different initial velocities for all the atoms, i.e. we average the data under 700 different samples to calculate VACF.

Figure 2 is the result of VACF near the center of mass of the upper cluster in our simulation. The upper envelope line is given by $f(x) = 0.0029x^{-1/2}$, which is consistent with the theoretical prediction.

5.2 The collision of two identical clusters

In this subsection, we show the results of out simulations for colliding two identical nanoclusters. We mainly simulate the two cases for the interaction between different clusters: the completely repulsive case with $a = 0.0$, and the weakly cohesive case with $a = 0.2$, where $a$ is the cohesive parameter in eq. (17) between different clusters.

Let us show the sequential snapshots of two colliding clusters. Figure 3 (a) and (b) show the collisional behavior in the case of $a = 0.0$ and $a = 1.0$, respectively. It should be noted that we demonstrate the case of $a = 1.0$ to emphasize the difference between the noncohesive collision and the cohesive collision. In Fig. 3 (b), we can observe the elongation of clusters along the $z-$axis before the separation, while we do not observe any elongation of clusters before the separation in Fig. 3 (a). This elongation in Fig. 3 (b) is the result of the cohesive interaction between two clusters.
Super-elastic collisions of thermal activated nanoclusters

Figure 3: Sequential snapshots of two colliding clusters in the cases of (a) a=0.0 and (b) a=1.0.

5.3 The relations between the restitution coefficient and the colliding speed

Here, we numerically investigate the relation between the restitution coefficient and the colliding speed. Figure 4 shows the relation between the restitution coefficient $e$ and the relative speed of impact $V/\sqrt{\epsilon/m}$ in purely repulsive collisions with $a = 0$. The initial configurations of two colliding clusters are assumed to be mirror symmetric. The cross points and error bars in Fig.4 are, respectively, the average and the standard deviation of 100 samples for each colliding speed. From Fig. 4, we confirm that the restitution coefficient $e$ decreases with the increase of the colliding speed $V/\sqrt{\epsilon/m}$. When the colliding speed is $V = 0.02\sqrt{\epsilon/m}$ at $T = 0.02\epsilon$, the average of $e$ becomes 1.04 which is slightly larger than unity. It is interesting that our result can be fitted by the quasi-static theory of low-speed impacts $1 - e \propto V^{1/5}[5, 6, 7]$ when the restitution coefficient in the limit $V \to 0$ is replaced by a constant larger than unity. Indeed, the solid and the broken lines in Fig. 4 are fitting curves of $e = \alpha_1 - \alpha_2 \left(V/\sqrt{\epsilon/m}\right)^{1/5}$, where $\alpha_1$ and $\alpha_2$ depend on material constants of colliding bodies and $T$.

We also briefly discuss the effect of the size dependence on the result. The results of our simulation for $N = 433$, which is a 11 layered spherical cut of FCC lattice, cannot be approximated by the quasi-static theory, where the restitution coefficient seems to be almost independent of the colliding speed in the wide range of the impact speed. On the other hand, we cannot find any systematic relation between the restitution coefficient and the colliding speed in the simulation for $N = 1466$ which is a 17 layered spherical cut of FCC lattice. This can be attributed to the
melting on the surface of the cluster. The details of the melting properties will be reported elsewhere.

Next, we investigate the weakly cohesive collisions with $a = 0.2$ between those two clusters. Figure 5 shows the relation between restitution coefficient and impact speed, where 100 samples are taken for each colliding speed at the initial temperature $T = 0.02\epsilon$. When there is the cohesive interaction between two colliding clusters, the relation has a peak as suggested by Brilliantov et al.[9]. In the figure, the open circles are the numerical results obtained by solving the equation developed by Brilliantov et al.[9]. To solve this equation, we evaluate the values $\gamma \simeq 0.026\sqrt{\epsilon m/\sigma}$ from the calculation of the attractive interaction between two clusters. The theoretical result in Fig. 5 suggests that the restitution coefficient is insensitive to the colliding speed for the large colliding speed, though the restitution coefficient slightly decreases with the increment of the colliding speed.

### 5.4 The frequency distribution functions of the restitution coefficient

Here, we show our numerical results on the frequency distribution function of the restitution coefficient, which strongly depends on the cohesive parameter. Figure 6 shows histograms of the restitution coefficients for both the purely repulsive collisions and the cohesive collisions $a = 0.2$. When there is no cohesive interaction between the two clusters, the frequency distribution function is roughly represented by the Gaussian distribution function. On the other hand, the frequency distribution function is irregular when the cohesion exists. It is notable that the anomalous events for $e$ to exceed the unity becomes rare when there is the attractive interaction between clusters, though a few percent of the collisions still exhibit the anomalous

---

1The surface tension $\gamma$ can be calculated from the attractive potential. The method of our evaluation will be reported elsewhere.
impacts. This is because two clusters are coalesced with each other in the slow impacts. Therefore, the frequency distribution function for $a = 0.2$ has a steep peak near $e = 1$.

In Fig.6(b), there are the first and the second peaks around $e = 0.4$ and $e = 0.65$, respectively. The collisional modes observed around these peaks are the rotational bounces after the collisions, while the most of bounces are not associated with rotations in the vicinity of the third peak around $e = 1$. It is reasonable that the excitation of macroscopic rotation lowers the translational energy to decrease the restitution coefficient.

![Figure 6](image)

Figure 6: Histograms of the restitution coefficients for (a) $a = 0.0$, $V = 0.02\sqrt{\epsilon/m}$, and (b) $a = 0.2$, $V = 0.1\sqrt{\epsilon/m}$. The guide line in the left figure is the Gaussian fitting of the data.

For cohesive collisions, we can categorize the rebound behaviors of the colliding clusters into four patterns (see Fig. 7): (a) $n = 0$ (complete adhesion), (b) $n > 1$, (c) $n = 1$ and $e < 1$, and (d) $n = 1$ and $e > 1$, where $n$ is the number of collisions in each impact process. The collision with $n > 1$ can take place, when the attractive interaction between the colliding clusters exists. Indeed, if the rebound speed is not large enough, the rebounded clusters are attracted to have the second collision. We call the case with $e > 1$ and $n = 1$ the anomalous impact, but there are some other characteristic collisions as can be seen in Fig. 7.

Similarly, we categorize the collisions into four groups as a function of the cohesive parameter under the fixing colliding speed $V = 0.02\sqrt{\epsilon/m}$ (Fig. 8). It is obvious that there are two categories, (c) and (d), in noncohesive collisions, while the probability to occur (a) or (b) increases as $a$ increases. It is interesting that Fig.8 is almost the mirror symmetric one of Fig. 7. This fact suggests that the cohesive parameter plays a role of the impact speed. The relation between the impact speed and the cohesive parameter will be discussed elsewhere.

6 Discussion and conclusion

In this paper, we study collisions of nanoclusters which are thermally activated. We also discuss the effects of cohesive force between the colliding two clusters. Although
the results are preliminary, we believe that our paper includes some potentially important results for the nanoscience. Let us briefly discuss our results. An anomalous impact with \( e > 1 \) occurs with a finite probability even for realistic situations (see Fig. 8). This is an important indication, though the cohesive force between the colliding clusters suppresses such events in the low speed collisions. We also find an interesting similarity in the roles of the impact speed and the cohesive parameter (Fig. 8). It is more interesting that the cluster is fluidized when the cluster is large. There is capillary instability at the surface of the large cluster, because the influence of the attractive binding force from the center of mass is weaker, the size of the cluster is larger. The quantitative discussion will be discussed elsewhere.

In conclusion, we study the impact of thermally activated nanoclusters numerically. We confirm that VACF satisfies \( \phi(t) \sim 1/\sqrt{t} \). The restitution coefficient seems to be consistent with the quasi-static theory when there is no attractive interaction between the two colliding clusters, while the restitution coefficient has a peak at a finite value of the impact speed, when the attractive interaction exists. The anomalous impacts which have \( e > 1 \) commonly take place in purely repulsive collisions, while such an impacts become rare in cohesive collisions. The frequency distribution function satisfies Gaussian for purely repulsive collisions and has some peaks in cohesive collisions.

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Simulation of microscopic compression-tension behavior of cohesive dry powder by applying DEM

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Abstract

The microscopic behavior of dry cohesive powders is considered by applying the DEM. Poly-disperse powder is composed by ultrafine (d ≥ 1µm) smooth spherical particles. Elastic–plastic–dissipative contact model with adhesion is applied to model the normal and tangential contact forces. Influence of contact velocity is considered in details. Micromechanical compression–tension behavior of powder is simulated by 1000 particles.

1 Introduction and background

The rapid increasing production of poly-dispersed dry cohesive ultrafine powders (d ≥ 1µm), e.g. adhering pigment particles, micro-carriers in biotechnology, auxiliary materials in catalysis, make technical problems much more serious like undesired adhesion in particle conversion or powder handling, and desired in agglomeration or coating. Thus, understanding the fundamentals of particle adhesion with respect to product quality assessment and process performance is very essential in powder technology. Cohesive powders like other granular materials are currently being studied by applying experimental, theoretical and numerical methods.

Recently, the discrete (distinct) element method (DEM) introduced by Cundall and Strack [1] has become a powerful tool for solving many scientific and engineering powder technology problems. It started with its first application to simulate the dynamic behaviour of non-cohesive granular material, which is presented as an assembly of grains. The DEM is based on the Langrangian approach, meaning that particles of the granular material are treated as individual objects and all dynamical parameters (position, velocity, orientation and etc.) of each particle are tracked during the simulation. Inter-particle contacts are described by normal and tangential forces and several approaches and models have been developed for description of contact behaviour. In major cases, the normal contacts are of repulsive character and the Hertz contact theory is usually used to describe repulsive contact forces.
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independently on particle size. Fundamentals of the DEM, particular models and import! ant details of simulation technique of non-cohesive granular material may be found in [2-8].

Investigation of the nature of smaller particles required to apply new models. Consequently, significance of the surface attraction or adhesive force increases for small particles when atomic and molecular forces became important. Actually, particle adhesion is caused by surface and field forces as well as material bridges between particle surfaces and interlocking. An expression of the normal force for spherical particles has been suggested by Johnson et al. [9]. This model assumes that the surface attraction force only results in a change of surface energy over the contact area. Derjaguin et al. [10] considered a model where surface attraction forces have a finite range and, therefore, act just outside the contact zone where surface separation is small. Independently on development of the discrete element method, first comprehensive physical models for fine particles were published by Molerus [11, 12].

The earliest discussions about simplest adhesion (surface attraction) models and the importance of these effects to the results of the simulation of granular material behaviour are presented by Thornton and Yin [13] and Kohring [14, 15]. Comprehensive research on cohesive powders is continued continued by Tomas and co-workers [16-18]. Fundamentals of cohesive powder consolidation and flow are generalised in [19]. Here, the model of ”stiff particles with soft contacts” was used for fine to ultra-fine particles. This model includes the elastic-plastic particle contact behaviours with adhesion and load-unload hysteresis. Some other interesting contribution and DEM simulations may be outlined. Shear behaviour of cohesive powders with friction was studied by Luding [20]. Cohesive powders combining contact elasticity and distant van der Waals-type attraction were simulated by Gilabert et al. [21]. Collision dynamics of granular particles with adhesion are considered by Brilliantov et al. [22] focusing basically on characterization of both restitutive collisions described by the coefficient of restitution as well as aggregative collisions described critical aggregative impact velocity.

Comprehensive literature reviews of recent developments are presented by Tomas [24-26]. Therewith, adhesion of ultrafine particles basing on micromechanical philosophy along with complex constitutive models was considered. Despite of increased interest and many years of experience investigation of cohesive powders are extremely difficult, while application of numerical simulations provide a feasible alternative to physical experiments. The microscopic behaviour of dry cohesive powders is considered by applying the DEM. Poly-disperse powder is composed by ultrafine \( d \geq 1\mu m \) smooth spherical particles. Elastic–plastic–dissipative contact model with adhesion is applied to model contact forces. Influence of contact velocity and adhesion force is simulated by considering binary contact of two particles and discussion on results is presented. Behaviour of cohesive powder is illustrated by simulation of 1000 particles.

2 DEM methodology

The DEM methodology considered in this paper is aimed to simulate dynamic behaviour of the cohesive powders. Actually, powders as granular material present a
3D space filled with spherical particles, termed hereafter as discrete elements. From modelling point of view, granular material is regarded as a system of finite number of deformable bodies with the given geometry and material properties. When moving, the particles, as the contacting bodies, impact and deform each other. The composition of the media is time-dependent because individual particles change their position due to the free rigid body motion or because of contacting with the neighbouring particles or walls. The motion of arbitrary particle \( i \) is characterized by a small number of global parameters: positions \( \mathbf{X}_i \), velocities \( \dot{\mathbf{X}}_i \) and accelerations \( \ddot{\mathbf{X}}_i \) of the mass center and force applied to it. Accordingly, Newton’s second law is applied to each particle \( i \) in order to describe its translational and rotational motion according to:

\[
\begin{align*}
\frac{d^2 \mathbf{X}_i}{dt^2} &= \mathbf{F}_i \\
\frac{d^2 \Theta_i}{dt^2} &= \mathbf{T}_i
\end{align*}
\]

where \( \mathbf{X}_i, \Theta_i \) are the vectors of the position of the centre of gravity and the orientation of the particle, \( m_i \) is the mass of the particle \( i (i = 1, N) \), \( I_i \) is the inertia moment of the particle, \( t \) is the time. Vectors \( \mathbf{F}_i \) and \( \mathbf{T}_i \) present the resultant contact forces and torques that act on the particle \( i \), respectively.

Methodology of calculating the forces in (1-2) depends on the particle geometry and mechanical properties as well as on the constitutive model of the particle interaction. Detailed description of models will be presented below. The solutions of differential equations (1-2) for each particle \( i \) at the time \( t + \Delta t \) (where \( \Delta t \) is the time step) is performed by numerical integration [2, 4]. The numerical simulation was performed by implementing the basic relations into the developed software DEM-MAT [7]. Standard Particle Flow code (PFC2D, from ITASCA) [25] was applied in particular cases.

### 3 Constitutive model for particles inter-action

The evaluation of the inter-particle as well as particle-wall interaction forces is focused on evaluation of separate force \( \mathbf{F}_{ij} \) acting between particles \( i \) and \( j \). Constitutive model comprising force–displacement and, if necessary, moment–angle, relations in form of algebraic functions has to be derived for these purposes. Because of different character, normal and tangential models are considered separately. Hence, the interaction force \( \mathbf{F}_{ij} \) found between two particles \( i \) and \( j \) is expressed in terms of the normal and the tangential components \( F^h_{ij} \) and \( F^t_{ij} \).

Generally, interaction comprises field and contact forces of various nature. Constitutive relationship will depend on individual properties of interacting particles and particular interaction mechanism. A comprehensive review on the constitutive models with adhesion may be read in papers presented by Tomas [23, 24].

The mechanical behaviour of cohesive powders is essentially different from non-cohesive granular material and may be characterized by insufficient flowability and large compressibility. Presence of the load dependent van der Waals adhesion force
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Figure 1: Simplest contact model with constant adhesion

and suitable micro-macro interaction rules is characteristic feature of dry cohesive powders.

Our focus is on the model of isotropic, stiff spherical particles that are approaching to soft contacts. Thus, contact displacement (overlap size) $h$ is assumed to be small compared to the size (diameter) $d$ of the stiff particle. Finally, the physical nature of universal models is basing on the elastic–plastic and dissipative particle contact behaviour with hysteresis.

Consequently, a normal interaction force during binary collision of particles comprises contact deformation force, adhesion force and dissipation force:

$$ F_{ij}^n = F_{adh}^n + F_{spring}^n + F_{diss}^n $$

(3)

Various linear and non-linear models may be applied to evaluate particular force components. Concept of the particle interaction with adhesion is explained by considering simple model, while complicated elastic-plastic-dissipative behaviour with nonlinear detachment by advanced model.

Concept of the constitutive relation and particular components in (3) with adhesion of two interacting spherical articles particles is explained hereafter by simple model in terms of load-displacement diagram. Here, pressure and compression are defined as positive but tension and extension are negative.

Simple model (Fig. 1) may be characterized by combining classical visco-elastic "spring-dashpot" contact model [1] supplied by reloading and constant adhesion.

When considering normal forces (3), the adhesive force is defined by constant value $F_{h0}$, which means the long-range adhesion force without any contact deformation (the so-called jump in). This model presents the simplest case of a realistic van der Waals force. The case $F_{h0} = 0$ responds to non-cohesive interaction.

Initially, assuming the elastic contact behaviour particles may be loaded from point $F_{h0}$ to final point $U$ and response force of spring $F_{spring}^n = F_{el}$ presents elastic force and may be governed by well-known expression

$$ F_{spring}^n = \frac{4}{3} \frac{E_{eff}^{ij}}{E_i + E_j} \left( R_{eff}^{ij} \right)^{2-\alpha} h_{ij}^\alpha $$

(4)

where $E_{eff}^{ij} = \frac{E_i E_j}{E_i (1-\nu_i^2) + E_j (1-\nu_j^2)}$ and $R_{eff}^{ij} = \frac{R_i R_j}{R_i + R_j}$ present the reduced contact elasticity modulus and reduced radius of particles i and j, while $E_i$ and $E_j$ are elasticity
moduli and $\nu_i$ and $\nu_j$ are Poisson’s ratios, respectively. Therewith, for the Hertzian contact model the power coefficient $\alpha = 3/2$, while for linear law $\alpha = 1$. Differences of both models for wide range of elasticity constants are demonstrated in [26].

In the stage of unloading, beginning at arbitrary point $U$, the elastically deformed, annular contact zone recovers along an initial deformation path (4). In presence of arbitrary dissipation mechanism, reloading will follow different path $U - A$. Historically, a partially latching-spring model with a hysteresis was proposed by Walton and Brown [27], where linear constant for reloading was calculated in terms of the restitution coefficient. If the adhesion limit at point $A$ in the diagram of Fig. 1 is reached, then the contacting surfaces detach.

Advanced elastic–plastic–dissipative model of normal contact is based on the resent developments of Tomas [23, 24]. It combines nonlinear elastic linear plastic contact behaviour in loading, reloading and nonlinear model of adhesion. Details of the constitutive relation and particular components in (3) are explained by binary interacting spherical particles in terms of load-displacement diagram (Fig. 2), retaining, however, concept of the simple model. This inelastic contact flattening leads to an increase of adhesion force $F_{adh}^n$ depending on the applied normal load $F^n$ or pre-consolidation history.

Consequently, expression (3) presents static normal force combining contact force and distant van der Waals-type attraction. As follows from the Fig. 2, adhesive force $F_{adh}^n$ is restricted between zero force $F^n \leq 0$ and detachment limit $F_{detach}$ represented by curve between points $A$ and $F_{h0}$ extended to $a_{F0}$. This curve contains two essential parameters: maximum attractive force $F_{h0}$ and minimum separation range $a_{F0}$. Particles $i$ and $j$ still attract each other if the gap $h$ between their surfaces is smaller than the separation range $0 \geq h \geq a_{F0}$. Typically, load-displacement diagram is plotted in the range of nanoscale.

Referring Fig. 2 it is obvious, that the contact may be loaded from point $F_{h0}$ to $Y$ and, as the response, is elastically deformed with an approximated circular contact area. In elastic stage, nonlinear contact behaviour is governed by Hertzian model.
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(4). With increasing external normal load the soft contact starts at a pressure $p_f$ with plastic yielding at the point $Y$.

Using some ideas generalised by Thornton and Ning [28], the author Tomas [16] had published a model for adhesive contact of ultrafine particles with elastic-plastic behaviour. Basing on this approach, yield point $Y$ is located below the abscissa, i.e. the contact force equilibrium $F^n = 0$ includes a certain elastic-plastic deformation as response of adhesion force $(1 + \kappa) F_{h0}$. Consequently, micro-yield surface is reached and this maximum pressure $p_f$ can not be exceeded and results in a combined elastic–plastic yield limit of the nanoplate-plate contact with an annular elastic zone and a circular centre. The total force can be obtained by the particle contact force equilibrium between attractio ($-$) and elastic as well as soft plastic repulsion ($+$).

Finally, the spring force in loading is defined by generalised expression

$$F^n_{spring} = \beta_{el} \cdot F^n_{el} + \beta_{el-pl} \cdot F^n_{el-pl}$$  \hspace{1cm} (5)

Coefficients $\beta_{el}$ and $\beta_{el-pl}$ depends on contact specification. When contact elastic $\beta_{el} = 1$ and $\beta_{el-pl} = 0$, when contact is elastic–plastic then coefficients exchanges. Plastic contact occurs when overlap $h_{elim}$ is exceeded

$$h_{elim} = R_{ij}^{eff} \left(3\pi p_f (\kappa_A - \kappa_p) / 2E_{ij}^{eff}\right)^2$$  \hspace{1cm} (6)

Here, $\kappa_A$ is dimensionless elastic–plastic contact area coefficient representing the ratio of plastic particle contact deformation area to total contact deformation area and includes a certain plastic displacement. The dimensionless plastic repulsion coefficient $\kappa_p$ describes a dimensionless ratio of attractive van der Waals pressure of a plate-plate model to a constant repulsive micro-yield strength.

Finally elastic–plastic contact force reads

$$F^n_{el-pl} = \pi \cdot r_{ij} \cdot p_f (\kappa_A - \kappa_p) \cdot h$$  \hspace{1cm} (7)

It is obvious that yield limit can not be exceeded; however, at certain point $U$ unloading can begin. Dissipation of energy during particle collision may be characterised by dissipation in loading-unloading cycle. Review and systematic analysis of known and the new extended models for normal contact and comparison to available experimental data are presented by Kruggel-Emden et al. [29]. Here, different dissipation mechanisms and their applicability are discussed, restricting, however, to non-cohesive interaction. As concerns cyclic irreversible dissipation, two basic indirect and direct approaches are available.

In order to reflect energy dissipation, the normal force (3) may directly contain the viscous dissipation term $F^n_{diss}$. These models belong to the class of the viscous force schemes. Kuwabara and Kono [30] intuitively proposed a fully nonlinear model combining spring and dissipative forces. It was based on analogy with that hold in the Hertz theory. Thus, non-liner damping force is

$$F^n_{diss} = C_{non} \cdot \dot{h}$$  \hspace{1cm} (8)
Here, nonlinear dissipation characteristic \( C_{\text{non}} \) was expressed through the effective damping constant \( B_{\text{eff}} \), effective radius \( R_{\text{eff}} \) and overlap \( h \) of particles \( i \) and \( j \) as

\[
C_{\text{nonK}} = 2B_{\text{eff}}\sqrt{R_{\text{eff}}h}
\]  

(9)

The effective damping constant is introduced in analogous manner to effective elasticity modulus, by replacing two elasticity constants with corresponding viscosity parameters. This model was also independently derived by Brilliantov et al. [31]. Here, derivation of the dissipative force was based by separation of components arising from both shear as well as from dilation rates. Finally, it was written in slightly different form compared to (9) and expressed in terms of non-linear constant comprising stiffness \( K_{\text{non}} \):

\[
C_{\text{nonBr}} = \frac{3}{2}K_{\text{non}}A\sqrt{h}
\]  

(10)

Here \( A \) is function not only of the material viscosity but also involves elastic properties. Tsuji et al. [32] proposed a Hertz-type force law including a slightly modified dissipative term with a different exponent

\[
C_{\text{nonTs}} = \alpha_d\sqrt{m_{\text{eff}}K_{\text{non}}h^{1/4}}
\]  

(11)

where \( \alpha_d \) is dimensionless damping coefficient.

Finally, the shear models relate the increment of shear force to the increment of shear displacement.

4 Investigation of normal contact

Normal contact during binary collision of two identical spherical particles is considered numerically by integrating equations of motion (1-2) and applying various combinations of elastic-plastic-dissipative contact models with adhesion. The mobile particle is initially subjected by the portion of induced energy while target particle is fixed during entire interaction period. Induced energy is predefined by initial velocity \( v_0 \) and serves the base for initial conditions.

Geometry of the moving particle is defined by constant radius \( R = 0.6\mu m \). Material properties of the particles are assumed to be elastic and defined by Young’s modulus \( E = 150\text{GPa} \) and Poisson’s ratio \( \nu = 0.28 \), while density is \( \rho = 2470\text{kg/m}^3 \). Particular parameters reflecting microscopic properties of adhesive force of cohesive powders are: adhesion force of the sphere-sphere contact \( F_{h0} = -2.64\text{nN} \), micro-yield strength \( \sigma_f = 300\text{MPa} \), plastic repulsion coefficient \( \kappa_p = 0.153 \), elastic-plastic contact area coefficient \( \kappa_A = 5/6 \). Influence of impact velocity was illustrated by considering two values of the impact velocity: \( v_0 = 2\text{mm/min} \) and \( v_0 = 2\text{m/min} \).

Original velocity-independent Tomas model is of static nature. Here, dissipation is considered indirectly and may be characterized by coefficient of restitution defined as area under curve. Simulation results for non-adhesive and adhesive collision
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Figure 3: Illustration of binary collision of particles by Tomas model when: $\nu_0 = 2 \text{mm/min}$ and $\nu_0 = 2 \text{m/min}$: a, c) without adhesion; b, d) with adhesion

using contact model of Tomas with reloading and for two different impact velocities are presented in Fig. 3. A typical normal force-displacement diagram comprising loading-unloading is recovered by considering time history during contact numerically. Detachment of particles after collision is implied by model is clearly indicated.

The normal contact model in loading (5-7) supplemented by velocity depended nonlinear viscous dissipative term $F^{n}_{\text{diss}}$ is considered. Different expressions suggested by Kuwabara and Kono (9), Brilliantov (10) and Tsuji (11) will be employed for evaluation of $F^{n}_{\text{diss}}$. Dissipation models applied were scaled by introducing damping factor $\alpha_d$ in order to reflect identical values of restitution. Basic of results of Kruggel-Emden et al. [29], these values $\alpha_d = 0; 20; 30; 40; 50$ were taken for Brilliantov and equivalent Kuwabara and Kono models, while for Tsuji model they are as $\alpha_d = 0; 0.2; 0.3; 0.4; 0.5$.

It should be noted that particle behavior in small velocity range is free of the negative force usually interpreted as anomalies. Presence of cohesive force diminishes this effect. Simulation results showed that differences between Brilliantov and Kuwabara and Kono models are insignificant. Results of the combined model by applying Briliantov damping are presented in Fig. 4 using the same style. Here, normal force comprises all inter-particle (right hand) forces, including dissipation. The pictures illustrate different character for different impact velocities. Higher
velocity results detachment of particles while low velocity leads to sticking. The similar character is exhibited by Tsuji model. Results combined with Tsuji model (11) are presented in Fig. 5.

Finally, variation critical sticking velocity as function of particle radii in logarithmic scale is illustrated in Fig. 6.

5 Simulation of particle assembly

Behaviour of the cohesive powder is considered by compression and tension of particle assembly. The two-dimensional computational domain containing particles presents a rigid box in a form of H shaped complicated geometry (Fig. 7). Basic physical parameters of the particles used throughout simulation are discussed above.

The following scenario is proposed for simulation of cohesive powders. The initially generated domain fulfilled by contact-less particles was subjected by uni-axial compression. The compaction is performed by the motion of rigid walls 1 and 7 and is controlled in time t by a constant rate \( v_0 \). The poly-dispersed assembly of 1000 particles with radii varying in a range of \( 1.0 - 1.5 \mu m \) was randomly generated. The
Simulation of microscopic compression-tension behavior of cohesive dry powder by applying DEM

Figure 5: Illustration of binary collision of particles by Tomas model combined with Tsuji damping when $\nu_0 = 2\text{mm/min}$ and $\nu = 2\text{m/min}$: a, c) without adhesion; b, d) with adhesion

initial location of particles is presented in Fig. 7a. Motion of particles is obtained by numerical integration of eq. (1-2). Particle interaction in our simulations are initially restricted, however, by simplest linear model.

Compaction comprises two different phases of the material behaviour. The initial contact-less phase may be considered as gas phase. The transformation to the solid phase was controlled by considering time variation of the side wall force (Fig. 7 d). In the gas phase, the wall force variation remains zero, while transformation to solid phase is indicated by the jump.

Intermediate final states of the compacted material are presented in Fig 7 b, c. The random structure have a tendency to be transformed into pyramidal (triangle) lattice. This tendency is not fully accomplished because of the lack of the free space and of the influence of boundaries. Triangle structure prevails in the middle part. The completely chaotic rearrangement is observed in the boundary of differently shaped subregions of the specimen. Quantitively, the packing structure is illustrated by contact force network.

The tension of the material is implemented by motion of walls 5 and 9. It should be noted that tension behaviour is affected by various parameters and models and description of details is still in development stage.
6 Concluding remarks

Various inter-particle elastic-plastic-dissipative contact models of spherical particles with adhesion were studied numerically by applying DEM. Emphasis of this investigation was focussed towards the influence of velocity.

Essential features of particular models were considered by simulating the normal contact of two particles. The applied stiff particles with soft contacts model as suggested by Tomas exhibit the plastic deformation behaviour with load-unload hysteresis. It was observed that hysteresis character depends on the particular dissipative model. Character of consolidation and influence of the velocity with respect to particle size is demonstrated.

Behaviour of the cohesive powder is considered by kinematically induced compression and tension of poly-dispersed 1000 particles. Formation of agglomerates
Simulation of microscopic compression-tension behavior of cohesive dry powder by applying DEM depending on the overlap depth was indicated.

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References


Application of Recurrence Quantification Analysis for the Time Series Study

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Abstract

With Recurrence Plots (RP) we can study the m-dimensional phase space trajectory through two-dimensional representation of its recurrences. Measures of complexity of RP could be computed by quantification of RPs graphical structures (diagonal and horizontal lines, separated dots). Possibilities of RQA are shown. RPs of the natural time series (Wolf numbers, aa-index) were built, RQA measures for these RPs were calculated.

1 Introduction

Natural processes can have a distinct recurrent behavior, e.g. periodicities or irregular cyclicities. Moreover, the recurrence of states, in the meaning that states are arbitrary close after some time, is a fundamental property of deterministic dynamical systems and is typical for nonlinear or chaotic systems.

Recurrence Plots (RP) is useful method of analysis of complex systems, which not requires long or stationary data. Recurrence plots allows us to speak about characteristics of system processes, influences of noise or drift, transitions, long and short time periodicities and cyclicities. The quantitative analysis of RPs gives us few numerical measures of recurrence plot complexity.

In this paper we first shortly describe recurrence plots and their quantification technique and introduce new measure of complexity. After that we apply this approach to the Wolf numbers and aa-index.

2 Recurrence Plots

Recurrence Plots [1] are introduced as a tool for visualization of recurrence of states \( x_i \) in phase space. This approach enables us to investigate the \( m \)-dimensional phase space through a two-dimensional representation of its recurrences. Recurrence of
state at time $i$ at different time $j$ is pictured on two-dimensional square matrix with black dot in position $i, j$ (both axes are time axes). If there is no recurrence of state, white dot should be used. Such an RP mathematically can be expressed as:

$$R_{m,\varepsilon}^{i,j} = \Theta(\varepsilon - \|\vec{x}_i - \vec{x}_j\|), \quad \vec{x} \in \mathbb{R}^m, \quad i, j = 1 \ldots N,$$

where $N$ is a number of considered states $x_i$, $\varepsilon$ is a threshold distance, $\| \cdot \|$ a norm and $\Theta(\cdot)$ the Heaviside function. In this paper a fixed threshold distance $\varepsilon$ and the maximum $L_\infty$ norm are used, resulting in a symmetric RP.

If we have only one observation $u_t$, we can use the Takens theorem [2] to reconstruct an equivalent phase space trajectory which preserves the topological structures of original phase space trajectory: $\hat{x}(t) = (u_t, u_{t+\tau}, \ldots, u_{t+(m-1)\tau})$, where $m$ is the embedding dimension and $\tau$ is the time delay (index based).

The view on RPs gives hints about the time evolution of studied trajectories using large and small scale patterns — typology and texture [1]. The typology gives us a global impression which can be characterized as homogeneous, periodic, drift and disrupted. The texture formed by small scale structures — single dots (not persist states), diagonal lines (similar local evolution of different parts of trajectory), horizontal or vertical lines (state does not change for some time).

### 3 The Quantitative Analysis of Recurrence Plots

Zbilut and Webber have developed the recurrence quantification analysis (RQA) to quantify an RP [3]. They define measures using the recurrence points density and the diagonal structures (through the frequency distribution of diagonal lines lengths $P_d^\varepsilon(l) = \bigcup_{l=1}^N P_\varepsilon(l)$, where $N$ is the absolute amount of diagonal lines) in the recurrence plot — the recurrence rate (RR), the determinism (DET), the maximal length of diagonal structures or its inversion — the divergence (DIV), the entropy (ENTR), the trend (TREND), the ratio (RATIO).

Marwan have developed measures based on horizontal (vertical) structures (through the frequency distribution of horizontal or vertical lines lengths $P_h^\varepsilon(v) = \bigcup_{v=1}^N P_\varepsilon(v)$, where $N$ is the absolute amount of horizontal or vertical lines) — the laminarity (LAM) and the trapping time (TT) [4].

Expressions for RQA measures are shown below.

$$\text{RR} = \frac{1}{N^2} \sum_{i,j=1}^N R_{m,\varepsilon}^{i,j},$$

$$\text{DET} = \frac{\sum_{l=l_{\min}}^N l P_d^\varepsilon(l)}{\sum_{i,j=1}^N R_{m,\varepsilon}^{i,j}},$$

where $l_{\min}$ is the threshold that excludes the diagonal lines which are formed by the tangential motion of the phase space trajectory. It is obvious $l_{\min} = 1 \Rightarrow \text{DET} = 1$.

$$L = \frac{\sum_{l=l_{\min}}^N l P_d^\varepsilon(l)}{\sum_{l=1}^N P_d^\varepsilon(l)}$$

(4)
is the average time that two segments of the trajectory are close to each other. This measure can be interpreted as the mean prediction time.

\[ L_{\text{max}} = \max \{ l_i; \ i = 1 \ldots N \}, \text{DIV} = \frac{1}{L_{\text{max}}}. \]  

(5)

\[ \text{ENTR} = - \sum_{l = l_{\text{min}}}^{N} p(l) \ln p(l), \text{where} p(l) = \frac{P^\varepsilon_d(l)}{\sum_{l=1}^{N} P^\varepsilon_d(l)} \]  

(6)

This measure refers to the Shannon entropy of the frequency distribution of the diagonal lines lengths. This measure reflects the complexity of the deterministic structure in the system.

\[ \text{RATIO} = N^2 \frac{\sum_{l = l_{\text{min}}}^{N} l P^\varepsilon_d(l)}{\left( \sum_{l=1}^{N} l P^\varepsilon_d(l) \right)^2}. \]  

(7)

is the ratio between DET and RR. This measure is useful to discover transitions when RR decrease and DET does not change at the same time.

\[ \text{LAM} = \frac{\sum_{v = v_{\text{min}}}^{N} v P^\varepsilon_h(v)}{\sum_{i,j}^{N} R^\varepsilon_{i,j}} \]  

(8)

is analogous to the definition of determinism (3). This measure is the ratio between the recurrence points forming the horizontal structures and the entire set of recurrence points. The computation of LAM is realized for horizontal line length that exceeds a minimal length \( v_{\text{min}} \).

\[ \text{TT} = \frac{\sum_{v = v_{\text{min}}}^{N} v P^\varepsilon_h(v)}{\sum_{v = v_{\text{min}}}^{N} P^\varepsilon_h(v)} \]  

(9)

shows average length of laminar states in the system.

4 The measure of trajectory cleanness

In periodical systems fluctuations and noise influence leads in separate points and very short diagonals. The measure cleanness (CLEAN) is the ratio between recurrence points in diagonals with lengths less than \( l_{\text{min}} \) and recurrence points in diagonal lines with lengths equal or more than \( l_{\text{min}} \):

\[ \text{CLEAN} = \frac{\sum_{l = 1}^{l_{\text{min}}-1} l P^\varepsilon_d(l)}{\sum_{l=1}^{N} l P^\varepsilon_d(l)}. \]  

(10)

The measure quantifies influence of noise and fluctuations on system trajectory and should be used if studied system shows periodic behavior.
5 RQA using windows moving along the main diagonal

A computation of RQA measures in small windows

\[ W_{i,j}^{w,S} = R_{i+w,j+w}, \quad i, j \in [1 \ldots S], \quad w \in [1 \ldots n = N - S] \]

moving along the main diagonal \( R_{i=j} = 1 \) of the RP yields the time dependent behavior of these variables. This method makes the identification of transitions in time series possible [5]. Frequency distributions of diagonal and horizontal lines lengths for each window are

\[ P_{\varepsilon,S}^{\omega}(l) = \bigcup_{i=1}^{S} P_i(l) \]

and

\[ P_{\varepsilon,S}^{\omega}(v) = \bigcup_{i=1}^{S} P_i(v) \]

correspondingly.

Equations (2...10) should be written as:

\[ RR_w = \frac{1}{S^2} \sum_{i,j=1}^{S} W_{i,j}^{w,S} \]

for recurrence rate (2);

\[ DET_w = \frac{\sum_{l=1}^{S-1} \sum_{i,j=1}^{l} W_{i,j}^{w,S}}{S(S-1)} \]

for determinism (3);

\[ L_w = \frac{\sum_{l=1}^{S-1} \sum_{i,j=1}^{l} W_{i,j}^{w,S}}{S} \]

for average length of diagonal lines (4);

\[ L_{\text{max}}_w = \max \{ |l_i; i = 1 \ldots S - 1\} \]

for divergence (5);

\[ \text{ENTR}_w = -\sum_{l=1}^{S} \ln \left( \frac{p_{\omega}^{S}(l)}{p_{\omega}^{S}(1)} \right) \]

for entropy (6);

\[ \text{RATIO}_w = \frac{S^2}{\sum_{l=1}^{S-1} \sum_{i,j=1}^{l} W_{i,j}^{w,S}} \]

for ratio (7);

\[ \text{LAM}_w = \frac{\sum_{v=\text{min}}^{S} \sum_{i,j=1}^{v} W_{i,j}^{w,S}}{\sum_{v=\text{min}}^{S} p_{\omega}^{S}(v)} \]

for laminarity (8);

\[ \text{TT}_w = \frac{\sum_{v=\text{min}}^{S} \sum_{i,j=1}^{v} W_{i,j}^{w,S}}{\sum_{v=\text{min}}^{S} p_{\omega}^{S}(v)} \]

for trapping time (9);

\[ \text{CLEAN}_w = \frac{\sum_{l=1}^{S-1} \sum_{i,j=1}^{l} W_{i,j}^{w,S}}{\sum_{l=1}^{S-1} \sum_{i,j=1}^{l} p_{\omega}^{S}(l)} \]

for cleanness (10).

Computation of measures in shifted window results in a set of quantification vectors \( Q^n \), where \( n = N - S \) is the amount of quantifications in window with size \( S \). Using of large window results in smooth measures graphs with less precision. Decreasing of window size allows us to enhance precision, but using of too small windows results in presence of false events on graphs. Our tests shows that good results could be obtained with window size \( S \approx N/5 \).

6 Application to the Wolf numbers and to the aa-index

RPs and quantification graphs are presented for the Wolf numbers on fig. 1 and 2; for the aa-index on fig. 3 and 4.

Both time series are monthly values from 1871, January to 1994, December. Recurrence Plots for this data was built using \( m = 3, \tau = 1, \varepsilon = 0.1 \), all measures quantified in window with size \( S = 312 \) points that is equal to 26 years. All graphs are approximated by splines with high precision.

On the graphs for the Wolf numbers (fig. 2) we first looks for transition between years 1934 and 1937 which is could be easily found by visual inspection of RP on
Figure 1: RP of the Wolf numbers

fig. 1 [6]. We can see extremely event at the end of the year 1935 on graphs of measures RR, DET, ENTR, RATIO and LAM (marked with dashed line). We also can see other extremes, for example at the end of year 1899 (marked with dotted line). It is possible to find this event on the RP but it looks not obviously like previous.

Graphs for the aa-index (fig. 4) are more interesting. We can see high sensitivity of measures for system behavior changes even if the signal is noised and fluctuated and periodic behavior looks not sharply (fig. 3). In fact, there is range from the middle of year 1934 to the middle of year 1938. Geomagnetic field perturbation changes during this period. There is mutual extreme of measures DET, L, ENTR, LAM and TT at the end of the year 1936. So, if our estimation about transition at the end of the year 1935 is correct, we can say that geomagnetic field reaction on appreciable change of solar activity was formed during one year delay.

The extreme found at the end of the year 1899 on graphs for the Wolf numbers also could be found on graphs for the aa-index. We should make attention on the following fact — this transition is not visible on the aa-index RP.
7 Conclusion

Using of Recurrence Quantification Analysis for time series study enables scientist to discover phase transitions even if they could not be found on the RP visually.

Application of described method to the Wolf numbers and to the aa-index gave us more accurate information about appreciable phase transition in the second half of 1930s. A number of other transitions were found. It is obvious that all measures react differently on different kinds of phase transitions.

We introduced new measure CLEAN as ratio between amount of recurrence points forms isolated dots and short diagonal lines and amount of recurrence points that forms long diagonals. This measure shows influence of noise and fluctuations on trajectories with periodic behavior.

References


Figure 3: RP of the aa-index


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Figure 4: RQA measures graphs of the aa-index RP
About analysis of the Entropy into kinematic and thermal conditions of Superplasticity

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Abstract

Analysis of the Entropy allows to consider process of deformation from positions of self-organizing dissipative structures in the nonequilibrium open systems.

As a result of research it is shown, that minimization of the entropy function is answered with formation ordered equiaxed the ultrafine-grained structure, allowing to predict occurrence of the structural situation promoting realization of the mechanism grain boundary sliding. Differently, by self-organizing in the conditions far from thermodynamic balance, process of the optimum structurization, accompanied by entropy isolation the open system is realized.

Advert to studying behaviour of entropy production in kinematic and thermal conditions of superplasticity.

Research of entropy function allows to consider process of deformation from positions of self-organizing dissipative structures in the nonequilibrium open systems [1]. Entropy function at known expression for free energy is defined by the formula [2]

\[ S = -\frac{\partial F}{\partial \theta}. \]  

(1)

We accept [3] that free energy and density of potential are connected by

\[ \Phi = \frac{F}{k\theta}. \]  

(2)

At the formulation of model [4] energy function of a condition has been accepted in the form of potential of accident of assembly in view of influence of an external field
Φ(η, β, q) = \frac{1}{4}m_0\eta^4 + \frac{1}{2}\beta(\xi)\eta^2 - q\eta, \quad (3)

were \( q = \frac{\sigma}{\sigma^*} - 1; \eta = \frac{\varepsilon}{\dot{\varepsilon}} - 1; \xi = \frac{\theta - \theta^*}{\theta^* - \theta^h}; m_0 - \text{const}; \beta = \beta(\xi) - \text{temperature function.}

For an increment of entropy production we shall receive

\[
\frac{\Delta S}{k} = 3 \frac{3}{4}m_0\eta^4 + \frac{1}{2}\beta\eta^2 + (\xi + \nu) \left[ \frac{1}{2} \frac{d\beta}{d\xi} \eta^2 - \beta(3m_0\eta^4 + 3m_0\eta^3 + \beta\eta^2 + \beta\eta) \frac{d\ln \sigma^*}{d\xi} \right],
\]

were \( k - \text{Boltzmann constant.} \)

Results of the calculations which have been carried out under the formula (4) are shown in graphic dependencies of an increment of entropy production \( \xi_0 = 0 \) from normalized temperatures (Fig.1) and control parameter (Fig.2,3).

Calculations were made for alloy AMg5. Character presented on Fig.1,...,3 dependencies qualitatively repeats and for other investigated aluminium alloys (D18T, 1561, AK6).

Let’s note following features of the received regularities. From Fig.1 it is visible, that change of an increment of entropy production on temperature within the limits of high-rate ranges of superplasticity has the fluctuating character inherent in the mechanism grain boundary sliding, adequating to a unstable structural condition and presence of dynamically raised structure [4]. Thus in the middle of a thermal range of superplasticity \( \xi = 0.5 \) it is had \( \Delta S/k = 0 \). Values \( \Delta S/k = 0 \) at \( \xi = 0; \xi = 1 \) reflect change of structural conditions - at \( \xi = 0 \) deformed or the cast structure starts to turn in ultrafine-grained, and \( \xi = 1 \) at transition to coarse-grained recrystallized to structure is carried out.

On Fig.2,3 dependences of an increment of entropy production from rate of deformation (\( \Delta S/k = 0 \sim \eta \)) in conditions of superplasticity are resulted at temperatures \( \xi = 0,0.1, ..., 0.5 \) (Fig.2) and \( \xi = 0.5, ..., 1 \) (Fig.3). The general for these temperatures is the tendency of aspiration to zero of entropy production on the average value of a high-rate interval of superplasticity \( \eta = 0 \) [5].

To the middle of thermal and kinematic ranges of superplasticity (\( \xi = 0; \eta = 0 \)) there corresponds zero value of an increment of entropy production.

In summary we shall note the following. At the formulation of model (3) [4] it was accepted, that superplasticity is considered a special (structurally unstable) condition of a deformable material in hierarchical change of conditions. The specified condition is treated as the effect which is carried out in conditions of structural nonequilibrium phase transition. Minimization of entropy is corresponded to formation ordered homaxonic ultrafine-grained structure [4], [7], allowing to predict occurrence of the structural situation promoting realization of the mechanism grain boundary sliding. Differently, by self-organizing in the conditions far from thermodynamic balance, process of the optimum structurization [5], accompanied by entropy allocation [7] the open system is realized.
Figure 1: Function of entropy production in thermal ranges of superplasticity.

Figure 2: Functional dependence of an increment of entropy production from rate deformation in conditions of superplasticity at $\xi = 0, 0.1, ..., 0.5$.

References

Figure 3: Functional dependence of an increment of entropy production from rate deformation in conditions of superplasticity at $\xi = 0.5, ..., 1$.
Oriented state of polymer in the gaps between filler particles in polymer nanocomposite

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Abstract

The theory is developed that can explain the appearance of oriented layers in the vicinity of filler surfaces in polymer nanocomposites which is based on the idea that the oriented regions of the polymer influence the oriented state of neighboring regions and tend to orient the polymer material in these regions. The orientation effect is transferred from one point to another, causing thus the essential propagation of the oriented polymer layer from the filler surface.

1 Continuum, probabilistic and discrete modeling

The layers of 2 to 10 nm (and more) thick that occur near the surface of filler particles play a large part in the formation of the mechanical properties of polymer nanocomposites. Despite the longstanding efforts of scientists to elucidate the cause of formation of these layers and to understand the mechanism of their influence on the mechanical properties of the material, the problem still remains to be solved. There is no answer to the question as to why the thickness of the layers formed near the surface of filler particles is so large that it achieves several nanometers. In the current study an attempt has been made to construct a mathematical model capable of providing the answer to this question.

For constructing the model, it is essential to determine mathematical parameters best suited to our study. The establishment of these parameters requires information about the preferential orientation of polymer links. To gain it, we use the notion of the orientation tensor. However, before proceeding to the description of the oriented state of the bulk medium, it is necessary to introduce the characteristic of the oriented state of a single link of one of the polymeric chains. Let all links of all polymer chains have a through enumeration: the first link of the first chain is designated as 1, and the last link of the last chain as N. The index j, running the values from 1 to N, takes the numbers of all links of all polymer chains.
As a characteristic of orientation of the polymer chain link with number \( j \), we offer to use the tensor \( \boldsymbol{\tau}_j \otimes \boldsymbol{\tau}_j \), in which \( \boldsymbol{\tau}_j \) denotes a unit vector defining the space orientation direction of the \( j \)-th link. Clearly, a change in the direction of the vector \( \boldsymbol{\tau}_j \) to the opposite produces no effect on the values of the tensor \( \boldsymbol{\tau}_j \otimes \boldsymbol{\tau}_j \). The proposed tensor is suitable for our purpose because its averaged value can be found for all possible links of polymer chains and the result of such averaging will not be equal to a zero tensor. It gives an estimate of the oriented state of the polymer. Its eigenvectors and eigenvalues have a clear physical meaning. The eigenvectors of the averaged tensor \( \boldsymbol{\tau}_j \otimes \boldsymbol{\tau}_j \) define the space directions along which the chain links are mainly oriented and the directions along which the links are rarely oriented. The eigenvalues of this tensor give a quantitative estimation of the orientation degree of polymer chains in corresponding directions. We assume that the interaction energy of the \( i \)-th and \( j \)-th links of polymer chains is represented as a potential:

\[
\begin{align*}
  u_{ij} &= \frac{c_u}{r_{ij}^6} \left( \frac{1}{3} - (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)^2 \right) = \frac{c_u}{r_{ij}^6} \left( \frac{1}{3} - \boldsymbol{\tau}_i \otimes \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \otimes \boldsymbol{\tau}_j \right),
\end{align*}
\]

where \( u_{ij} \) is the interaction energy of the \( i \)-th and \( j \)-th links, \( c_u \) is the material constant, and \( \mathbf{I} \) is a unit tensor. Its physical meaning can be treated as follows. The interaction energy of polymer chain links depends on the distance between the centers of mass of the interacting links of polymer chains and the angle between the directions of these links.

For modeling the oriented polymer region formation, one can use continuum, discrete and probability models. Let us consider these models.

**PROBABALISTIC MODELS.** For analyzing the mechanical behavior of the medium, one or several chains may be considered. The influence of the remaining chains will be replaced by their effective action and formulated using the selfconsistent methods, the probability theory or the theory of random processes. In further calculation, we will use the Gibbs distribution of probability density \( \psi \) of the state of the \( i \)-th link in equilibrium, which takes the form

\[
\psi = C \exp \left( -\frac{1}{c_B \theta} \sum_{j=1, j \neq i}^{N} u_{ij} \right),
\]

where \( C \) is the normality constant, \( c_B \) is the Boltzmann constant, \( \theta \) is temperature. In accordance with equation (1), the energy of interaction of the \( i \)-th link with the other links is defined as

\[
\sum_{j=1, j \neq i}^{N} u_{ij} = \frac{c_u}{3} \left( \sum_{j=1, j \neq i}^{N} \frac{1}{r_{ij}^6} \right) - c_u \boldsymbol{\tau}_i \otimes \boldsymbol{\tau}_i \cdot \left( \sum_{j=1, j \neq i}^{N} \frac{\boldsymbol{\tau}_j \otimes \boldsymbol{\tau}_j}{r_{ij}^6} \right).
\]

**DESCRETE MODELS.** The method of molecular dynamics allows one to analyze the motion of all polymer chains taking into account their interaction. Such calculations are cumbersome, time consuming and require high-performance memory computers. Because of that it is reasonable to use discrete models for justifying the validity of simpler models and calculating the appropriate constant, rather than for studying physical processes. Hence, the best way to carry out investigations is to use simpler continuum models.
For further construction of the model we should use the notion of averaging of the
tensor function over the bulk material. If we deal with the probability and discrete
models then for calculating the energy of interaction of the \(i\)-th link of the polymer
chain with the remaining links we should use the space averaging
\[\langle \mathbf{\tau}_i \otimes \mathbf{\tau}_j \rangle_V,\]
which can be obtained as
\[\langle \mathbf{\tau}_i \otimes \mathbf{\tau}_j \rangle_V = l^6 C_N \sum_{j=1, j \neq i}^N \frac{\mathbf{\tau}_j \otimes \mathbf{\tau}_j}{r_{ij}^6},\]
and by the normality condition
\[l^6 C_N \sum_{j=1, j \neq i}^N \frac{1}{r_{ij}^6} = 1,\]
where \(C_N\) is the normality constant. It is easy to define that for a tetrahedron grid
this constant is
\[C_N = 0.0824,\]
where \(l\) is the distance between the mass centers of the polymer chain links. The
normality condition allows us to describe the energy of interaction of the \(i\)-th link
of the polymer chain with the remaining links:
\[\sum_{j=1, j \neq i}^N u_{ij} = \frac{c_u}{l^6 C_N} \left( \frac{1}{3} - \mathbf{\tau}_i \otimes \mathbf{\tau}_i \cdot \langle \mathbf{\tau}_j \otimes \mathbf{\tau}_j \rangle_V \right) .\]
The volume averaging is carried out using the weight coefficient \(r_{ij}^{-6}\) which takes
into account the contribution of the \(j\)-th link (being at the distance \(r_{ij}\) from the
considered \(i\)-th link) to the general energy of interaction of the \(i\)-th link with the
bulk material.

In the following, for construction of equations in the frame of continuum models
we will use analogous mathematical expressions.

CONTINUUM MODELS. Among other models, continuum models are simplest.
They essentially reduce the time of solution of the problems and facilitate the analy-
sis of physical processes, because there is no need to consider the motion of separate
polymer links in the bulk material. In these models instead of the tensor \(\mathbf{\tau}_i \otimes \mathbf{\tau}_i\),
defined in the centers of mass of polymer chains, it is necessary to use a smooth tensor
function specified for all points of the polymer material. For this purpose, we will
use the suppositions, which allow us to construct the phenomenological equations
of the continuum model and to relate them with the molecular interactions in the
material.

First supposition. We assume that there is a continuous twice differentiated
tensor function \(\mathbf{O}(t, \mathbf{x})\), which provides calculation of the energy of interaction of
the \(i\)-th link with the remaining material, as it is usually fulfilled in the context of
probability and discrete models
\[\sum_{j=1, j \neq i}^N u_{ij} = \frac{c_u}{l^6 C_V} \left( \frac{1}{3} - \mathbf{\tau}_i \otimes \mathbf{\tau}_i \cdot \langle \mathbf{\tau}_j \otimes \mathbf{\tau}_j \rangle_V \right) ,\]
Oriented state of polymer in the gaps between filler particles in polymer nanocomposite

where the space averaging in the frame of the continuum model is defined by the expression

\[ \langle \tau_j \otimes \tau_i \rangle_V = l^6 C_V \int_V \frac{O(t, x + \Delta x)}{r^6} \, dV \]  

(5)

and the normality condition

\[ l^6 C_V \int_V \frac{1}{r^6} \, dV = 1, \]  

(6)

where \( dV = d\Delta x_1 d\Delta x_2 d\Delta x_3 \), \( l^6 C_V \) is the normality constant, \( t \) is the current moment of time, \( x \) is the vector defining the space location of the center of mass of the considered \( i \)-th link. The current variables in the integrand are the components \( \Delta x_1, \Delta x_2, \Delta x_3 \) of the vector \( \Delta x = \Delta x_1 i_1 + \Delta x_2 i_2 + \Delta x_3 i_3 \), whose origin is placed in the considered space point, and its end passes through all the points of the volume \( V \). The symbols \( i_1, i_2, i_3 \) designate the unit basis vectors of the rectangular Cartesian coordinates.

In our investigation, by the volume \( V \) we mean the entire volume except for the small spherical region in the vicinity of the considered space point. Let the radius of this small spherical region be denoted as \( \delta \). This region is eliminated from the integration process because two links of polymer chains cannot exist in it simultaneously and, thus, the interaction between the links placed at a distance less than \( \delta \) is impossible. That is the reason why we can take into account (during the averaging process) the influence of only those regions that are able to interact with the considered point. The way to define the radius size will be described in the Section devoted to the discussion of the requirement of equivalence between continuum and deterministic averaging processes.

The integral in equation (6) is calculated analytically and has the following value:

\[ \int_V \frac{1}{r^6} \, dV = \int_\delta^\infty \int_0^{2\pi} \int_0^\pi \frac{1}{r^4} \sin \theta \, d\theta \, d\alpha \, dr = \frac{4\pi}{3} \delta^3. \]

Hence, the constant \( C_V \) is

\[ C_V = \frac{3 \delta^3}{4\pi l^6}. \]  

(7)

2 Equivalence requirement of continuum and deterministic averaging

For the purpose of our investigation, the operators of continuum and discrete averaging should operate equally when they will be used to define the appropriate limited twice differentiated function \( A = A(x) \) of the vector \( x \). We assume that
in the vicinity of the considered space point the function \( A = A(x + \Delta x) \) can be approximated with high accuracy by the following quadratic relation:

\[
A(x + \Delta x) = A + \sum_{i=1}^{3} \frac{\partial A}{\partial x_i} \Delta x_i + \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial^2 A}{\partial x_i \partial x_j} \Delta x_i \Delta x_j.
\]  

(8)

We deal with the region of the material where the weight coefficient \( r^{-6} \) in the operator of the continuum averaging cannot be treated as a small value. Substituting the approximation (8) in the continuum averaging operator gives

\[
\langle A(x) \rangle_V = l^6 C_V \int_V \frac{1}{r^6} \left( A + \sum_{i=1}^{3} \frac{\partial A}{\partial x_i} \Delta x_i + \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial^2 A}{\partial x_i \partial x_j} \Delta x_i \Delta x_j \right) dV.
\]

Similarly the discrete averaging of the function \( A = A(x) \) over the space points, in which the centers of mass of polymer links are located, yields

\[
\langle A(x) \rangle_V = l^6 C_N \sum_{j=1, j \neq i}^{N} \frac{1}{r_{ij}^6} \left( A + \sum_{k=1}^{3} \frac{\partial A}{\partial x_k} (x_k^j - x_k^i) + \frac{1}{2} \sum_{k=1}^{3} \sum_{n=1}^{3} \frac{\partial^2 A}{\partial x_k \partial x_n} (x_k^j - x_k^i)(x_n^j - x_n^i) \right) dV,
\]

where \( x_j^i = x_j^1 i_1 + x_j^2 i_2 + x_j^3 i_3 \) is the vector defining the space location of the center of mass of the \( j \)-th link. As mentioned above, we consider the case when the center of mass of the \( i \)-th link is in the considered space point whose place is defined by the vector \( x \). It is easy to verify that the equivalence requirement of continuum and deterministic averaging for the tensor function \( A = A(x) \) can be fulfilled only if the the following conditions are satisfied:

\[
l^6 C_N \sum_{j=1, j \neq i}^{N} \frac{1}{r_{ij}^6} = l^6 C_V \int_V \frac{1}{r^6} dV,
\]

\[
l^6 C_N \sum_{j=1, j \neq i}^{N} \frac{(x_k^j - x_k^i)^2}{r_{ij}^6} = l^6 C_V \int_V \frac{\Delta x_k^2}{r^6} dV, \quad k = 1, 2, 3.
\]  

(9)

The first equation is satisfied automatically as a consequence of the normality condition. To fulfill the equation (9), we need to define correctly the size of the small spherical region in the vicinity of the considered space point, which is eliminated from the bulk polymer when calculating the integral. The above considerations will be useful for a correct choice of the radius \( \delta \), about which we have mentioned earlier when introducing the notion of the averaging operation in the context of continuum models. The radius \( \delta \) is determined under the assumption that the centers of mass of polymer links are placed in the nodes of a regular grid. It is evident that for construction of the radius \( \delta \) we can use any of the equations of formula (9). The choice of the number \( k \) does not affect the calculation results

\[
l^4 \sum_{j=1, j \neq i}^{N} \frac{(x_3^j - x_3^i)^2}{r_{ij}^6} = 4.10.
\]  

(10)
The integral in equation (6) is calculated analytically and has the following value:

\[
\int_{V} \frac{\Delta x_3^2}{r^6} \, dV = \int_{\delta}^{\infty} \int_{0}^{\frac{2\pi}{3}} \int_{0}^{\cos^2 \theta} \frac{\cos^2 \theta}{r^2} \sin \theta \, d\theta \, d\alpha \, dr = \frac{4\pi}{3\delta^3}.
\]  

(11)

It follows from (3), (7), (10), (11) that the sphere radius \( \delta \), being eliminated in taking the integral over the polymer volume, is equal to

\[ \delta = 0.581. \]

3 Main causes of orientation tensor time evolution

The model describing the time-dependent formation of the layers near filler particles in elastomeric nanocomposites is constructed under the following assumption.

**Second supposition.** We assume that the time evolution of the orientation tensor in the considered space point is determined by two factors: a) the orientation influence of the neighboring points on the considered point; and b) the influence of the thermal motion of polymer chains which tend to bring the material into the state without orientation. Thus, the evolution equation can be written in the form

\[
\frac{1}{b} \frac{D}{Dt} \langle O \rangle = a_1 t^6 C V \int_{V} O(t, x + \Delta x) \frac{1}{r^6} \, dV - O + \left( \frac{I}{3} - O \right),
\]

(12)

where \( D/Dt \) is the objective time derivative, and \( a_1 \) and \( a_2 \) are the non-negative functions of the parameters of the medium state. The first term in the right-hand part of the equation (12) indicates the following. The more the tensors \( \langle \tau_i \otimes \tau_j \rangle \) and \( O \) differ from one another, the faster the material tends to change this nonequilibrium state. In other words, the more the polymer orientation in the considered point differs from that dictated by the neighboring points, the faster the orientation in the considered point changes to the orientation required by the neighboring points. The presence of the second term points to the fact that the bigger the difference of the polymer oriented state in that point from the state of full chaos (the state without orientation), the stronger the thermal motion tends to take the material off this state and to destroy the existing orientation of polymer chain links. These two factors define the rate of change in the oriented state of the polymer.

Let us transform equation (12). The first square bracketed term in the right-hand side of the equation must be written in an easy-to-use form. To this end, we expand the tensor function \( O(t, x + \Delta x) \) in a Taylor series and discard in it the terms of third and higher orders of smallness. This operation is possible because the integrand has the multiplier \( r^{-6} \) that makes the integration result unaffected by almost all values of the function \( O(t, x + \Delta x) \) except for the small vicinity of the space point (its location is given by the vector \( x \). Having factored the independent
expressions outside the integral sign, we obtain the formula

$$C_V \int_V \frac{O(x + \Delta x)}{r^6} \, dV = O \left( C_V \int_V \frac{1}{r^6} \, dV \right) + C_V \int_V \frac{\partial O}{\partial x} (x + \Delta x) \, dV + \frac{3}{2} \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial^2 O}{\partial x_i \partial x_j} \left( C_V \int_V \frac{\Delta x_i \Delta x_j}{r^6} \, dV \right).$$

In view of the normality condition (6) and the fact that integrals with odd integrands are equal to zero, we have the equality

$$t^6 C_V \int_V \frac{O(x + \Delta x)}{r^6} \, dV = O + C_\Delta \sum_{i=1}^3 \frac{\partial^2 O}{\partial x_i^2}, \quad (13)$$

where

$$C_\Delta = \frac{1}{2} t^6 C_V \int_V \frac{\Delta x_i^2}{r^6} \, dV > 0.$$

Using (7) and (11), we have

$$C_\Delta = \frac{1}{2} \delta^2.$$

Finally, equation (12) takes the form

$$\frac{1}{b} \frac{DO}{Dt} = a C_\Delta \sum_{i=1}^3 \frac{\partial^2 O}{\partial x_i^2} + \left( \frac{1}{3} - O \right). \quad (14)$$

For the solution of the problems dealing with the formation of oriented layers near filler particles in polymer nanocomposites, the functions $a$ and $a_2$ must be represented in a special way.

4 Specification of function $a$

**Third supposition.** We assume that in equilibrium the tensor $O$ provides calculation of the medium energy just the same as value $\tau_i \otimes \tau_i$. It is possible only in case of equation fulfilment

$$\langle \tau_i \otimes \tau_i \rangle_V \cdot O = \langle \tau_i \otimes \tau_i \rangle_V \cdot \int \tau_i \otimes \tau_i \, C \exp \left\{ - \frac{c_u}{c_B \theta_l^3 C_V} \left( \frac{1}{3} - \tau_i \otimes \tau_i \cdot \langle \tau_i \otimes \tau_i \rangle_V \right) \right\} \, d\Gamma,$$

where $\Gamma$ is the phase space of possible states of the considered system. This yields the tensor that defines the oriented state of the medium. The index $\Gamma$ near the bracket implies that the averaging is carried out over a variety of possible states of the system. In view of equations (4), (5), (13), and (14), free material energy can be
written as

\[
\mathbf{u} = \left\langle \sum_{j=1, j \neq i}^{N} \mathbf{u}_{ij} \right\rangle_{\Gamma} = \left\langle \frac{c_u}{16C_V} \left( \frac{1}{3} - \mathbf{\tau}_i \otimes \mathbf{\tau}_i \cdot \left\langle \mathbf{\tau}_j \otimes \mathbf{\tau}_j \right\rangle_{V} \right) \right\rangle_{\Gamma} = \\
= \frac{c_u}{16C_V} \left[ \frac{1}{3} - \mathbf{O} \cdot \left( \mathbf{O} + \frac{1}{a} \left( \mathbf{O} - \frac{1}{3} \right) \right) \right] = \frac{c_u}{16C_V} \left( 1 + \frac{1}{a} \right) \left( \frac{1}{3} - \mathbf{O} \cdot \mathbf{O} \right).
\]

The results of application of this model are shown in Figures 1,a and Figures 1,b which illustrated the equal-level lines for internal energy of interaction of polymeric chains links. In this figures we can see the equal-level lines along one particle’s sufrace of filler (Figure 1,a) and — in the gap between filler particles (Figure 1,b). The material constant is \( c_u = 2.5e^{-21} \).

Fig. 1. Equal-level lines for internal energy of interaction of polymeric chains links. The material constant is \( c_u = 2.5e^{-21} \). a – along one particle’s sufrace of filler; b – in the gap between filler particles.

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Deformation and fracture of ceramics with various pores structure under mechanical loading

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Abstract

The development of deformation and fracture under mechanical loading in porous ceramic materials with the pore space having regular and stochastic structures of various types has been studied by the method of movable cellular automata. The influence of the porous structure on the dynamics of damage nucleation and development is been analyzed, and a correlation between the effective stiffness of porous samples and the rate of damage accumulation is found. It is concluded that brittle materials can exhibit quasi-ductile fracture determined entirely by the pore space structure.

Introduction

In recent decades, sintered ceramic materials have found wide application in various fields. Owing to the features of powder technology, these materials possess a porous structure, which, on the one hand, imparts useful practical properties (low weight, permeability) but, on the other hand, complicates the understanding and prediction of behavior under various working conditions. If the pores have known shapes and a periodic arrangement, the elastic properties of a given material can be determined using the methods of averaging. According to this approach, a real porous body (structure) is considered as an anisotropic continuous medium characterized by effective elastic moduli. Unfortunately, the equations of motion are much more complicated for anisotropic media than for the isotropic ones. In the region of elastic deformation, these equations can still be solved. But the description of plastic behavior and fracture processes requires the introduction of additional criteria and the development of particular theoretical models. In case of a substantially aperiodic spatial distribution of pores, the averaging methods give the dependence of effective moduli only on the total porosity. Moreover, these theoretical dependences adequately describe the behavior only within rather narrow range of porosity [1, 2, 3, 4]. The main drawback is that these methods do not allow the
character of fracture of a porous sample and its response even to the initial damage to be evaluated.

In this context, a certain advantage is offered by methods of direct numerical simulation of the behavior of porous materials under preset loading conditions, which make possible the study of the laws of their deformation and fracture. One of the most advanced and effective approaches to solving such tasks is offered by the method of movable cellular automata [5, 6, 7].

1 Investigation of deformation and fracture of porous media under shear loading

This part of paper presents the results of numerical simulation of the behavior of porous ceramic (ZrO$_2$) samples with various porous structures, including both regular (Figs. 1a–d) and stochastic (Fig.1e). In all cases, the pores had identical dimensions and shapes, being extended in the direction of loading. The total porosity in all samples was 25%, the samples had dimensions 1.14x0.625 mm, and the movable automata were 0.01 mm in size. The loading was simulated by setting identical velocities to all automata in the uppermost front layer. The value of this velocity gradually increased from 0 to 1 m/s in sinusoidal manner during the initial period of 1.5 ms and then remained constant. This regime ensured a quasi-static character of loading and allowed dynamic effects to be avoided until the appearance of the first damage. All samples had periodic boundary conditions in the direction of loading. The problem was solved under plane strain conditions. The response function of automata corresponded to the diagram of loading for nanocrystalline ZrO$_2$(Y$_2$O$_3$) (yttria-stabilized zirconia) with a total porosity of 2% and an average pore size comparable with the grain size [8].

![Figure 1](image)

Figure 1: The initial structures of model samples with various porous arrangements: a–d — periodic; e — stochastic.

A regular pore structure was modeled in four ways. In the first case, the pores were periodically arranged both along the vertical axis, with a period equal to the pore height, and in the horizontal direction, with a period equal to their width. Arranged in this manner, the pores formed high-porosity vertical strata alternating with monolithic layers (Fig. 1a). In the second, third, and fourth ways, the pores were arranged in a checkerboard pattern (Figs. 1b–d, respectively) with various densities of the resulting porous space. The difference between these porous structures consisted in density of pores per square of sample.

Fig. 1a shows the stress-strain diagrams of loading obtained by numerical calculations. The diagrams for the samples with periodical pores arrangement had no regions with numerous “breakdowns” and exhibited abrupt character of falling
branches of diagrams (close to vertical) in contrast to one of the sample with stochastic pore arrangement. Such a feature of these diagrams was explained by sharp macro-crack propagation in the samples and simultaneous dropping their strength (curves a, d) or further deformation of samples with interlocking of their fragments in the vicinity of the main crack under constrained boundary conditions in the vertical direction. In that case the stress-strain diagrams included the region with numerous “breakdowns”, which correspond to the elastic deformation of sample alternating with generation and accumulation of structural damage.

The results of calculations showed that, the samples with periodical arrangement of pores (Figs. 1a–d), exhibited higher ultimate stress and strain as compared to the sample with randomly distributed pores (Fig. 1e). This could be explained by more uniform distribution of stresses in the samples with regular porous structure.

The samples with a regular porous structure had different effective elastic shear moduli (1.48–13 GPa), possessing the same total porosity. That is related to the peculiarities of pores arrangements in the samples. In fact, these samples are the frameworks (skeletons). Mechanical properties of these frameworks are characterized substantially by their structural peculiarities and by the direction of loading. The samples with pores arranged in a checkerboard pattern (Figs. 1b–d) exhibited an increase in the effective stiffness with decreasing the number of pores per cell. Therefore the sample in Fig 1d had the maximum effective stiffness. The strength properties of the samples were increased with growth of effective stiffness. The samples Figs. 1b,c in contrast to the samples Figs. 1a,d still resisted to shear loading even after the first macrocrack propagation (Fig. 2) along with damage accumulation.

Evaluation of the elastic energy “injected” into the sample till the first macro-crack nucleation (characterized by the area under the $\tau - \gamma$ curve) showed that such energy for the sample Fig. 1a is about 3 times higher than for the sample Fig. 1e, while the effective elastic moduli of these samples exhibited inverse behavior. The samples Figs. 1b,c, having the difference in the shear moduli about 20%, exhibited the difference in the “injected” elastic energy about 25%. It should be noted, that the greater is value of elastic energy the lower is effective stiffness (Fig. 1b), because
Deformation and fracture of ceramics with various pores structure under mechanical loading

it corresponds to greater value of relative deformation proper the first macrocrack nucleation. In general, the samples with a regular arrangements of pores exhibited rather greater values of elastic energy “injected” into the sample till the first macrocrack nucleation than the samples with random distribution of pores.

The character of fracture can be directly evaluated from an analysis of bonds between automata, which are presented as networks (Fig. 3). The samples with regular porous structure exhibited fracture patterns of three types. The common features for all these samples are symmetry of damages (because of regularity of the porous structure) and strongly horizontal macrocracks. The first two types of fracture are realized for specimen depicted in Figs. 1a,c,d. In these cases damages nucleation and macrocrack propagation had place in the vicinity of the loading surfaces. It should be noted, that the samples in Figs. 1c,d kept meshing of their fragments in the vicinity of the main cracks, in contrast to the sample in Fig. 1a, and it led to further damage accumulation. The third type of fracture is realized for specimen in Fig. 1a. In this case, damage nucleation took place over the entire sample with further development of macrocrack in the middle part of the specimen. The reason of further damage nucleation in all the samples after loosing the completeness is the constrained boundary condition in the vertical direction.

Figure 3: Fraction of the broken bonds between automata $\eta$ versus relative shear deformation $\gamma$. The crosses on the curves correspond to the moments of first macrocrack development in the sample. The notation of curves corresponds to that of the samples in Fig. 1.

Dynamics of damage nucleation and accumulation in a sample can be quantitatively characterized in terms of ratio of the number of broken bonds between automata to the initial number of bonds versus the relative deformation of the sample (Fig. 3). Each curve corresponding to the sample with regular porous structure in Figs. 1a–d consists of several horizontal and ascending regions. The first ascending region corresponds to the nucleation of the damages over the entire sample (curve b) or to the nucleation of the damages and macrocrack propagation (curves a, c, d). In the $\tau-\gamma$ curves, this is the region with sharp breakdowns of stress (Fig. 2). The next ascending regions of the curves in Fig. 3 correspond to the further nucleation of the damages mainly in the vicinity of macrocracks (curves c, d) or to the development and propagation of first macrocrack (curve b). The horizontal parts of the curves
Figs. 3b–d correspond to elastic deformation of the sample fragments (curves b–d) or of the entire sample (the first horizontal region of curve b). In the stress–strain curves, this is the region in which the shear stress increases monotonically. The ascending regions of curves in Fig. 3 correspond to drop of the shear stress or to its fluctuation near certain value.

Thus, the calculation results show, that the rate of damage accumulation in the brittle specimens with regular pores exhibit threshold character. This fact agrees with experimental data [9], which demonstrate that after local fracture ceramics is been deformed by the same rule as before. At the same time there is a correlation between the macrostresses and the parameters of local strain distribution in ceramics (Fig. 4). The regions of this dependence, corresponding to the uniform accumulation of shear strain by the sample, alternate with stick-slip regions, which first lead to local fracture in specimen and then to the macrofracture of the entire specimen. It should be noted, that both experimental and theoretical investigations were performed for pore size distributions which contain one strong maximum peak.

Figure 4: The dependence of average shear stress $\tau$ on the intensity of shear strain $I_\varepsilon$ in the sample. The moments of local and macro-fracture is signed by the arrows [9].

2 Investigation of deformation and fracture of porous media under uniaxial compression

This part of paper presents the results of numerical simulation of the behavior of porous ceramic ($\text{ZrO}_2$) samples with mentioned types of porous structures under uniaxial compression (Fig. 5). It was established [7] that the samples with this orientation of pores with respect to the axis of loading possess the minimum rigidity and strength. The total porosity in all samples was 25%. The samples had dimensions $0.6 \times 1.25$ mm. A regular pore structures were modeled in four types, which were described in detail above (see the second part of the paper).

Fig. 6a shows the stress-strain ($\sigma - \varepsilon$) diagrams of loading constructed using the results of numerical calculations. As can be seen from Fig. 6, each curve (corre-
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The regions of elastic deformation in the stress–strain diagrams of loading constructed using the results of numerical calculations. As can be seen from Fig. 6, each curve (corresponding to a sample of particular type) can be divided into three regions. The first region, with a low slope, corresponds to the stage of production of the primary separate damages and their development. In the $\sigma - \varepsilon$ curves, this is the region in which a horizontal plateau with repeated breakdowns is attained (Fig. 6a). In the samples with regular porous structures, the length of this region is proportional to the effective stiffness, while the rate of damage accumulation (i.e., the slope) is inversely proportional to the stiffness. The second region features the formation and development of a system of macrocracks in the samples. This stage is characterized by the maximum rate of growth in the number of broken bonds. In the stress–strain curves, this region extends over most of the plateau and a certain part of the descending branches. It should be noted that the slope of the descending branch is proportional to the rate of damage accumulation in a given sample. The third region corresponds to the fragmentation of a sample and the formation of additional damaged sites, typically in the vicinity of the main crack.

The character of fracture in the model samples could be directly evaluated from
the analysis of bonds between automata, which are imaged by network patterns (Fig. 5). The samples under consideration exhibit fracture patterns of two types. The sample with a regular porous structure depicted in Fig. 1a exhibits the nucleation of damage, multiple cracking, and material fracture in the regions of loading surfaces. Then, the material exhibits bulging at the side faces, and the sample separates into layers with the accumulation of damage in the central part (Fig. 5a). The samples with checkerboard pattern of pores are characterized by the formation of a system of symmetric macrocracks, which propagate in the directions of maximum tangential stresses (Figs. 5b–d). In the sample with a stochastic distribution of pores, the first damage usually appears far from the loading surfaces, at the weakest sites characterized by the maximum local porosity. In this sample, the system of macropores shows no symmetry. The formation of the main crack in this case requires additional energy, since the paths of crack propagation from the weak sites are not rectilinear and exhibit a random character.

For the same total porosity, the samples with a regular porous structure (Figs. 5a–d) exhibited higher strength and had greater effective elastic moduli (i.e., slopes of the stress–strain curves) as compared to the sample with a stochastic distribution of pores (Fig. 5e). This trend was especially pronounced for the sample presented in Fig. 5a. The samples with pores arranged in a checkerboard pattern (Figs. 5b–d) exhibited an increase in the effective stiffness and strength at a certain decrease in the ultimate strain (Fig. 6a) with increasing number of pores per cell. Possessing the same total porosity but having a different type of regular structure, the samples with a checkerboard pattern exhibited lower strength and elastic moduli as compared to those of the sample with a vertically stratified structure (Fig. 5a).

The regions of elastic deformation in the $\sigma - \varepsilon$ diagrams are followed by regions with numerous “breakdowns (Fig. 6a), which correspond to the generation and development of structural damage. Calculations showed that, for both the sample with a random distribution of pores and the samples with a checkerboard order of separate pores, this region is rather extended (plateau). In the samples with regular pore structures, the “breakdowns are observed at higher relative deformations than in the sample with a stochastic porosity. This difference can be related to (i) a more uniform distribution of stresses and (ii) a more pronounced “smearing of stress concentrators in the samples with regular porous structure than in the randomly-porous medium. In the samples with regular structures of different types (Figs. 5a–d), the onset of damage production is observed at various levels of deformation. The same trend is observed in the samples with a checkerboard pattern of pores (Figs. 5b–d).

After the appearance of microcracks, the stress–strain diagrams exhibit descending regions, which correspond to the loss of strength. Evaluation of the elastic energy pumped into the sample (characterized by the area under the $\sigma - \varepsilon$ curve) showed that this energy is greater in all samples with regular porous structures than in the case of a stochastic distribution of pores and is proportional to the effective stiffness of each sample.

The dependence of the ratio of the number of broken bonds between automata to the initial number of these bonds, determined as a function of the relative deformation of the sample is depicted in Fig. 6b. As can be seen from Fig. 6b, each curve (corresponding to a sample of particular type) can be divided into three re-
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regions. The first region, with a low slope, corresponds to the stage of production of the primary separate damages and their development. In the \( \sigma - \varepsilon \) curves, this is the region in which a horizontal plateau with repeated breakdowns is attained (Fig. 6a). In the samples with regular porous structures, the length of this region is proportional to the effective stiffness, while the rate of damage accumulation (i.e., the slope) is inversely proportional to the stiffness. The second region features the formation and development of a system of macrocracks in the samples. This stage is characterized by the maximum rate of growth in the number of broken bonds. In the stress–strain curves, this region extends over most of the plateau and a certain part of the descending branches. It should be noted that the slope of the descending branch is proportional to the rate of damage accumulation in a given sample. The third region corresponds to the fragmentation of a sample and the formation of additional damaged sites, typically in the vicinity of the main crack.

As can be clearly seen, the maximum rate of damage accumulation (i.e., the maximum slope in Fig. 6b) among the samples with checkerboard pattern of pores (Figs. 5b–d) is observed for the sample with minimum effective stiffness (Fig. 5d). As the effective stiffness decreases, the rate of damage accumulation increases. It should be noted that this trend is observed only for samples with porous structures of the same type. For example, samples with periodic structures of different types (Figs. 5a and 5d) and effective stiffness values differing by a factor of about 2 exhibit close dynamics of damage accumulation in the second stage (Fig. 6b).

The sample with a stochastic distribution of pores exhibits a substantially different dynamics of damage accumulation. Indeed, the slope of the corresponding \( \sigma - \varepsilon \) curve (Fig. 6b) rather insignificantly varies along this curve, and the second stage (corresponding to the propagation of macrocracks in other samples) in this case is virtually degenerated. The total number of broken bonds in the stage of strength loss for this sample is about five times as small as that in most other samples.

3 Conclusions

To summarize, the results of numerical simulations lead to the conclusion that ceramic samples with stochastic porosity can miss the stage of rapid propagation of the main crack and a sharp drop in the strength, which is typical of brittle materials. This makes possible a quasi-ductile fracture of such brittle materials, which is determined entirely by the pore space structure.

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Atomic mechanisms of thermal energy transformation into mechanical one by non-closed nanostructures

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Abstract

The structural response peculiarities of non-closed nano-sized structures composed of bilayer metallic films under thermal action are investigated. The investigation was based on the molecular dynamics method. The interatomic interactions were described by potentials obtained by the embedded atom method. The calculation data have shown that simulated non-closed nanostructures can transform the supplied thermal energy into the mechanical one. The typical structural changes responsible for the formation of nano-sized structures made of initial bilayer films and for their behavior under thermal action are investigated. Two types of atomic system collective behavior of non-closed nanostructures are revealed.

Introduction

At present, much attention is paid to the investigation of different properties of nanostructures and its use in nanodevices of different functionalities [1]. Nevertheless, the questions connected with atomic mechanisms responsible for nanostructure formation processes are still urgent. The methods of control over nanostructure motions are not sufficiently investigated as well as over capability of these structures to transform supplied energy. The study of the given subjects is the key stone in solution of many fundamental problems. It is of great importance for the practical use of nano-sized structures, for instance, in nanomachines and when designing the nanorobots and nanodevices.

1 Formulation of the problem

The given paper is aimed at studying the atomic mechanisms of structural changes, determining the behavior of non-closed nanostructures formed of bilayer metallic films during the formation process and under thermal loading.
All the calculations in the given paper were made under the molecular dynamics method [2], using the multiparticle interatomic potentials calculated by the embedded atom method [3].

2 Results of numerical simulation

The subject of the given research is the non-closed nano-sized structures formed on the basis of bilayer metallic films with crystalline structure. The simulation of nano-sized structure formation process composed of inclusions with regular internal structure is described in detail [4]. Each inclusion is composed of atoms of a kind; in particular, one type of inclusions was composed of aluminum atoms, another one - of copper atoms. The final shape of simulated non-closed nanostructures was determined by initial parameters of initial nano-sized films. When varying the geometric sizes of copper inclusions and their mutual arrangement in the initial aluminum film, one can obtain the non-closed nanostructures of different shape. In order to accelerate the rolling process of nanostructures, the etching processes of "victim layer" were neglected in papers [4, 5, 6, 7, 8]. It was assumed that initial nano-sized film under stress condition is already separated from substrate. Figure 1 presents the simulation results of non-closed nanostructures, composed of aluminum and copper inclusions.

Figure 1: Shapes of non-closed nanostructures. Copper inclusions of different length are found: a-d on opposite sides of aluminum film; e-g on one side of aluminum film; h is the nanostructure with one inclusion. The copper atoms are shown by light grey color; the aluminum atoms are shown by dark-grey color.

The behavior of non-closed nanostructures, presented in Fig. 1, was investigated under heating over the temperature interval from 50 to 500 K. The edges of these structures start oscillating under heating as far as the thermal-expansion coefficients of layers and their temperature dependence differ considerably. The edge oscillation frequencies of simulated nanostructures are essentially independent of heat intensity. At the same time, the length of copper inclusions and their mutual arrangement...
in the aluminum film affect on frequency and oscillation amplitude. Increase of inclusion length can lead both to the oscillation frequency increase of non-closed nanostructures (inclusions are found on one side of the film (Fig. 1,e-g)), and to the oscillation frequency decrease (inclusions are found on opposite sides of the film (Fig. 1,a-c)).

The calculation results have shown that oscillation amplitude of edges is increased due to the increase in heating temperature and decreased when cooling the non-closed nanostructure. It points to the fact that a part of supplied thermal energy is transformed into the mechanical oscillation energy of free edges. The oscillation frequencies are found in the gigahertz interval for simulated nanostructures. Thus, when varying the arrangement geometry and copper inclusion sizes in films, one can change a response of the simulated non-closed nanostructure under thermal action.

The investigation of questions on supplied thermal energy transformation by the non-closed nanostructures, is not only of scientific interest, but also is very important from the point of view of design and production of nanoengines and energy converters. For this purpose, the simulation of thermal energy transformation into mechanical one by the example of the nanostructure presented in Fig. 1,f.

The temperature interval of performed calculations varied over the range of 130 to 230 K. In the model under investigation, the viscosity forces of the medium surrounding the nanostructure was not taken into account, and energy dissipation of mechanical motion (as well as thermal energy supply) was carried out due to the gradual decrease (increase) in nanostructure kinetic temperature by 100 K. Fig. 2,a,b presents the dependences of free edge displacement of the simulated structure on time. The curve sections numbered 1 and 3 correspond to the nanostructure condition with a kinetic temperature of 230 K while the fields numbered 2 and 4, correspond to the nanostructure condition with a kinetic temperature of 130 K. Thus, when varying the temperature of studied nanostructure, it is possible to change the oscillation amplitude of its edges. The influence of heat duration (cooling) for simulated system on the oscillatory motion behavior was also investigated. Heat (cooling) duration varied from one to three periods of nanostructure oscillation. The calculation results have shown that oscillation frequency of the nanostructure edges poorly depends on thermal action duration over the indicated temperature interval (Fig. 2,a,b).

It should be noted that the viscosity forces affecting the oscillatory edges should be accounted under heating for the more realistic behavior of non-closed nano-sized structures.

In order to take into account the viscosity characteristics of the medium, wherein the simulated nanostructure is arranged, the viscosity force was applied to the surface atoms of oscillatory edges (shown by light grey color in Fig. 3). The viscosity force affecting the surface atoms, was determined by the formula: \( \vec{F} = -k \vec{V} \). Where \( \vec{V} \) is the atom velocity; \( k \) is the proportionality coefficient.

For test determination of \( k \) in this expression, the oscillation damping behavior of nanostructure was investigated for different viscosity values (\( k \) varied over the interval from 0 to \( 6 \cdot 10^{-11} \text{ Ns/m} \)). The calculation results are presented in Fig. 4. For test calculations on studying the simulated structure response on pulse heating \( k \) is set to \( k = 26 \cdot 10^{-14} \text{ Ns/m} \). The test calculations were made in order to investigate the princi-
ple possibility of initial amplitude recovery for nanostructure oscillations (see Fig. 3) in the viscous medium by means of periodical pulsed heating. For this purpose in a certain time interval (here in about three oscillation periods) the simulated structure was heated up for one period. Note that, use of pico- or nanosecond lasers can be one of the methods for pulsed heating of the nanostructures in practice. The initial temperature of simulated nanostructure made 140 K. The oscillation amplitude of edges decreased approximately by 50 % over three periods, and kinetic temperature of the whole nanostructure decreased down to 90 K due to the viscous forces. Then due to the uniform artificial heating, the temperature increased up to 400 K. Under this heating, the oscillation amplitude of edges increased approximately by 40 % relative to its value at the previous section (Fig. 5).

Figure 2: Dependences of free edge displacement of the non-closed simulated nanostructure on time. The duration of heating (cooling) made: a is the one oscillation period; b is the three oscillation periods

Analysis of using these systems as nanoengines of different functionality is one of the most important aspects of non-closed nanostructure simulation under thermal action. The atomic mechanisms of structural changes in the simulated nanostructures should be investigated, starting from the initial moment of its rolling and finishing with oscillations of the already formed nanostructures. The peculiarities of the atomic system behavior were studied as applied to the Al-Cu films.

The simulation results have shown that collective vortex motions of atoms are formed when separating the film from substrate. Figure 6,a presents the atomic displacement fields for the Al-Cu film with a thickness of 10 atomic planes from the moment of its separation from substrate. The figure shows that vortex motions with a diameter of several lattice parameters cover both layers along the full thickness of the films. The vortex motion duration of atoms is rather small (for the Al-Cu system with a thickness of 10 atomic planes made several picoseconds), herein the vortex displacement occur at distances from 8 to 11 lattice parameters. For the fields of displacement presented in Fig. 6,a, the perturbation originates at the film edge during its lifetime and then propagates towards the center.

When no external resistance exists, the formed structure starts oscillating. Although the oscillation amplitude dependence on time has a certain periodicity for the nanostructure, the oscillation mode is unstable and there are sharp breakdowns on the curve. The atomic mechanisms of structural changes in the film under the given oscillation mode are expressed by collective vortex motions of atoms (Fig. 6,a).
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Figure 3: Shape of nanostructure used for studying its behavior in the viscous medium. The aluminum atoms are shown by black color, copper atoms are shown by dark grey color; the surface atoms of nanostructure affected by viscous force are shown by light grey color.

Figure 4: Dependences of free edge displacement of non-closed simulated nanostructure on time in mediums with different viscosity characteristics. The proportionality coefficient value of viscous force (k) made: 1- k = 0 $\text{N} \cdot \text{s} / \text{m}$ (nanostructure oscillates without viscosity forces); 2 k = $26 \cdot 10^{-12} \text{N} \cdot \text{s} / \text{m}$; 3 k = $26 \cdot 10^{-14} \text{N} \cdot \text{s} / \text{m}$

However, when approaching the nanostructure oscillations to the harmonic mode, the vortex character of atomic displacements is replaced by the collective motion of the film atomic groups (Fig. 6,b). These atomic groups are characterized by the atomic displacement vectors, tangentially directed to the studied film surface.

3 Conclusions

Thus, the performed calculations showed an opportunity of using the non-closed nano-sized structures as elementary energy converters. By means of matching the corresponding shape and elemental composition of non-closed nanostructure, pulsed heating mode, choice of the medium viscosity characteristics, one can significantly recover the oscillation amplitudes of the non-closed nanostructure edges. Relaxation and redistribution of elastic stresses in the initial film at rolling is carried out due to the collective motion of atomic groups. It is shown that there are two types of collective motions of the atomic system, determining the behavior at formation and subsequent oscillations.
Figure 5: Variation of nanostructural oscillation amplitude in the viscous medium under pulsed heating: 0 is the nanostructure oscillations disregard of the viscous force; 1 is the nanostructure oscillations in the viscous medium \(k = 26 \cdot 10^{-14} \frac{N \cdot s}{m}\); 2 is the pulsed heating of the nanostructure for one oscillation period; 3 is the nanostructure oscillations in the viscous medium \(k = 26 \cdot 10^{-14} \frac{N \cdot s}{m}\).

Figure 6: The displacement fields of film atoms and its structure presented for different periods of time: a - \(t=(48.38-48.86)\) ps; b - \(t=(435.42-483.8)\) ps. Displacements and structure are introduced for the film free edge, whose length correspond: a -30 % of its initial length; b -50 % of its initial length. The colors of atoms and their displacements are marked: by black for aluminum atoms and by light grey for copper atoms.
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The definition of the deform hardening curve of metal materials under load-displacement diagram of conic indenter

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Abstract

The new technique of the hardening curve definition which is approximated by three-parametrical function under the results of tests for pressing of three conic indenter with various corners of conicity was developed. This procedure allows to investigate metal materials with the expressed limit of fluidity. The technique has passed verification in laboratory conditions on steels St3, 08Cr18N10T and pure copper. The experiments were carried out on the servohydraulic testing machine Instron 8801.

There are three standardized tests — the stretching, the compression and the torsion of speci-mens which are basically applied to define the mechanical properties of metals. These methods give the authentic information about material properties. It is necessary to cut out a part of mate-rial from billet, product or construction unit for manufacturing specimen therefore considered tests concern to so-called destructive methods. However in some cases it is not obviously possible to make samples of the necessary sizes or quantity, or it is not expedient from the economic or technical requirements. It is just for constructions and machines which are in service, when it is necessary to evaluate of the current status of technical objects to define an opportunity of their further operation. In these cases nondestructive methods or without specimen methods of test realization are applied. Such test methods which will be carried out directly on the examined products and do not cause its destruction concern to without specimen test methods, for example the methods based on measurement of hardness.

The method of kinetic indentation based on a conic indenter penetration in a product surface [1, 2] which uses the indentation diagram of load penetration \( P \) from the penetration indenter depth \( h \), is perspective. This relation is well described by the parabolic of Kick’s law [3]

\[
P = ch^2
\]
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where \( c \) is a factor which is dependent from the indenter corner \( \alpha \) and elastic-plastic properties of a material into which indenter is pressed and which is practically does not depend on indentation depth.

Generally the hardening curves of metals and alloys are approximated by power dependences. The three-parametrical dependences approximate the curve of hardening of metals and alloys with obviously expressed yield strength more exactly than two-parametrical dependences.

For the majority of metals the hardening curve is possible to approximate by three-parametrical power dependence as

\[
\sigma_s = \sigma_0 (1 + a_1 \Lambda)^{a_2}
\]

where \( \sigma_0 \) is the yield point; \( \Lambda \) is the degree of shear strain; \( a_1 \) and \( a_2 \) are the empirical factors.

For development of definition technique of hardening curve parameters by the results of conic indenter pressing it is necessary to execute computer modeling of conic indenter pressing in elastic-plastic semispace, to check up adequacy of modeling results to the experimental data and to receive the necessary volume of calculated data for selected set of the hardening curve parameters. The modeling of conic indenter pressing to the elastic-plastic semispace has been executed by finite element method by the computer program developed in Institute of Engineering Science. The adequacy modeling criterion has good coincidence of the calculated and experimental indenter diagrams and the pile-up which is formed during indenter penetration in metal.

As the large strains take place during the indenter pressing the hardening curve is reasonable determined by results of tests for sample compression. Thus it is necessary to define it precisely on the initial stage of deforming. The true hardening curve were received from the experiments of cylindrical specimens compression to test materials: steels St3, 08Cr18N10T and pure copper. These metals were annealed previously. The received curves are given in a fig. 1.

![Figure 1: The deform hardening curve](image)

The axially symmetric deformation was considered. A material has described by model of elastic-plastic isotropic and isotropic hardening environment. The elas-
tic deformations were small and satisfied to the Hook’s law. Plastic strains were large and submitted to the associated law of plastic flow with loading function of Mizes. The change of volume was only elastic. Numerical algorithm of the computer program based on quadrilateral isoparametric elements, step-by-step change of loading by small increments of indenter moving, principle of virtual capacity in the high-speed form and method of initial deformations.

Indenter has been considered as an absolutely rigid body. On a surface of environment which contacting with indenter, the friction law of Pradtly-Ilyushin [4] was set which unites the friction laws of Coulomb and Zibel. The friction factors in last laws have set equal 0,1 and 0,4 accordingly. In a fig. 2 the fragment of initial geometry of a finite element grid is shown. A grid set by regular dimension 70×70 of cells and a variable step.

![Figure 2: A grid of finite element modeling](image)

For example the calculated diagrams of indentation and shapes of pile-up for steel St3 for the corners of indenter equals 94°, 120° and 143° are shown in a fig. 3 and 4 by dashed lines.

![Figure 3: Experimental (continuous lines) and calculated (dashed lines) indentation curve for steel St3: 1 – α = 94°; 2 – α = 120°; 3 – α = 143°](image)
The experiments on conic indenter pressing in test materials have executed on the servohydraulic test machine Instron 8801. The specimens which were subject of pressing have been polished.

During experiment the indentation diagrams were continuously recorded. In a fig. 3 continuous lines show results of experiment for steel St3. The precision of the experimental and calculated indentation diagrams testifies to good accuracy of the used computer program.

![Figure 4: The average shapes of overlap for steel St3 and indenter corners equals 94° – 1, 120° – 2, 143° – 3](image)

The shapes of pile-up in two mutually transverse directions from dimple depth for each material and indenter corner were measured by interferometric microscope Wyko NT 1100. In a fig. 4 continuous lines show the average experimental shape of pile-up for steel St3. The precision of pile-up shape also testifies to adequate accurate results of computer modeling.

Generally the parameter $c$ in the equation (1) depends on hardening curve (2) coefficients $\sigma_0$, $a_1$, $a_2$, Young’s modulus and conic indenter corner $\alpha$:

$$c = c(\sigma_0, a_1, a_2, E, \alpha).$$

Under the dimension analysis and P-theorem given dependence have presented as

$$c = E\Phi(a_0, a_1, a_2, \alpha)$$

where $a_0 = \frac{\sigma_0}{E}$, function $\Phi$ and its arguments $a_0, a_1, a_2$ are nondimensional values.

For the estimation of function $\Phi$ the penetration of the conic indenter with the given corner $\alpha$ in elastic-plastic medium was multiple simulated by the finite element method for set of parameter values $a_0, a_1, a_2$. The Young’s modulus and Poisson ratio for all materials have been considered equal 200 GPa and 0.3 accordingly. The calculations have been executed for indenter corners equals 94°, 120° and 143° to ensure the verification of the technique to indentation experimental data received on the test machine Instron 8801. A calculated indentation curve was approximated by the Kick’s law (1).
The function $\Phi$ values have been received by division of factor value $c$ onto the Young’s modulus $E$. The calculated data have been approximated by analytical dependence as

$$\Phi = \varphi a_1^n a_2^m$$  \hspace{1cm} (4)

where $\varphi (a_0) = b_0 + b_1 a_0$, $m (a_0) = -b_2 + b_3 a_0$, $n (a_2, a_0) = b_4 + (b_5 - b_6 a_0) a_2$, $b_i = d_i + g_i \alpha$, $i = 0, \ldots, 6$, $d_i$, $g_i$ — numerical factors.

The average squared deviation of calculated values of function $\Phi$ from approximated data is equal 2.2%.

The factor values of $c_i$ ($i = 1, 2, 3$ where $i$ is number of indenter) in the Kick’s law have defined from experiments of pressing of three indenters with various corners, so we received the system of three nonlinear equations according to (3), (4)

$$u_i = \varphi a_1^{n_i} a_2^{m_i}, i = 1, 2, 3,$$  \hspace{1cm} (5)

where $u_i = \frac{u_i}{E}$, the index $i$ defines values of factors $b_0 - b_6$ for the appropriate corner of a cone.

As the equation (5) is nonlinear, its decision was found by a trial-and-error method [5] by minimizing discrepancy

$$\rho = \frac{1}{E} \sqrt{\sum_{i=1}^{3} \left[u_i - \varphi a_1^{n_i} a_2^{m_i}\right]^2} \to \text{min}.$$

The hardening curves of test materials received from upset experiments (dashed lines) and on developed technique (continuous lines) are shown in a fig. 5. It points to the fact that the given curves sufficiently good coincide with experimental hardening curves on the variation interval of degree of shear strain $\Lambda < 1$ for steel St3 and pure copper and $\Lambda < 0.8$ for steel 08Cr18N10T.

Figure 5: Experimental (dotted lines) and approximated (continuous lines) hardening curves for steel St3 (a), steel 08Cr18N10 (b) and pure copper (c)

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The definition of the deform hardening curve of metal materials under load-displacement diagram of conic indenter


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Finite element meshing in modeling of the initial crack growth from defects in a plate under cyclic loading

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Abstract

Recently, a lot of attention is paid to the investigations of process of origin and growth of defects in the material under cyclic loading. One of effective methods to solve different complicated tasks in this field is Finite Element Method (FEM). However there are certain problems on this way and one of these problems is the parasitic influence of the finite element grid on the trajectory of the growing defect.

This paper is the first stage of the investigations devoted to the minimization of influence of the finite element grid to the trajectory of growing defect. At this stage the general principles are formulated and the types of grids which meet these principles and let minimizing the influence of the finite element grid on the trajectory of the growing defect are presented.

The object of investigations is the trajectories of growing defects in a plate under cycling loading. The task is solved in the context of linear elasticity and linear fracture mechanics.

It was found that the traditional rectangular finite element grid doesn’t allow the defect growth trajectory to deflect from the straight line.

In this paper general principles of creating a finite element grid in the task of defects propagation in a plate under cyclic loading are formulated and one of the most efficient realization of grid is presented. Its efficiency, in terms of absence practically any influence the geometry of grid on the defect growth trajectory, is confirmed by serial calculations with different types of loading.

1 Statement of the problem

Currently, a serious attention is been paid to the process of origination and growth of defects in material under cyclic loading. Based on experimental findings, an effective proved the finite element method (FEM) of analysis. However there are certain
Finite element meshing in modeling of the initial crack growth from defects in a plate under cyclic loading

problems in modeling the material behavior and turning of defects into cracks, and one of these is the remarkable influence of the finite element grid on the trajectory of the growing defect (crack).

In the following the first stage of analysis is displayed focused on the minimization of influence of the finite element grid on the trajectory of growing defect in a component under cyclic loading. At this stage the general principles will be formulated and the types of grids which meet these principles and would allow reducing the influence of the finite element type and mesh on the growing defect paths are presented.

A thin rectangular plate uniformly cyclically loaded at the infinity is selected appropriate mechanical model. The plate is considered a composition of finite elements representing material elements with randomly distributed resistance to fatigue, as if they were grains with randomly distributed orientation of slip planes with respect to direction of loading. Defects in material structure are assumed grains characterized by insignificant resistance to fatigue loading. Although fatigue behavior implies development of nonlinear processes in material microstructure, the problem is analyzed first in the context of linear elasticity and linear fracture mechanics.

Fatigue process was modeled as the sequence of damage accumulation in FE’s affected using the Palmgren-Miner rule:

$$D = \sum_i \frac{n_i}{N_i}$$

where $D$ - is the formally assessed damage index (within the frames of the rule), $n_i(S_i)$ – is the number of load cycles with the stress range, $S_i$ – characteristic of an “i” element, accordingly its location in the FE model, $N_i(S_i)$ - is the number of cycles prior failure of the “i” element, this value is the characteristic of the stress field in every finite element.

The fatigue properties of finite (material) elements are described by the known Basquin’s equation:

$$N(S) = C/S^m$$

where $C$ and $m$ – are the material empirical “constants”, to be obtained from the experimental data, $S$ – is the stress range (in a particular FE).

Respectively, the damage accumulated in every of the elements in the course of cycling and crack extensions:

$$D = \sum_i \frac{n_i}{N_i} = (1/C) \sum_i n_i S_i^m$$

Crack propagation is assumed a process of successive failure of elements; when the damage in a sequential element becomes , stiffness of the element is decreased by several decimal orders, allowing the crack extension. When the progress of damage, crack growth rate, is essentially accelerated the process phase is regarded the specimen failure.


2 Common grid

Firstly, the plate under the scope is approximated with a regular finite element grid of 4-nodes constant stress elements. Fig. 1 shows the initial distribution of the defects in the plate and the final state with growing defects preceding failure defined as in above.

Crack growth path shown in Fig.1 is seemingly in accordance with the crack mechanics because in this case normal opening fracture mode is realized, and the defect propagates perpendicular to the applied stress flow direction.

However, in a more general case, when one crack grows in vicinity of another crack its trajectory may be strongly influenced by the stress flow, caused, in particular, by the deviation of the principal stresses and development of shear stress at the crack tip. As seen in Fig.1b the apparent disturbance of the stress field at the "main trace" due to nearest defect did not affect the straightforward crack extensions.

The due analysis of the stress field at the blunt, rectangular "crack tip" provided by the above procedure shows that it is almost impossible to fit the crack path allowing for the stress field deviation, since the most significant stress raise is computed in the consecutive finite element.

Apart from that, application of linear elasticity ideology implies that the stress in the vicinity of the crack tip is infinite. In numerical simulation there is no stress infinity at the crack tip due to averaging over the element, but the stress remains very high. According to the Basquin's equation the failure is expected to occur in the element with the highest stress. It is easily seen that the highest stresses will be computed only in the element which has two common nodes with the crack tip (because of the extremely high stresses in the vicinity of the crack in comparison
Finite element meshing in modeling of the initial crack growth from defects in a plate under cyclic loading

with its neighborhood). And there is the only element with such characteristic - it is the element on the defect’s extension line. Attempts to find a straightforward solution via applying successively finer mesh occurred misleading, and it means that the mesh type controls the crack extension direction.

To illustrate the highly influence of mesh types on the crack extension direction fig.2 is presented.

Figure 2: The influence of the mesh type on the crack extension direction

So far, the attempts were focused on development the mesh type which would provide the crack deviation under influence of diversity of the fatigue properties of material (finite) elements.

It can be done by creating triangle elements at the tip of the crack because only triangle elements have only one common node with the element at the tip. In this case the further crack propagation can be provided only accordingly the chosen criteria.

It should be mentioned that in principle it might be possible to allow the crack deviation by consecutive re-designing of the mesh and deleting the nodal connections. However, the changing of initial mesh during the crack propagation analysis should be avoided because of the initial distribution of the fatigue strength in the finite elements and this distribution has not to be changed during the crack propagation.

By this reason the only means to provide the possibility for crack trajectory to deviate during successive extensions is to design the mesh of equally distributed special ”blocks” made of triangle elements. In this case the crack growth path between the ”blocks” will be a straight one, while in the ”blocks” the direction of further propagation might be allowed according to selected criteria. Such blocks might be designed so as to provide the smooth crack deviations, e.g. at 15 degrees or even smaller. And, finally, if these blocks would be small enough with respect to
the plate dimensions, the crack trajectory might be expected a realistic one.

Another important issue is that it is necessary to provide the regularity and isotropy of the grid.

The regularity of the finite element mesh is one of the ways to increase the accuracy of the stress analysis. It should be noted that rectangular elements are preferred in the mesh design, because the rectangular element with the equal or close to equal sides has higher degree of accuracy in comparison with the triangles in which one side is much bigger than another, a needle-like ones. And one more point is development of an isotropic grid may provide avoiding the appearance of the ”main” direction that will result in a great influence on the crack growth trajectory.

3 Advanced grid

Based on these principles a number of versions of finite element grid were created and analyzed under different combinations of loading. With the help of optimization a grid type was found which met the above principles. The characteristic cell designed of rectangles is shown in Fig.3.

![Figure 3: a cell of the finite element grid](image)

The geometry of the cell shows the two levels in this model. The first level consists of ”large circles” with the triangles elements in the center which allows the trajectory of the crack to deviate. The second level consists of small ”circles”, also with triangles in the center. The role of the second level is to provide for the crack path to turn even if it propagates along the edges of the big ”circles”.

So far, this configuration of finite element grid has to provide the deviation of the crack trajectory to under influence of the particular stress flow and of the fatigue properties of material (finite) elements in a smooth way.

Analysis have shown that the above ideas and the type of meshing occurred effective in assessing the crack growth within the principles of modeling the fatigue behavior of components. The developed type of meshing macroscopically provides a high degree of regularity, symmetry and isotropy essentially important when the elements are allotted with different prescribed fatigue properties which would prevent or complicate the mesh re-designing in the course of crack propagation simulation.

To illustrate the said and the efficiency of the designed meshing, one of the results of the modeling the crack development from a defect and further propagation with the means of the special grid is presented at Fig.4. The elements are randomly allotted with the differing fatigue properties, in this case, with different values of the material constant C in approximation of the fatigue curve (2). The left hand part,
Fig. 4, a shows the location of defects and early stage of the damage development accordingly the rule (3). Respectively the elements’ fatigue resistance one of the initial defects in material structure becomes the governing and gives “birth” to the principal “crack” (Fig. 4, b). The other irregularities of the structure occurred in this analysis less effective because of composition of fatigue properties of surrounding elements and resulted in non-propagating cracks.

![Figure 4: a cell of the finite element grid](image)

The trajectory of the growing defect demonstrates the efficiency of the developed finite element grid. The simulated crack now can deviate according to the structure of the local stress field. In the presented example the crack propagation is deflected from the straight line due to scatter of fatigue properties and the rate of accumulated damages, in a sense, affected by the small crack at the bottom of the plate which are "felt" by the main crack. It means that the grid influence on the crack growth trajectory may be regarded as essentially reduced.

To conclude, the present paper formulated and realized several principles of development a finite element grid in simulation of fatigue crack initiation from material structure defects and propagation in a thin plate under cyclic loading. The principles are: the necessity to provide the crack direction deviation in the course of its propagation under influence of the local stress flow and fatigue resistance of material elements, and the necessity to provide the regularity and the isotropy of the grid. Based on these principles a two-level finite element grid is designed, the geometry of which is presented in Fig. 3. This grid has drastically reduced the influence of the mesh geometry on the crack growth trajectory. Its efficiency is confirmed by serial calculations with different types of loading.
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Plasticity nucleation at atomic level in crystal materials under dynamic loadings

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Abstract

Molecular dynamics simulation of plastic deformation nucleation peculiarities was carried out. Influence of external conditions and different schemes of loading were studied. It was shown that local structural distortions called protodefects always preceded conventional structural defects formation.

1 Introduction

One of the key tasks in the modern physics of plasticity is connected with the search for a thermodynamic parameter whose variation would define local stability loss of the crystal. The influence of atomic density or, which is the same, atomic volume on the structural-phase state of solids has long been discussed [1, 2, 3, 4]. As paper [4] demonstrates, atomic density is one of the thermodynamic variables that govern the phase state of condensed matter. The introduction of this parameter in an explicit form has allowed one for the first time to validate a new type of phase diagrams. The diagrams are plotted in the variables of temperature — concentration — atomic density. The use of the diagrams not only expands our notions about the conditions of phase coexistence at varying atomic density, but also explains instability of the lattice and its mechanical melting when a solid expands to a critical specific volume [4]. Molecular dynamics studies [5, 6] also show that volume expansion is a cause of lattice instability; in so doing, as follows from [4], it is not important how the excess volume is achieved, whether due to heating or mechanically.

Notice that all the above-given results have been obtained on the assumption about homogeneous (uniform) expansion of the volume. It would natural to ask what effects can be induced by local volume change. First of all, whether the change will precede the formation of lattice defects and if yes, what defects exactly. Paper [7] show that under mechanical loading of fcc metals one can see the generation of
specific local structural distortions that correspond to a local structural transition of fcc-hcp type. The local structural distortions may be considered as protodefects, because, as follows from [7], they give rise to defects of a higher level (partial dislocations, stacking faults, etc.). The formation mechanism of such local structural distortions is not understood. In view of the aforesaid, the question arises whether the formation of such protodefects is related with local volume expansion?

To study this question, we have performed molecular dynamics simulation of the behavior of a preloaded specimen at the relaxation stage, which allows excluding effects of dynamic nature.

The calculations were carried out at finite temperature (T = 300 K) for a 3D parallelepiped copper crystallite. The coordinate axes were oriented along the [110], [110], and [001] crystallographic directions. Along the [110] crystallographic direction we simulated periodic boundary conditions, free surface were oriented normally to the [110] direction. Preloading (tension at constant rate 50 m/s) was performed along the [001] direction. To simulate relaxation processes at a certain strain, the calculations were carried out with zero tension rate. Interatomic interaction was described in the framework of the embedded atom method [8].

2 Protodefects formation

As is shown in [7], there is a certain threshold strain value at which the growth of zones with local structural changes is almost avalanche-like. The calculations suggest that the threshold value is in the range from 1014% and depends on temperature and loading conditions. Note that increase in strain rate (load intensity) leads to the fact that relaxation processes have no time to provide the generation of local structural changes. As a consequence, the generation begins at higher strains. We may therefore expect that at long relaxation of the preloaded crystallite protodefect generation will start at lower strains. This is justified in the present study which demonstrates that really during relaxation local structural changes begin when the prestraining value achieves 8.5%. Notice that the loading conditions and temperature were assumed to be the same as in [7].

The calculation results for the number of atoms involved in local structural transformations during relaxation of a tensile specimen prestrained by 8.8% are given in Fig. 1. The same Figure illustrates respective changes in potential energy per one atom. Notice that the coordinated behavior of the both curves unambiguously points to the fact that the generation of local structural changes is one of the mechanisms of internal stress relaxation.

A detailed analysis of atomic displacements at the stage of nucleation of local structural distortions (protodefects) has revealed that their formation is related with specific rearrangement in the first and second coordination spheres of one of the atoms. Local structural distortion around the atom corresponds to the local topology of the hcp structure; hence in the subsequent discussion we will identify such atoms as centers of protodefects. Fig. 2 schematically illustrates the typical sequence of atomic displacements, which causes the formation of a protodefect in the vicinity of one of such atoms (denoted by α). It is clearly seen that one of the atoms of the second coordination sphere (denoted by β) is displaced to the first
Plasticity nucleation at atomic level in crystal materials under dynamic loadings

coordination sphere, while one of the atoms of the first coordination sphere (denoted by \( \gamma \)) leaves it.

![Figure 1: Growth in the number of atoms (N) involved in local structural transformations and potential energy variation during relaxation of the crystallite prestrained to 8.8%](image)

Figure 1: Growth in the number of atoms (N) involved in local structural transformations and potential energy variation during relaxation of the crystallite prestrained to 8.8%

![Figure 2: Schematic of structural transformations that cause the generation of a zone of local structural changes (protodefect formation): a) — initial crystal; b) — intermediate stage; c) — stage when neighbors of the central atom already have the hcp topology. The lines indicate the bonds of atom (\( \alpha \)) with the first coordination sphere atoms](image)

Figure 2: Schematic of structural transformations that cause the generation of a zone of local structural changes (protodefect formation): a) — initial crystal; b) — intermediate stage; c) — stage when neighbors of the central atom already have the hcp topology. The lines indicate the bonds of atom (\( \alpha \)) with the first coordination sphere atoms.

To investigate the role of excess volume in protodefect formation during relaxation, we studied atomic volume variation for all atoms of the simulated system. The calculations have shown that for the atom \( \alpha \), which is in the state corresponding to that indicated in Fig. 2a, the atomic volume is almost equal to equilibrium and the local structure corresponds to the fcc packing. When the environment of the atom \( \alpha \) goes to the state illustrated in Fig. 2b, the atomic volume grows by 5-6%. It is the atomic configuration that characterizes the local unstable state of the lattice. The calculations have also shown that this atomic configuration can either return to the initial fcc packing (Fig. 1a) or transform into the hcp packing (Fig. 2c). The latter leads to protodefect formation. In the both cases, the atomic volume reduces
to the corresponding equilibrium value. Herein the deviation induced by thermal-fluctuation processes does not exceed 1-2%. The absence of a visible residual change of the atomic volume is due to the fact that both the fcc and hcp structures are close-packed. Note that the described mechanism holds true for all atoms which are centers of protodefects.

Figure 1 clearly depicts the stage-by-stage variation of potential energy and increase in the concentration of local structural distortions during relaxation. Notice that the stage-by-stage character coincides for the both curves in Fig. 1. In order to understand its cause, we studied in detail the generation of protodefects and evolution of their spatial distribution (see the results in Fig. 3). For clarity, all atoms in Figs. 3a-c except those which are the centers of local structural changes were made invisible, thus visualizing the formed structures.

At the first stage the crystallite relaxes, which is accompanied by a slight increase and subsequent decrease of its potential energy. Protodefects are not generated in this case, while the potential energy decrease occurs due to the formation of local lattice distortions that precede protodefect generation. At the second stage one can see protodefect generation and evolution, which governs corresponding potential energy reduction. In the considered case, the nucleation of protodefects begins close to a free surface (Fig. 3a) and then they condense into paired plane structures (Figs. 3ac). Fig. 3c illustrates the structure corresponding to the completion of relaxation, which is manifested in flattening out of the time dependence of potential energy (third stage).

Two cases are clearly observed in Fig. 3c: 1) the close-packed planes with condensed protodefects are adjacent, and 2) the same planes are separated by a defect-free plane.

In the first case, analysis of alternating close-packed planes has shown that protodefects form a classic stacking fault (Fig. 3d). This follows from the fact that
the sequence of close-packed planes ABCABCABC, which is typical of a perfect fcc crystal, transforms into the sequence ABCACABC. Notice that the stacking fault is bounded by a partial dislocation. In the second case, there is extrinsic stacking fault.

3 Complex loading

Another interesting task is the investigation of protodefect formation in species under complex loading. To study this question we used following boundary conditions: in one direction we used periodic boundaries, in the second — free and in the third direction loadings were applied. For implementation of complex loading there were strain loading plus shearing stress.

Simulation showed that there is a threshold deformation value when protodefect begin to nucleate near free surface. While strain rate is growing several disturbed fragments beginning to appear separated by stacking faults and by free surfaces (Fig. 4).

Figure 4: Fragmented structure while strained on 7.5%. Atoms with hcp-topology with nearest neighbours are marked with big balls.

It should be noted that in species with grain boundary disturbed fragments are separated with stacking faults both types and, hypothetically, microtwins (Fig. 5).

Formation of fragments is folowing: in the upper corner of the Fig 6 one can see region with displacements greatly exceeds mean displacements. This region is situated near jaw. In the places with maximum displacement gradients stacking faults formed from protodefects begin to arise. This stacking faults serve as buffer between regions with different orientations and provide integrity of the matter. On the Fig 6b it clearly can be seen another region with high displacements. The simulation shows that in contact region the stacking fault will appear.

4 Summary

The obtained results show that the formation of structural defects with crystalline structure as a plastic deformation mechanism is complex and multistage. It is realized in the conditions of local expansion of the atomic volume. The formation of a
local excess volume depends on many factors: crystallographic direction of loading, intensity of external actions, temperature of the simulated specimen, presence of interfaces in the specimen and other. In materials with perfect structure the formation of the excess atomic volume has a thermal-fluctuation nature [7]. It should be noted that the excess atomic volume formation always precedes the nucleation of protodefecs that may be considered as elementary carriers of structural distortions. During relaxation the local structural distortions do not disappear, moreover they condense giving rise to the formation of plane defects (like stacking faults) and partial dislocations. It should be noted that interfaces of different nature play significant role in nucleation and development structural defects. Complex loading can lead to fragmented structure formation.

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Figure 6: Fragmented structure while strained on 6.1% (a) and 6.2% (b)
Modeling of graphene crystal lattice

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Abstract

The work is devoted to investigation of different graphene lattice models. The methods of exploring equations describing the elastic moduli of graphene are examined. The material is represented as a set of particles that interact with each other and this interaction is produced by means of linear and angular springs. The closest neighbour’s interaction is considered. One- and two-parametric models of graphene layer are built. The connection between the elastic moduli and the stiffnesses of the springs is obtained via energy and force approaches. Investigated models allow to express micro parameters via macro parameters and as the result to receive the correspondence with the experimental data.

1 Introduction

Graphene is one-atom-thick planar sheet of carbon atoms that are densely packed in a honeycomb crystal lattice. Each atom is covalently bonded to three other. Stable sheet of graphene was first obtained in 2004 by a research group from the University of Manchester (Manchester, UK) and the Institute for Microelectronics Technology (Chernogolovka, Russia) [1]. It attracts a great deal of attention because of its fundamental nature: graphene is the constituent of all carbon-based systems (graphite is a stack of graphene layers, carbon nanotubes a made of rolled-up sheets of graphene, fullerenes are spheres of wrapped-up graphene). One atom thick graphene membranes offer many exciting directions for future research. Those obtained experimentally are not perfectly flat: the surface normal varies by several degrees and out-of-plane deformations reach 1 nm. This comes to an accordance with the fact that perfect 2D atomic crystals cannot exist in the free state [2], [3]. In this work out-of-plane deformations are not taken into consideration.
2 Description of the model. Energetic approach.

Let us consider two-dimensional single crystal (fig. 1). Covalent interactions between the atoms of graphene lattice’s crystal structure can be described by methods of molecular dynamics. Let us represent material as a set of particles located in the vertexes of rectilinear hexagons. The interaction between the particles is carried out by linear and angular springs: each particle is bonded to the three other by means of linear springs and these springs are connected by means of angular spring. The interaction between the closest neighbours is taken into consideration. Elementary cell contains two particles.

![Figure 1: Model of graphene layer](image)

Let us use energetic approach while calculating the system. It is very convenient when small deformations are considered. Energy accounting for one particle can be presented by the following equation:

\[
W = \frac{1}{V_0} \left( G_1 \sum_{\alpha} \kappa_\alpha^2 + G_2 \sum_{\alpha,\beta} \xi_{\alpha \beta}^2 \right). 
\]

Here \( V_0 \) is the volume of the elementary cell (is depicted on Figure (1) with dotted line), \( \kappa_\alpha \) and \( \kappa_\beta \) – deformations of the bonds \( \alpha \) and \( \beta \), \( \xi_{\alpha \beta} \) – change of the angle between the bonds [4].

Using formulas from [4] we can calculate the Poisson ratio, bulk modulus, Young
modulus:
\[ \nu = \frac{c - 6c_\gamma}{c + 18c_\gamma}, \quad K = \frac{3ca^2}{4V_0}, \quad E = \frac{36ca^2c_\gamma}{V_0(c + 18c_\gamma)}, \]

where \( c \) — stiffness of the linear spring, \( a \) — its length, \( \gamma \) — stiffness of the angular spring, \( c_\gamma = \frac{\gamma}{a^2} \). For graphene lattice \( V_0 = \frac{3\sqrt{3}}{2} a^2 \).

And now let us consider one-parametric model. Each atom forming a lattice is bonded to three other via absolutely stiff rods. Assuming the stiffness \( c \) of the linear springs in the first model tending to infinity the following results can be achieved:

\[ \nu = 1, \quad K = \infty, \quad E = 36\frac{\gamma}{V_0}. \]

3 Force approach and its comparison to energetic one

![One-parametric model of graphene layer](image)

Figure 2: One-parametric model of graphene layer

Force approach while investigating one-parametric model was also examined. Within the framework of this approach the deformation that is responsible for the changes of the angles between the bonds is represented by linear springs with stiffness \( \tilde{c} \) to simplify the model. To the atoms located at the end of the crystal constant tensile stresses \( \sigma_x \) and \( \sigma_y \) are applied. Two uniaxial stress states are considered: \( \sigma_x = 0, \sigma_y \neq 0 \) and \( \sigma_y = 0, \sigma_x \neq 0 \). While considering the first state let us mentally cut the crystal along the horizontal straight line (x axis) and consider one nod located close to this line. The stress \( \sigma_y \) can be expressed via the total normal
force $F_y$ exerted on this nod by its closest neighbours:

$$\sigma_y = \frac{F_y}{S_y}, \quad (4)$$

where $S_y$ — distance between the closest nods along the horizontal line. $F_y$ can be related via micro parameters $\tilde{c}$, $a$, $\tilde{a}$ — distance between the vertex and a point of fastening the linear spring, $\alpha$ describes the change of the angle between the closest ties. $S_y$ can be related via $a$ and $\alpha$. After calculating these values, putting it in (9) and linearizing, $\sigma_y$ can be expressed. The expression for $\sigma_x$ depending on the micro parameters can be achieved in a similar way. The result is

$$\sigma_y \big|_{\sigma_x=0} = 4\tilde{c} \left( \frac{\tilde{a}}{a} \right)^2 \alpha, \quad \sigma_x \big|_{\sigma_y=0} = -4\tilde{c} \left( \frac{\tilde{a}}{a} \right)^2 \alpha. \quad (5)$$

Let us denote the strains of the crystal along x and y axes by $\varepsilon_x$ and $\varepsilon_y$, respectively. They depend only on parameter $\alpha$:

$$\varepsilon_x = -\frac{2}{3} \alpha \sqrt{3}, \quad \varepsilon_y = \frac{2}{3} \alpha \sqrt{3}. \quad (6)$$

The Poisson ratio $\nu_x$ and the Young modulus $E_x$, characterizing the tension along the x axis and the respective values $\nu_y$ and $E_y$ characterizing the tension along the y axis are [5]:

$$\nu_x = -\frac{\varepsilon_y}{\varepsilon_x} \bigg|_{\sigma_y=0}, \quad E_x = -\frac{\sigma_x}{\varepsilon_x} \bigg|_{\sigma_y=0},$$

$$\nu_y = -\frac{\varepsilon_x}{\varepsilon_y} \bigg|_{\sigma_x=0}, \quad E_y = -\frac{\sigma_y}{\varepsilon_y} \bigg|_{\sigma_x=0}. \quad (7)$$

After putting (4),(5),(6) into (7) one can see that the Poisson ratio and the Young modulus corresponding to both of uniaxial stress states are the same:

$$\nu = 1, \quad E = \frac{2}{\sqrt{3}} \tilde{c} \left( \frac{\tilde{a}}{a} \right)^2. \quad (8)$$

The bulk modulus $K$ can be calculated using the relation

$$K = \frac{E}{2(1-\nu)} \Rightarrow K = \infty. \quad (9)$$

To make the comparison to the results (3) a relation between the stiffnesses $\gamma$ and $\tilde{c}$ was achieved:

$$\gamma = \frac{1}{4} \tilde{c} \tilde{a}^2. \quad (10)$$

After putting this relation in (3) one can see that the results of the force approach coincide with ones obtained using energetic approach. Force approach has an important advantage: it allows to consider non-small deformations.
4 Determination of micro parameters

For graphene lattice components of stiffness tensor’s experimental data:

\[
\begin{align*}
\frac{C_{11}}{h} &= 1060 \text{GPa}, \\
\frac{C_{12}}{h} &= 180 \text{Gpa},
\end{align*}
\]

where \( h = 0.34 \text{nm} \) is the distance between the graphene sheets in graphite [6].

Using relations \( C_{11} = \lambda + 2\mu \), \( C_{12} = \lambda \) parameters \( \lambda \) and \( \mu \) can be calculated:

\[
\begin{align*}
\mu &= 149.6 \frac{\text{N}}{\text{m}}, \\
\lambda &= 61.2 \frac{\text{N}}{\text{m}} \quad \Rightarrow
\end{align*}
\]

\[
\begin{align*}
K &= 210.8 \frac{\text{N}}{\text{m}}, \\
E &= 350 \frac{\text{N}}{\text{m}}, \\
\nu &= 0.17.
\end{align*}
\]

From (2) the following relation can be obtained:

\[
\chi = \frac{1}{6(K/E - 3)},
\]

where \( \chi = \frac{\gamma c a^2}{\text{ca}^2} \) and it can also be expressed via Poisson ratio:

\[
\chi = \frac{1 - \nu}{6(3\nu + 1)}.
\]

From (2), (13) and using the relation (15) micro parameters for two-dimensional model can be expressed:

\[
c = 730.2 \text{N/m}, \\
c_\gamma = 66.9 \text{N/m}.
\]

And now let us calculate \( c_\gamma \) that corresponds to the one-parametrical model using the relation (3):

\[
c_\gamma = 25.3 \text{N/m}.
\]

The stiffness \( c_\gamma \) in case of two-parametrical model is 2.6 times more than in case of one-parametrical one. In case of stiff rods \( c \) is equal to \( \infty \) and as follows from (3) \( \gamma \) is positive.

5 Results and conclusions

One-parametrical and two-parametrical models of graphene’s layer were considered. These models allow to obtain simple analytical expressions connecting their microscopic and macroscopic parameters and to determine micro parameters applying the accordance with the experimental data.

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The influence of small scale dispersion and dissipation on nonlinear waves in elastic media.

The problem of solution non-uniqueness in hyperbolic approximation

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Abstract

The simultaneous effects of dissipation and dispersion on nonlinear wave behavior in elastic media are considered when the effects are small and manifested only in narrow high-gradient regions. If one constructs solutions of self-similar problems in “hyperbolic” approximation using Riemann’s waves and admissible discontinuities (i.e., discontinuities with structures) one obtains many solutions the number of which unlimitedly grows with growing the relative influence of dispersion (as compared to dissipation) in discontinuity structures.

The numerical analysis (based on PDE with dispersion and dissipation) of nonself-similar problems with self-similar asymptotics is performed to determine which of self-similar solutions is an asymptotic form for the nonself-similar solution.

1 Introduction

The equations of nonlinear elasticity theory are hyperbolic equations expressing the conservation laws. In solutions to these equations discontinuities appear and this is a possible source of solution nonuniqueness. The conservation laws should be satisfied on discontinuities (when there are no external surface effects). It is well known that not all discontinuities which don’t contradict to the conservation laws can be considered as really existing.

We refer to a hyperbolic system of equations together with a particular set of discontinuities (called admissible) as a hyperbolic model. In a reasonable model a set of admissible discontinuities should be given in such a way that it should involve discontinuities which one could consider as realizable under the conditions for
The influence of small scale dispersion and dissipation on nonlinear waves in elastic media. The problem of solution non-uniqueness in hyperbolic approximation which the model was defined. There are widely accepted rules to choose admissible discontinuities: the entropy nondecreasing, \textit{a priori} evolutionness conditions (Lax conditions) and the requirement for a stationary discontinuity structure to exist. The last condition leads to a dependence of the rule to select admissible discontinuities on assumptions concerned with the processes in discontinuity structures (there are no such assumptions when the hyperbolic problem is formulated).

2 Nonlinear quasi-transverse small amplitude waves in elastic media

One-dimensional unsteady solutions (depending on cartesian coordinate $x$ and time $t$) to nonlinear elasticity problem are considered. There are three families of characteristics along which perturbations propagate to each of sides. If in planes $x = \text{const}$ nonlinearity and anisotropy are small the characteristic velocities $c_1$ and $c_2$ corresponding to two quasi-transverse waves appear to be close. To describe small amplitude quasi-transverse waves propagating through the uniform state in positive $x$–direction the system of equations was obtained \cite{1,2}

\[
\frac{\partial u_\alpha}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial R(u_1, u_2)}{\partial u_\alpha} \right) = 0, \quad \alpha = 1, 2
\]  

\[R(u_1, u_2) = \frac{1}{2} f(u_1^2 + u_2^2) + \frac{1}{2} g(u_1^2 - u_2^2) - \frac{1}{4} \kappa (u_1^2 + u_2^2)^2, \quad f, g, \kappa = \text{const}
\]

Here $u_\alpha = \partial w_\alpha/\partial x$, $w_\alpha$ – the displacements in directions normal to the $x$–axis, $x$ – the lagrangian coordinate, $f$ – the characteristic velocity in the absence of nonlinearity and anisotropy, $g$ – the anisotropy parameter, $\kappa$ – the constant to characterize nonlinearity. The function $R(u_1, u_2)$ is determined by medium elastic properties. This expression corresponds to the general case when $u_1, u_2$ and anisotropy are small.

The conditions on a discontinuities corresponding to system (1) and following from the conservation laws for the transverse momentum are of the form

\[W[u_\alpha] = \left[ \frac{\partial R}{\partial u_\alpha} \right]
\]

$W$ is the Lagrangian velocity of the discontinuity.

Square brackets denote a jump of a function. A set of states $u_1, u_2$ behind various possible discontinuities propagating through a given state is called a shock adiabatic curve. Such a curve is shown in Fig.1.

3 The hyperbolic model No 1

Consider a model based on hyperbolic system (1) and a set of discontinuities for which in the framework of the Voight model a stationary viscous structures exist. The equations for quasi-transverse waves are written as follows
\[ \frac{\partial u_\alpha}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial R(u_1, u_2)}{\partial u_\alpha} \right) = \mu \frac{\partial^2 u_\alpha}{\partial x^2}, \quad \mu = \text{const} \number{3} \]

The equations (3) differ from equations (1) by terms on the right hand side.

The discontinuity with a structure is looked for in the form of a traveling wave, for which functions \( u_\alpha(\xi), \quad \xi = -x + W t \) take values corresponding to states behind and in front of the discontinuity as \( \xi \to \pm \infty \). It is shown [2,3] that the requirement for a viscous stationary structure to exist is equivalent to the requirement of discontinuity evolutionness with boundary conditions (2) (Lax conditions). This means that one of the following inequality systems should be satisfied

\[ c_1^{-1} \leq W \leq c_2^{-1}, \quad 0 \leq W < c_1^+ \number{4} \]

\[ c_2^+ \leq W, \quad c_1^+ \leq W < c_2^+ \number{5} \]

Here \( c_1 \) and \( c_2 \) are the characteristic velocities of system (3), superscripts “+” and “-” are referred to the states behind and in front of discontinuity, respectively, and \( W \) is the discontinuity velocity.

In Fig.1 the intervals AJ and EK of the shock adiabatic curve correspond to states behind fast shock waves (inequalities (5)) while the interval AF corresponds to states behind slow shock waves (inequalities (4)).

The set of discontinuities involving fast and slow shock waves together with equations (1) for continuous solutions form the hyperbolic model No 1.

3a. The problem of arbitrary discontinuity desintegration (the Riemann problem). The typical problem for hyperbolic equations is a problem of arbitrary discontinuity desintegration. Initial data for \( t = 0 \) are given in the form \( u_\alpha = U_\alpha \) for \( x \geq 0 \) and \( u_\alpha = u_\alpha^* \) for \( x \leq 0 \). One should find the solution of the form \( u_\alpha = u_\alpha(x/t) \) involving admissible discontinuities and continuous waves (the Riemann waves).
3b. Solution nonuniqueness for the model No 1. It is shown that the region of parameter values $U_\alpha, u_\alpha^*$ exists for which the model No 1 makes it possible to construct more than one solutions of the problem of arbitrary discontinuity desintegration [2,4,5].

3c. Nonself-similar problems with self-similar asymptotics for a viscous elastic media. For system (3) the problem with initial data $u_\alpha^0$ in the form of continuous functions tending to $U_\alpha$ as $x \to +\infty$ and to $u_\alpha^*$ as $x \to -\infty$ is analyzed. For high values of time the size of a region $L$ where initial data differ essentially from constant values appears to be small as compared to the region size $L$ where perturbations propagate. Therefore the solution considered as a function of $x/t$ and $t$ should tend to a self-similar limit determined by the hyperbolic model.

The above formulated nonself-similar problem was numerically analyzed [6,7]. It is shown that when the model No 1 has a nonunique solution the nonself-similar solutions tends to one or other asymptotic depending on the form of functions $u_\alpha^0$ which smooth the discontinuity in initial conditions. The dependence of the arising asymptotic on the choice of these functions was qualitatively analyzed.

4 The hyperbolic model No 2

A set of admissible discontinuities is defined as a set of discontinuities with a stationary structure described by the system of equations [8]

$$
\begin{align*}
\frac{\partial u_1}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial R(u_1, u_2)}{\partial u_1} \right) &= \mu \frac{\partial^2 u_1}{\partial x^2} + m \frac{\partial^2 u_2}{\partial x^2} \\
\frac{\partial u_2}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial R(u_1, u_2)}{\partial u_2} \right) &= -m \frac{\partial^2 u_1}{\partial x^2} + \mu \frac{\partial^2 u_2}{\partial x^2}
\end{align*}
$$

(6)

$\mu, m = \text{const}$

So defined the set of admissible discontinuities together with equations (1) from hyperbolic model No 2.

This system of equations describes quasi-transverse waves for some types of elastic composites in the case of viscous dissipation. Terms with the coefficient $m$ simulate wave dispersion. If the value $m/\mu$ is rather high the discontinuity structure is of oscillatory form. The admissible discontinuity set on the shock adiabatic curve takes the form shown in Fig.2 by solid intervals and separate points. The appearance of separate points $C_i$ corresponding to special discontinuities with discrete set of discontinuity velocities $W_i, i = 1, ..., n$ is an essential peculiarity of the discontinuity set when dispersion effects in structures are taken into account. The velocities $W_i$ are such that the special discontinuities don’t catch up fast waves (continuous waves or shocks), but no slow waves catch them up. The number of various types of special discontinuities and the number of separate intervals on the interval AF of the shock adiabatic curve (corresponding to admissible shocks) depends on the ratio $m/\mu$ and grows unlimitedly with the growth of $m/\mu$. 
4a. Solution nonuniqueness for the model No 2. For given states to the right and to the left of the initial discontinuity there is a possibility to construct solutions involving fast and slow waves (continuous waves or shocks), and between them a special discontinuity corresponding to any of points $C_i (i = 1, ..., n)$ can be situated. Besides, in the solution several special discontinuities can follow each other. This means that the number of possible solutions of the problem depends on $m/\mu$ and grows unlimitedly when the ratio $m/\mu$ grows.

4b. Nonself-similar problems with self-similar asymptotics for viscous elastic media with dispersion. Problems with initial conditions in the form of a step smoothed in a various way were numerically analyzed [8]. It was shown that by choosing way to smooth one could obtain any of possible asymptotics described in point 4a. For the same conditions at infinity the solutions can tend to different asymptotics for various smoothing functions in unital data.

Qualitative conclusions were made on conditions for self-similar solutions to tend to one or other asymptotic when time growing.

5 The hyperbolic model No 3

Longitudinal nonlinear waves in rods with complicated nonlinearity are considered. The equation of small amplitude long waves propagating in the positive $x$–direction can be written as follows

$$\frac{\partial u}{\partial t} + c(u) \frac{\partial u}{\partial x} = 0, \quad c(u) = \frac{\partial \phi(u)}{\partial u} \quad (7)$$

The function $\phi(u)$ is determined by the dependence of a rod elongation on its tension and the plot of the function is assumed to have two inflection points. The hyperbolic model No 3 involves equations (7) for continuous solutions and a set of discontinuities with stationary structures described by the equation [9]

$$\frac{\partial u}{\partial t} + \frac{\partial \phi(u)}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2} - m \frac{\partial^3 u}{\partial x^3} \quad (8)$$

Here $\partial w/\partial x, w$ - the longitudinal displacement of rod points, $\mu$ and $m$ are the viscosity and dispersion coefficients, respectively. Dispersion is a result of non-one-dimensional motions of rod points. Previously this model was considered for the case without dispersion ($m = 0$) [10].

Equation (8) (as well as (7)) expresses the conservation law, therefore the relation on a discontinuity can be written in the form

$$W = \frac{[\phi(u)u]}{[u]} \quad (9)$$

Here $W$ is the discontinuity velocity, square brackets denote a difference between values of functions behind and in front of the discontinuity.
The influence of small scale dispersion and dissipation on nonlinear waves in elastic media. The problem of solution non-uniqueness in hyperbolic approximation

A complicate nonlinearity provides the existence of three different shock waves propagating through the same state at the same velocity to exist. If effects of small scale dispersion are essential (as compared to viscous effects) the stationary discontinuity structure becomes to be oscillatory. As in the case of quasi-transverse waves the set of admissible discontinuities becomes complicate and special discontinuities appear, this leads to multiple nonuniqueness of solutions in the hyperbolic model.

5a. Nonself-similar solutions with self-similar asymptotic described by the hyperbolic model No 3. Numerical solutions to equation (8) with initial data in the form of a smoothed step shows [11] that one can choose a smoothing function in such a way that the solution tends to asymptotic represented by any of self-similar solutions of the hyperbolic model. However, if initial data are monotonically smoothed the asymptotic arises which involves the special discontinuity with the simplest structure in all cases when the condition at infinity admits such a self-similar solution. But a self-similar solution with such a special discontinuity exists not for any conditions for $x \to \pm \infty$. In the cases when there is no such a self-similar solution, there are self-similar solutions involving special discontinuities with more complicate structures. In these cases when solving nonself-similar problems for equation (8) with initial data in the form of monotonically smoothed step we obtain quite different asymptotic involving the single shock wave with unsteady structure inside of which periodic nondecaying in time oscillations occur. Discontinuities with such structures should be included into the set of admissible discontinuities.

6 Conclusions

It is shown that the hyperbolic models can be put in correspondence to complicate equations with dissipation and dispersion taken into account (equations (3), (6), (8)). In this case one should often (but not always – see point 5a) choose discontinuities with stationary structures as admissible ones. Hyperbolic models make it possible to construct self-similar solutions representing asymptotics to solutions of original complete equations. In many cases such solutions appear to be nonunique, the nonuniqueness being multiple when effects of dispersion are more essential then effects of dissipation. For appropriate initial conditions these solutions are stable asymptotics to solutions of original complicate equations for appropriate initial conditions. To which of self-similar solutions of a hyperbolic model the solutions of complete equations tend depends on such details of the problem formulation which are missing from hyperbolic models.

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Equation of state for Gaussian chain

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Abstract

The behavior of nonlinear one-dimensional chain is considered. The approach based on particle dynamics method is used. The assumption of Gaussian distribution of thermal fluctuations in the chain is proposed. Within the scope of this assumption the exact equation of state is obtained in the integral form. The dependence of Gruneisen function for two typical values of volume on thermal energy is obtained. The verification of the assumptions is carried out by means of molecular dynamics simulation.

1 Introduction

Equations of state (EOS) which connect pressure, volume and temperature can be obtained by various ways. Classical methods of continual mechanics based on the use of laws of thermodynamics and general principles can give only main limitation for EOS [1, 2]. Thus one can obtain only approximate equations which are applicable for a narrow range of parameters.

Another way was proposed in papers [3, 4, 5]. Here modelling was based on particle dynamics method. According to this method the medium is represented by a great number of interacting particles. The particles are moving in accordance with the laws of classical dynamics of Newton [5, 6, 7, 8]. Further microscopic analogues of pressure, thermal energy and other macroscopic values were introduced. Time averaging and expansion into a series in terms of small thermal parameter were carried out. Thus for models considered in works [3, 4, 5] Mie-Gruneisen equation was derived and the dependence of Gruneisen function on volume was obtained. In particular it was shown that Mie-Gruneisen EOS does not work for large tensile deformations. The more accurate EOS were derived. However, the smallness of thermal motion plays a key part in mentioned papers.

The idea of this paper is to generalize the method [3, 4, 5] to the case of relatively large thermal motions. The assumption about the distribution of particles displacements is introduced. Within the scope of this assumption accurate EOS are derived. The verification of assumption using computer simulation is carried out.
2 Main designations

Let us consider 1D chain which consists of identical particles interacting via the potential $\Pi$ of Lennard-Jones type. Let us limit our consideration to the case when each particle interacts only with two nearest neighbors. In order to obtain the desired EOS for pressure, volume and thermal energy, the microscopic analogues of such values should be defined. Following the ideas of paper [4] let us first introduce the averaging operator

$$\left\langle F_n \right\rangle \overset{\text{def}}{=} \frac{1}{\tau \Lambda} \int_0^{n+\Lambda/2} \sum_{k=n-\Lambda/2}^{n} F_k(t) \, dt,$$  

where $N$ is total number of the particles in the chain, $\tau$ and $\Lambda$ satisfy the following conditions

$$T_{\text{min}} \ll \tau \ll T_{\text{max}}, \quad 1 \ll \Lambda \ll N,$$  

where $T_{\text{min}}$ and $T_{\text{max}}$ are the smallest and the largest periods of the system. Further let us assume that any averaged values for the chain do not depend on particle’s number.

Let us introduce the specific thermal energy $E_T$ corresponding to the single particle as a sum of kinetic $K_T$ and potential $U_T$ parts

$$E_T = K_T + U_T, \quad K_T = \frac{1}{2} \left\langle m \dot{u}_k^2 \right\rangle, \quad U_T = \frac{1}{2} \left\langle \Pi(b + \Delta_k) - \Pi(b) \right\rangle,$$  

where $u_k$ is displacement of the particle number $k$, $\Delta_k = u_k - u_{k-1}$ is deformation of the bond caused by thermal motion, $b$ is average distance between two nearest neighbors. Let us define the pressure and divide it into “cold” component $p_0$ and thermal component $p_T$ as follows

$$p = \left\langle f(b + \Delta_k) \right\rangle, \quad p_0 = f(b), \quad p_T \overset{\text{def}}{=} p - p_0,$$  

where $f = -\Pi'$ is interaction force.

In paper [3] it was proposed to expand the formulae (3), (4) into a series with regard to $\Delta_k$. The following system was obtained

$$p = \sum_{k=0}^{\infty} \frac{f(2k+1)(b)}{(2k)!} \left\langle \Delta_n^{2k} \right\rangle, \quad E_T = -\frac{1}{2} \sum_{k=0}^{\infty} \frac{(k + 2) f(2k+1)(b)}{(k+1)(2k+1)!} \left\langle \Delta_n^{2k+2} \right\rangle.$$  

According to the system (5) the thermal state of the chain is determined by infinite number of parameters $\left\langle \Delta_n^{2k} \right\rangle$. However in classical thermodynamics there is only one parameter, e.g. temperature, responsible for the thermal state. Therefore, parameters $\left\langle \Delta_n^{2k} \right\rangle$ should be dependent. In paper (5) it was proposed to introduce the following dependence

$$\left\langle \Delta_n^{2k} \right\rangle = \lambda_k \theta^k, \quad \theta^2 = \left\langle \Delta_n^2 \right\rangle.$$  

Here $\lambda_k$ are dimensionless parameters which are assumed to be constant. Obviously $\lambda_1 = 1$. 

3 Integral representation of the equation of state

Let us rewrite system (5) using expression (6):

\[
p_T = \sum_{k=1}^{\infty} \frac{f^{(2k)}(V)}{(2k)!} \lambda_k \theta^{2k}, \quad E_T = -\frac{1}{2} \sum_{k=0}^{\infty} \frac{(k+2)f^{(2k+1)}(V)}{(k+1)(2k+1)!} \lambda_{k+1} \theta^{2k+2}
\]

Here \( V \overset{\text{def}}{=} b \) is specific volume. In paper [3] only fourth order terms were taken into account. Thus an approximate equation of state was obtained. Let us find the exact relation between thermal pressure and thermal energy using the following identity

\[
\psi(x) = \sum_{k=0}^{\infty} \psi_k x^k \implies x\psi'(x) = \sum_{k=0}^{\infty} k \psi_k x^k
\]

Using formula (7) the following differential relation can be obtained:

\[
\frac{\partial E_T(V, \theta)}{\partial V} = -p_T(V, \theta) - \theta^2 \frac{\partial p_T(V, \theta)}{\partial \theta^2}
\]

Equation (9) can be solved with respect to \( p_T(V, \theta) \) taking into account the following condition: \( p_T(V, 0) = 0 \). Then one can obtain

\[
p_T(V, \theta) = -\frac{1}{\theta^2} \int_0^{\theta^2} \frac{\partial E_T(V, \theta)}{\partial V} d\theta^2.
\]

Thus if thermal energy is a certain function of theta then the pressure can be calculated using equation (10).

4 Gaussian distribution

The central problem of the investigated approach is to determine \( \lambda_k \). Let us assume that \( \Delta_n \) is normally distributed random value with zero mean and dispersion equal to \( \theta^2 \). Changing time averaging to the averaging by all possible values of \( \Delta_n \) leads to the following expression for \( \langle \Delta_n^{2k} \rangle \).

\[
\langle \Delta_n^{2k} \rangle = \frac{1}{\sqrt{2\pi}\theta^2} \int_{-\infty}^{+\infty} \Delta_n^{2k} \exp \left(-\frac{\Delta_n^2}{2\theta^2}\right) d\Delta_n = \frac{1}{\sqrt{\pi}} \Gamma \left( k + \frac{1}{2} \right) 2^k \theta^{2k},
\]

where \( \Gamma \) is Euler gamma function. Comparison of the last formula with formula (6) gives the following expression for \( \lambda_k \).

\[
\lambda_k = \frac{1}{\sqrt{\pi}} \Gamma \left( k + \frac{1}{2} \right) 2^k = (2k - 1)!!
\]

Numerical verification of this formula is carried out in the next paragraph. Substituting equation (12) into equation (5) one can obtain

\[
p = \frac{1}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{f^{(2k)}(b)}{(2k)!} \Gamma(k + \frac{1}{2})(2\theta^2)^k,
\]

\[
E_T = -\frac{1}{2\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(k+2)f^{(2k+1)}(b)}{(k+1)(2k+1)!} \Gamma(k + \frac{3}{2})(2\theta^2)^{k+1}
\]
According to the definition of gamma function the expression for thermal pressure (13) can be rewritten in the following manner

\[ p = \frac{1}{\sqrt{\pi}} \sum_{k=0}^{\infty} \int_{0}^{\infty} \frac{e^{-t} f^{(2k)}(b)}{\sqrt{t}} (2t\theta)^k dt, \]  

(14)

Let us change the integration and summation in the last formula and make the following transformations

\[ \sum_{k=0}^{\infty} \frac{f^{(2k)}(b)}{(2k)!} (2t\theta)^k = \sum_{k=0}^{\infty} \frac{((-1)^k + 1) f^{(k)}(b)}{k!} (\sqrt{2t\theta})^k = \]

\[ = \frac{1}{2} \left( f(b + \sqrt{2t\theta}) + f(b - \sqrt{2t\theta}) \right) \]  

(15)

Substituting equation (15) into (14), one can obtain

\[ p = \frac{1}{2\sqrt{\pi}} \int_{0}^{\infty} \frac{e^{-t} \left( f(b + \sqrt{2t\theta}) + f(b - \sqrt{2t\theta}) \right)}{\sqrt{t}} dt, \]  

(16)

Analogous expression can be derived for the thermal energy

\[ E_T = -\frac{\theta}{2\sqrt{2\pi}} \int_{0}^{\infty} e^{-t} \left( f(b + \sqrt{2t\theta}) - f(b - \sqrt{2t\theta}) \right) dt - \]

\[ + \frac{1}{2\sqrt{\pi}} \int_{0}^{\infty} \frac{e^{-t} \left( \Pi(b + \sqrt{2t\theta}) + \Pi(b - \sqrt{2t\theta}) - 2\Pi(b) \right)}{\sqrt{t}} dt, \]  

(17)

The system of equations (16), (17) represents the accurate EOS in the implicit form. This EOS is applicable in the range of thermal energies where assumptions (6), (11) are true.

5 Computer simulation

Molecular dynamics simulation was carried out in order to verify assumption (11). One-dimensional chain containing 10000 particles with periodical boundary conditions was considered. Interactions between particles were described by Lennard-Jones potential. Initial velocities of particles were uniformly distributed in the interval \([-v_0; v_0]\).

Parameters \(\lambda_k\) were calculated using formula (6). The dependence of \(\lambda_k\), \(k = 2..6\) on the deformation of the chain and on the value of the initial random velocity \(v_0/v_d\) is shown in figures 1, 2. Here \(v_d \overset{\text{def}}{=} \sqrt{2D/m}\) is dissociation velocity. It can be seen that the difference between theoretical prediction of \(\lambda_k\) and its value obtained from the simulation is increasing with \(k\). The biggest difference is approximately 10%. It can be also concluded that the dependence of \(\lambda_k\) on volume is rather weak and thus can be neglected. The dependence on the intensity of thermal motion is more essential. However, as it will be shown in the next section, the influence of \(\lambda_k\) on the EOS is rapidly decreases with the increase of \(k\). Thus it can be supposed that the errors in \(\lambda_k\) (\(k >> 1\)) will not influence the final results.
One of the wide-spread EOS is Mie-Gruneisen equation [10], [11]. It declare the following linear relation between pressure and thermal energy

\[ p = p(V, E_T) = p_0(V) + \Gamma(V) \frac{E_T}{V}, \]  

(18)
where $\Gamma(V)$ is so-called Gruneisen function of volume $V$. The expression $\Gamma(V)$ for the chain was obtained in various papers [3], [4], [9]. The result is as follows

$$\Gamma = -\frac{bf''(b)}{f'(b)}. \quad (19)$$

The key assumption of Gruneisen is that $\Gamma$ does not depend on the thermal energy. However, more accurate equations of state proposed in [3], [4] show that the Mie-Gruneisen EOS is not accurate in the case of strong tensile deformations. It was proposed to leave only terms till forth order in the expressions (5). The following dependence of thermal pressure on thermal energy was obtained.

$$p_T = \frac{4f_4}{3f_3}E_T + 2\frac{3f_2f_1 - 4f_1f_4}{9\lambda_2f_3^2} \left( \sqrt{f_4^2 + 3\lambda_2f_3E_T} - f_1 \right). \quad (20)$$

Thus in general case the dependence of Gruneisen function on thermal energy should be taken into account.

Let us introduce the following generalization of Mie-Gruneisen EOS

$$p_T = \tilde{\Gamma}(V, E_T) \frac{E_T}{V}, \quad \tilde{\Gamma}(V, E_T) \overset{\text{def}}{=} \frac{p_TV}{E_T}. \quad (21)$$

On the one hand, generalized Gruneisen function can be calculated using the exact equations (16), (17). On the other hand, it can be calculated using equation (20), which takes into account only $\lambda_2$. The dependence of $\tilde{\Gamma}$ on thermal energy for different volumes is shown in Fig. 3, 4. One can see that in case of critical deformation

![Figure 3: The dependence of Gruneisen parameter on thermal energy in case of undeformed chain ($b = a$). Solid line — equations (16), (17), dashed line — equation (20)](image)

of the chain Gruneisen parameter strongly depends on thermal energy. Thus in such
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Figure 4: The dependence of Gruneisen parameter on thermal energy in case of large deformation of the chain ($b = 1.1a$). Solid line — equations (16), (17), dashed line — equation (20)

cases the use of Mie-Gruneisen EOS can lead to the serious errors. Also one can see that for the case of undeformed chain the difference between predictions of the exact EOS ((16), (17)) and equation (20) is about 5%. In case of large deformation the maximum difference is approximately 15%.

7 Conclusion

The behavior of a nonlinear one-dimensional chain was considered. The expansions of thermal pressure and thermal energy into a series in terms of small thermal parameter were used. The assumption about distribution of thermal displacements of particles was proposed. Verification of the assumption using molecular dynamic simulations was carried out. It was shown that for relatively small thermal motions the assumption is applicable. Using this assumption the exact EOS in the implicit form was derived. The dependence of Gruneisen coefficient on thermal energy was calculated in case of Morse potential. It was shown that in case of undeformed chain the dependence is relatively weak in comparison with the accuracy of the experimental data. In contrast in case of strong tensile deformation the dependence become principal and can not be neglected even for the small thermal energies. The comparison with approximate EOS was carried out. It was shown that the difference between predictions of both equations is about 5% for undeformed chain and 15% for strong tensile deformation. Such accuracy is enough for most practical cases.
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Comparison of approaches based on statistical physics and particle dynamics for equations of state derivation

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Abstract

Behavior of a particle in a potential well is considered. Methods of statistical physics are used. Method for statistical sum calculation is proposed. Expression for the statistical sum in the form of power series is derived. Mie–Gruneisen and more precise equations of state are derived. Comparison of the obtained results with the exact and approximate solutions obtained by the particle dynamics method is conducted.

1 Introduction

The problem of equation of state (EOS) obtaining is still a serious challenge for the modern physics of condensed matter. Laws of thermodynamics and general principles can give only main limitation for EOS [1, 2]. Thus one has to use various empirical equations, which can lead to certain instabilities and physically incorrect results [3].

An attractive way of solving this problem is to develop simple mechanical models which allow analytical obtaining of the desired equations. The simplest model of this kind is a particle in the potential well, which can be considered as approximation of the dynamics of an atom of crystal. One of the classical ways of the EOS obtaining is to analyze the statistical sum of the system [4]. In case of harmonic potential of the interatomic interactions this approach allows to the desired EOS in Mie-Gruneisen form which declare the following linear relation between pressure and thermal energy

\[ p = p(V,E_T) = p_0(V) + \Gamma(V) \frac{E_T}{V}, \]

(1)

where \( \Gamma(V) \) is so-called Gruneisen function of volume \( V \). The anharmonic correction to the Gruneisen function was considered in [5].
Another way was proposed in works [6, 7, 8], where EOS obtaining was based on particle dynamics method [8, 9, 10, 11]. According to this method the medium is represented by a great number of interacting particles. The particles are moving in accordance with the laws of classical dynamics of Newton. Further microscopic analogues of pressure, thermal energy and other macroscopic values are introduced. Time averaging and expansion into a series in terms of small thermal parameter are carried out. Thus for models considered in works [6, 7, 8] Mie–Gruneisen equation was derived and the dependence of Gruneisen function on volume was obtained. In particular it was shown that Mie–Gruneisen EOS does not work for large tensile deformations. The more accurate EOS was derived. The exact EOS for the particle in the potential well was obtained in [12].

This paper is devoted to the comparison of the approaches mentioned above. The new method of statistical sum calculation is proposed. The influence of anharmonical terms in the potential of interatomic interactions is investigated. The generalization of Mie–Gruneisen EOS, essential for large tensile deformations and thermal energy, is obtained.

2 Main designations

Let us represent the material as a large number of independent anharmonic oscillators. Interactions between different oscillators can be approximately taken into account if we assume that the oscillator behaves like a particle in the potential well with random value of energy. Let us also assume that particle interacts with walls of the well by means of potential $\Pi$. Then the hamiltonian of the system has the following form

$$H = \frac{p^2}{2m} + U(x), \quad U(x) = \Pi(b + x) + \Pi(b - x),$$  \hspace{1cm} (2)

where $p$ is momentum of the particle, $x$ is its coordinate ($x = 0$ corresponds to the middle of the well), $b$ is half of the distance between walls. Let us denote the specific volume as $V = 2b$ and the potential energy as a sum of “cold” component $U_0(V)$ and thermal component $U_T(V, T)$. “Cold” component corresponds to the deformation of the potential well. It is function of volume only. Thermal component depends on both volume and temperature.

$$U_T \overset{def}{=} U - U_0, \quad U_0 = 2\Pi(b)$$  \hspace{1cm} (3)

Following the book [4], let us introduce the statistical sum $Z$

$$Z = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\beta H(p, x)} dp dx, \quad \beta = 1/kT$$  \hspace{1cm} (4)

where $\hbar$ is Plank constant, $k$ is Boltsman constant, $T$ is temperature. Integrating equation (4) with respect to $p$, one can obtain

$$Z = \frac{Z_0}{\sqrt{\beta}} e^{-\beta U_0} \int_{-\infty}^{\infty} e^{-\beta U_T} dx.$$  \hspace{1cm} (5)
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where \( Z_0 = \sqrt{\frac{m}{2\pi\hbar^2}} \). According to the definition [4] Helmholtz free energy can be
calculated by the following formula.

\[
F \overset{\text{def}}{=} -\frac{1}{\beta} \ln Z = U_0 - \frac{1}{\beta} \ln \sqrt{Z_0} - \frac{1}{\beta} \ln \int_{-\infty}^{\infty} e^{-\beta U_T} \ dx
\]  

(6)

The classical definitions of pressure and internal energy are as follows [4]

\[
p = -\left( \frac{\partial F}{\partial V} \right)_T, \quad E = \left( \frac{\partial \beta F}{\partial \beta} \right)_V.
\]

(7)

Following [5], let us divide pressure and internal energy into “cold” and thermal
components. Using formulae (6) and (7), one can obtain

\[
p_0 \overset{\text{def}}{=} p|_{T=0} = -\frac{\partial U_0}{\partial V}, \quad p_T \overset{\text{def}}{=} p - p_0 = -\frac{\int_{-\infty}^{\infty} \frac{\partial U_T}{\partial V} e^{-\beta U_T} \ dx}{\int_{-\infty}^{\infty} e^{-\beta U_T} \ dx},
\]

\[
E_0 \overset{\text{def}}{=} E|_{T=0} = U_0, \quad E_T \overset{\text{def}}{=} E - E_0 = \frac{1}{2} kT \int_{-\infty}^{\infty} U_T e^{-\beta U_T} \ dx.
\]

(8)

Thus equations (8) represent the EOS in an implicit form. They can be rewritten
in more compact form using the following averaging operator \( \left< f(x) \right> \overset{\text{def}}{=} \int_{-\infty}^{\infty} f(x) n(x) \ dx \)

\[
p_T = -\frac{1}{2} \left< \Pi'(b + x) + \Pi'(b - x) \right>, \quad E_T = \frac{1}{2} kT + \left< \Pi(b + x) + \Pi(b - x) \right> - 2\Pi(b).
\]

(9)

where \( n(x) \) is distribution function with respect to coordinates [13]

\[
n(x) \overset{\text{def}}{=} \int_{-\infty}^{\infty} e^{-\beta U} \ dx.
\]

(10)

In paper [7] the analogous expressions were obtained using time averaging of the
equations of motion.

Cold characteristics are usually well known in contrast to the thermal one.
The wide spread way of calculating the thermal characteristics is to use so-
called quasiharmonic approximation [5]. Within the scope of this approximation
\( \Pi = \frac{1}{2} C (b - a + x)^2, \ C \) is function of volume, \( a \) is equilibrium distance. Then
thermal component of potential energy has the following form

\[
U_T = C(V)x^2,
\]

(11)

where \( V = 2b, V_0 = 2a \). In this case the integral in formula (8) can be calculated.
Then one can obtain the expression for the thermal pressure in Mie–Gruneisen form

\[
p_T = \frac{\Gamma(V)}{V} E_T, \quad \Gamma(V) = -\frac{V C'(V)}{2C(V)}, \quad E_T = kT.
\]

(12)

The expression for Gruneisen function is equal to the result of the paper [6]. Thus
one can assume that for the case of linear oscillations (small thermal energies) time
and coordinate averaging are equivalent.
3 Equation of state in the form of series

In order to estimate the influence of anharmonical terms on the EOS let us divide the potential energy into harmonic and anharmonic parts.

\[ U_T = Cx^2 + U_{ah}, \quad U_{ah} \overset{\text{def}}{=} U_T - Cx^2. \]  

(13)

Substituting formula (13) in formula (5) and expanding \( e^{-\beta U_{ah}(x)} \) in power series in terms of \( x \) one can obtain

\[
Z = \frac{Z_0 e^{-\beta U_0}}{\sqrt{\beta}} \int_{-\infty}^{\infty} \sum_{i=0}^{\infty} e^{-\beta Cx^2} U_i(V, \beta) x^{2i} dx, \quad U_i(V, \beta) \overset{\text{def}}{=} \frac{1}{(2i)!} \frac{d^{2i}(e^{-\beta U_{ah}})}{dx^{2i}} \bigg|_{x=0}.
\]  

(14)

Note that only such kind of expansion can give one opportunity to obtain the expression for statistical sum. For example, the direct expansion of \( e^{-\beta U_T} \) in formula (5) into power series leads to divergent integrals.

Let us interchange the integration and summation in formula (14). Also let us take into account the following identity

\[
\int_{-\infty}^{\infty} e^{-\beta Cx^2} x^{2i} dx = \frac{\gamma(i + 1/2)}{\sqrt{\pi} \beta^{i+1/2}(i+1/2)!},
\]  

(15)

where \( \gamma \) is Euler gamma function. Then substituting (15) in (14) one can obtain

\[
Z = \frac{Z_0 e^{-\beta U_0}}{\sqrt{\pi} \beta} \sum_{i=0}^{\infty} U_i(V, \beta) \frac{\gamma(i + 1/2)}{(i+1/2)!} \left(\frac{\beta}{C}\right)^i.
\]  

(16)

Using formula (16) one can calculate the exact formulae for pressure and internal energy. However, only finite number of terms are usually the matter of interest from the practical point of view. In appendix A it is shown that \( U_i(V, \beta) \) are polynomials of the \([i/2]\) degree in terms of \( \beta \). Therefore term number \( i \) in the sum (16) has the following order

\[
U_i(V, \beta) \frac{\gamma(i + 1/2)}{(i+1/2)!} \beta^{[i/2] - i} \sim \beta^{[i/2] - i}.
\]  

(17)

Equation (17) gives one an opportunity to estimate the terms which are neglected.

Let us leave only terms of order till \( T^2 \) in expression (16).

\[
Z \approx \frac{Z_0 \sqrt{\pi} e^{-\beta U_0}}{\sqrt{C}} \frac{kT}{2} \left( 1 - \frac{1}{32} \frac{U_{ah}(4)}{C^2} kT \right),
\]  

(18)

It is obvious that first anharmonic term is essential in case of large temperatures. Let us calculate the thermal pressure and thermal energy accurate within \( T^2 \). Using formulae (2), (13) one can represent \( p_T \) and \( E_T \) in terms of interatomic potential \( \Pi \)

\[
\begin{align*}
 p_T &= -\Pi''' \frac{kT}{4\Pi''} - \frac{\Pi''(5)\Pi'' - \Pi''(4)\Pi'''}{64\Pi''^3} (kT)^2, \\
 E_T &= kT - \frac{1}{32} \frac{\Pi''(4)}{\Pi''^2} (kT)^2.
\end{align*}
\]  

(19)
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Excluding the temperature from the system (19) one can obtain the desired EOS in the explicit form

\[ p_T = -\frac{\Pi'''}{4\Pi''}E_T + \frac{\frac{3}{2}\Pi^{(4)}\Pi''' - \Pi^{(5)}\Pi''}{64\Pi''^3}E_T^2. \]  

(20)

Let us compare EOS (20) with the result of paper [6]. The following EOS was obtained in paper [6] using particle dynamics method

\[ p_T = f_2\sqrt{f_1^2 + \frac{3}{2}\lambda_3 E_T} - f_1, \quad f_k = \frac{(-1)^{k+1}\Pi^{(k+1)}}{k!}, \quad \lambda = \frac{\langle x^4 \rangle}{\langle x^2 \rangle^2}, \]  

(21)

where \( \langle \rangle \) denotes time averaging. Computer simulations have shown that \( \lambda \approx 1.6 \) and depend on temperature and volume weakly. Expanding equation (21) in a series in terms of \( E_T \) one can obtain

\[ p_T = -\frac{\Pi'''}{4\Pi''}E_T + \frac{\lambda\Pi^{(4)}\Pi'''}{64\Pi''^3}E_T^2. \]  

(22)

One can see that the second terms in equations (20) and (22) are different. However the derivation of formula (22) was based on the assumption that \( \lambda \) does not depend on thermal energy. Computer simulation shows that this dependence can be neglected only for relatively small thermal energies. Thus one can use formulae (22) and (20) in order to determine \( \lambda \).

4 Critical deformation of the potential well

In paper [6] it was shown that EOS for the particle in the potential well strongly depends on the deformation of the well. Let us consider the deformation of the potential well, which corresponds to the maximum of the cold pressure. This case corresponds to the simplest model of the behavior of an atom in the elementary cell in the vicinity of failure. The critical distance between walls can be obtained from the following equation

\[ C(b_{cr}) \overset{\text{def}}{=} \Pi''(b_{cr}) = 0 \]  

(23)

By the analogy of the previous section let us divide the potential energy into two parts.

\[ U_T = C_1x^4 + \tilde{U}_T(x), \quad \tilde{U}_T \overset{\text{def}}{=} U_T - C_1x^4. \]  

(24)

Then one can obtain the following expression for statistical sum

\[ Z = \frac{Z_0 e^{-\beta \tilde{U}_T}}{2 C_1^2\beta^{\frac{3}{2}}} \sum_{i=0}^{\infty} \gamma(\frac{1}{2} + \frac{1}{4}) \tilde{U}_i(\mathcal{V}, \beta) \frac{1}{(C_1\beta)^{\frac{i}{2}}}, \quad \tilde{U}_i(\mathcal{V}, \beta) = \frac{1}{(2i)!} \frac{d^{2i} e^{-\beta \tilde{U}_T}}{dx^{2i}}, \]  

(25)
where identity was used
\[
\int_{-\infty}^{\infty} e^{-\beta C_1 x^4} x^2 \, dx = \frac{1}{2} \frac{\gamma (\frac{1}{4} + \frac{1}{4})}{(C_1 \beta)^{\frac{3}{2} + \frac{1}{4}}},
\]

Then using equations (7) one can obtain the desired EOS in the implicit form.

\[
\begin{aligned}
&\begin{cases}
\pi_T = -\frac{\pi^{(5)}}{8\pi^{(4)}} kT - A \frac{\pi^{(7)} \pi^{(4)} - \frac{3}{2} \pi^{(5)} \pi^{(6)}}{\pi^{(4) \frac{3}{2}}} (kT)^{\frac{3}{2}} \\
E_T = \frac{3}{4} kT - A \frac{\pi^{(6)}}{\pi^{(4) \frac{3}{2}}} (kT)^{\frac{3}{2}}.
\end{cases}
\end{aligned}
\]

(26)

where \( A = \frac{\sqrt{3\gamma (3/4)^2}}{40\sqrt{2\pi}} \approx 0.015 \). Solution of the system (26) shows that dependence \( \pi_T(E_T) \) has form

\[
\pi_T = D_1 E_T + D_2 E_T^{\frac{3}{2}}.
\]

(27)

On the other hand, the same dependence can be obtained by substituting \( f_1 = 0 \) into equation (21).

\[
\pi_T = -\frac{\pi^{(3)}}{\sqrt{\lambda \pi^{(4)}}} \sqrt{E_T}.
\]

(28)

One can see that results given by equations (27) and (28) are qualitatively different even for the small thermal energy.

5 Exact EOS in the case of Morse potential

In case of a particular interatomic potential one can calculate the exact dependence of the thermal pressure on thermal energy using equations (8). Let us assume that particle interacts with walls by means of Morse potential.

\[
\Pi = D (e^{-2\alpha(r-a)} - 2e^{-\alpha(r-a)}) ,
\]

(29)

where \( D \) — bond energy, \( a \) — equilibrium distance, \( \alpha \) — parameter which characterizes the width of the potential well.

Then formulae (3) has the following form

\[
\begin{aligned}
&U_0 = 2D (e^{-2\nu} - 2e^{-\nu}) \\
&U_T = 2D (e^{-2\nu \text{ch}(2\alpha x)} - 2e^{-\nu \text{ch}(\alpha x)}) - U_0,
\end{aligned}
\]

(30)

where \( \nu = \alpha(b - a) \). Substituting formula (30) into equations (8) one can obtain the dependence of thermal pressure and thermal energy on temperature.

The exact EOS for the case of Morse potential was derived in paper [12]. The approach proposed in [6], based on the particle dynamics method was used. Within
the scope of this approach the following dependence of thermal pressure on thermal energy was obtained

\[ p_T = 2\alpha D \int_0^{z_m} \frac{[e^{-2\nu}\text{ch}(2z) - e^{-\nu}\text{ch}(z)] \, dz}{\sqrt{E - 2D [e^{-2\nu}\text{ch}(2z) - 2e^{-\nu}\text{ch}(z)]}} - 2\alpha D (e^{-2\nu} - e^{-\nu}), \]

\[ z_m = \text{Arch} \left( \frac{e^{\nu}}{2} + \frac{\sqrt{e^{2\nu}(\frac{E_T}{D} + 1) + 2}}{2} \right), \quad E = E_T + 2D (e^{-2\nu} - 2e^{-\nu}). \]

In order to compare the predictions of equations (8) and (31) let us plot the dependence \( p_T(E_T) \). The desired dependence for undeformed well \( b = a \) and for the case of critical deformation \( b = (1 + \ln 2/6)a \approx 1.1a \) is shown in figure 1. The value of parameter \( \alpha a \) was taken equal to 6. One can see that in case of undeformed potential well the results of formulae (8), (31) are almost equal. However in case of critical deformation there is a differences about 10\%. The comparison of the approximate EOS (26), (28) with the exact shows that the approximate EOS obtained by the methods of statistical physics is qualitatively different from the exact one.
6 Discussion

It can be seen in figures 1, 2 that there are essential differences between the results of the statistical physics approach and the exact solution. Let us note some “weak” places of the previous derivations. First of all, one can ask: “Is the statistical approach applicable to a single particle?” The answer is: “No, it is not”. Motion of a single particle in the potential well is determined. From the formal point of view the expression for the statistical sum (4) loses sense because the total energy of the particle is constant and hence integral (4) is equal to infinity. However, one can consider the following model. The medium is represented by a large number of independent particles in the potential wells. The interactions between the particles are weak, so one can consider the behavior of a single particle. This approach solves the problem mentioned above. However, it is not the only problem. One can see that in all formulae for statistical sum ((4) et. all) the infinite limits on integral were used. Following the book [4] the integration is carried out by all phase space of the system. In the considered case coordinate of the particle is limited by the distance between walls. Therefore the limits on integrals should be equal to ±b. However, the integrated function exp(−βU(x)) is rapidly decreasing with x for real potentials. Thus the use of the infinite limits can not lead to the serious errors.

Also let us note the difference between approximate and exact EOS obtained by methods of statistical physics. One can suppose that the reason is in the proposed method of approximation. However at least from the mathematical point of view all derivations are correct.
7 Conclusion

A simple model for elementary cell of 1D crystal was considered. The statistical approach was used. The new way of calculation of the statistical sum calculation was proposed. The expression for statistical sum in the form of a series with respect to temperature was obtained. In case of quasiharmonic approximation Mie–Gruneisen equation of state was derived. It was shown that the dependence of Gruneisen function on volume is similar to the prediction of paper [6]. The more precise equations of state were derived for different values of volume. It was shown that for both cases the equation of state is different from the results of paper [6]. The difference becomes principal in case of critical deformation of the potential well. Comparison of the results of statistical approach with the exact equation of state in case of Morse potential was carried out. It was shown that the results are close to each other for undeformed well. In case of critical deformation of the well 10% error was obtained. It was shown that approximate EOS obtained by the particle dynamics method is qualitatively equal to the exact one. In contrast approximate EOS obtained by the methods of statistical physics is qualitatively different from the exact one.

8 Appendix A

Let us consider functions $U_i(V, \beta)$. According to the definition (14) they have the following form

$$U_i(V, \beta) = \frac{1}{(2i)!} \frac{d^{2i}(e^{-\beta f(x)})}{dx^{2i}} |_{x=0}$$  \hspace{1cm} (32)

It can be shown that $U_i(V, \beta)$ are polynomial functions with respect to $\beta$. Let us denote

$$u_{2i} = \frac{d^{2i}(e^{-\beta f(x)})}{dx^{2i}} |_{x=0}$$  \hspace{1cm} (33)

and carry out the following transformations

$$u_{2i} = -\beta \frac{d^{2i-1}(f' e^{-\beta f})}{dx^{2i-1}} |_{x=0} = -\beta \sum_{n=0}^{2i-1} C_{2i-1}^n f^{(n+1)}(e^{-\beta f})^{(2i-1-n)} |_{x=0} =$$

$$= -\beta \sum_{n=0}^{2i-1} C_{2i-1}^n f^{(n+1)} u_{2i-n-1} |_{x=0},$$  \hspace{1cm} (34)

where $C_{2i-1}^n = \frac{n!(2i-1)!}{(2i-n-1)!}$. One can see from equation (34) that $u_{2i}$ are polynomials with respect to $\beta$. The degree of $u_{2i}$ increases with increase of $i$. Let us determine the degree of $u_{2i}$. Let us assume $f = U_{ah}$. It has the following properties

$$f^{(i)}(0) = 0, \quad i = 0, 1, 2, 3.$$  \hspace{1cm} (35)
Then equation (34) can be rewritten as

\[ u_{2i} = -\beta \sum_{n=3}^{2i-1} C_{2i-1}^n f^{(n+1)}(0) u_{2i-n-1} \] (36)

Let us denote the degree of \( u_{2i} \) as \( d_{2i} \). Then one gets following equation for \( d_{2i} \)

\[ d_{2i} = d_{2i-4} + 1. \] (37)

Solution of the last equation is \( d_{2i} = [i/2] \), where \([ \cdot ]\) denotes the integer part. Thus \( U_i(\mathcal{V}, \beta) \) is a polynom of \([i/2]\) degree with respect to \( \beta \).

**References**


Comparison of approaches based on statistical physics and particle dynamics for equations of state derivation


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Molecular dynamics modeling of heat wave propagation in crystals

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Abstract

Description of process of heat exchange in crystal structures in terms of the classical heat conduction equations frequently encounter serious problems. Our investigation of heat conduction in nano-sized crystals with defects [4] shows that classical theory does not work in the case of low defects density. Here we continue study of heat transfer processes by the example of thermal waves distribution in nonuniformly heated ideal crystals.

1 Problem statement

A rectangular crystal is considered. One side of the crystal (left) is subjected to an immediate heating, which models influence of a laser source. The heat propagation in the crystal is investigated and the temperature at the opposite side of the crystal (right) is being registered and compared to the temperature induced by the laser at the left side. The main questions of this investigation is if the temperature at the right side can be comparable with the temperature at the left side and what is the mechanism that can transfer the energy through the crystal. Here we are interested in a fast energy transfer with a speed close to the speed of sound waves in the crystal. As it is known, sometimes this fast heat transfer which can not be explained by classical heat conductivity can be registered in real experiments.

2 Simulation technique

The simulation procedure applied in this work is close to that used at the previous papers, for more details the references [1, 2, 3] can be followed. The material is represented by a set of particles interacting through a pair potential \( \Pi(r) \). The equations of particle motion have the form
\[
\mathbf{m}\ddot{r}_k = \sum_{n=1}^{N} \frac{f(|\mathbf{r}_k - \mathbf{r}_n|)}{|\mathbf{r}_k - \mathbf{r}_n|} (\mathbf{r}_k - \mathbf{r}_n),
\]

where \( \mathbf{r}_k \) is the radius vector of the \( k \)-th particle, \( m \) is the particle mass, \( N \) is the total number of particles, and \( f(r) = -\Pi'(r) \) is the interparticle interaction force. Main notations: \( a \) is the equilibrium distance between two particles, \( D = |\Pi(a)| \) is binding energy, \( C = \Pi''(a) \equiv -f'(a) \) is the stiffness of the interatomic bond at equilibrium, and \( t_0 = 2\pi\sqrt{m/C} \) is the period of vibrations of the mass \( m \) under the action of a linear force with stiffness \( C \), \( v_d = \sqrt{2D/m} \) is dissociation velocity (the minimum velocity required to escape from the potential field). The temperature is taken to be proportional to an average of the kinetic energy of a set of particles (supposing that the average velocity of this set is zero).

\[
T = \tilde{k} \left\langle \frac{m v^2}{2} \right\rangle = \frac{\tilde{k} m}{2} \left\langle v^2 \right\rangle,
\]

where \( \tilde{k} \) is Boltzmann constant, \( \langle \ldots \rangle \) stands for averaging over the selected set of particles.

We will consider the classical Lennard-Jones potential:

\[
\Pi_{LJ}(r) = D \left[ \left( \frac{a}{r} \right)^{12} - 2 \left( \frac{a}{r} \right)^{6} \right],
\]

\[
f_{LJ}(r) = -\Pi'_{LJ}(r) = \frac{12D}{a} \left[ \left( \frac{a}{r} \right)^{13} - \left( \frac{a}{r} \right)^{7} \right],
\]

where \( D \) and \( a \) the binding energy and the equilibrium interatomic distances, introduced earlier.

The cut-off distance used in calculations is set as \( a_{\text{cut}} = 1.4a \), in this case only the first neighbors are interacting for the close-packed structures. This simplifies comparison with analytical considerations, where only the first neighbors are taken into account and also allows to speed-up the calculations. Here we study the principal possibility of describing the heat transfer rather than simulate the behavior of a certain material; therefore, the proposed simplified potentials are sufficient. Our results can be extended to more complex potentials describing the properties of materials more exactly.

3 Initial set-up

The specimen is a 3D rectangle with particles arranged in face-centered cubic (FCC) crystal lattice - see Fig.1, where specimen containing about 100 000 particles is shown. The surfaces of the rectangle are taken to be parallel to the faces of the lattice. Initial temperature distribution in the specimen is shown in Fig.2 (\( x \) is longitudinal coordinate, \( L \) is length of the specimen). Nearly 14\% (approximately 1/7 of the crystal) at the left has temperature \( T_1 \), and the rest of the specimen (at the right) has temperature \( T_0 \) (Fig.2). In all the experiments the temperature
$T_0$ is taken equal to $T_0 = 0.01T_d$, where $T_d = k v_d^2 / 2$, $v_d = \sqrt{\alpha f(\alpha) / \delta}$ is the dissociation velocity. Temperature $T_1$ is varying in the range between $0.1T_d$ and $T_d$. The dissociation temperature $T_d$ can be considered as a rude approximation to the melting temperature.

Figure 1: *Initial state of the specimen. The material near the left surface is heated closely to the melting temperature, the rest of the specimen has low temperature and ideal crystal lattice.*

After the initial conditions are applied, the molecular dynamics simulation is performed to investigate the propagation of the temperature wave and dependence of the temperature $T_2$ at the right surface of the specimen at the moment of the wave arrival from the initial temperature at the left surface $T_1$.

Figure 2: *Initial temperature distribution.*

### 4 Results

A series of computations was performed in which the temperature $T_1$ was varying in the range from $0.1T_d$ to $T_d$. It was obtained that for the sufficiently high temperature $T_1$ a shock wave is formed, which is propagating to the right side of the crystal. At the front of the shock wave a temperature increase is being excited (the temperature wave), which is result of coupling between the mechanical and thermal motions of the media. If the temperature $T_1$ is close or less then $0.1T_d$, then the shock wave is not observed and the temperature wave is absent. In Fig.3 the sequential stages of the propagation of the shock wave for the case $T_1 = 0.5T_d$ is shown. The black curve shows velocity profile in the specimen, the gray curve — the temperature profile. It is visible that the initial temperature is propagating into the specimen due to
Molecular dynamics modeling of heat wave propagation in crystals

thermal conductivity, but this process is much slower than propagation of the shock wave. The shock wave itself generates the temperature wave, which is much lower than the initial temperature disturbance, but still noticeable.

Figure 3: Propagation of the shock and temperature wave for the case $T_1 = 0.5T_d$. Black color shows the dimensionless temperature (divided by dissociation temperature), gray — dimensionless velocity (divided by dissociation velocity).

Fig. 4 shows the temperature after the shock wave arrival at the right surface $T_2$ as a function of the initial temperature $T_1$. The obtained dependence can be approximated by the following empirical formula: $T_2/T_d = 0.016(T_1/T_d)^{3/2}$.

Figure 4: Dependence of the temperature at the right surface after the shock wave arrival $T_2$ from the temperature of the initial disturbance $T_1$. 
5 Conclusions

In the presented paper it was shown that the temperature transfer through the specimen can be explained by the coupling between the mechanical and thermal properties of the medium. If the laser source is strong enough to generate the temperature disturbance more then approximately 10% of the melting temperature then the noticeable temperature can be detected at the opposite side of the specimen, brought by the shock wave generated in the material. In the further investigation it is planned to study influence of the parameters of the excitation and the length of the specimen on the efficiency of the heat transfer. Also it is planned to investigate influence of the heat transfer between atoms and electrons by using the two-component medium approach.

References


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Researching of formation process of cylindrical shell consisting of glass and metal

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Abstract

This article displays mathematical model of three-layer cylindrical glass and metal based shell formation. Following problems are solved: shell temperature distribution and it’s cooling in given cooling conditions; initial displacement and stress in condition of given materials properties.

1 Simulator

Cylindrical shell consists of metal layer including glass layer according to patented way of glass and metal base production.[1]

Mathematical model covers period of time from the moment of glass base transition into glassy state to the moment of total cooling of glass and metal base.

Disconnected problem of shell heat deformation is solved, according to the fact that heat stream of glass and metal base layers is much more that energy of strain its. At the same time cooling thermal process is base on thermal conductivity equation without taking shell deformation into consideration. Cooling thermal process calculation influences shell deformation with mechanical material operation factors and thermal coefficient.

Two problems were solved: small diameter tube cooling and large diameter cylindrical shell cooling which are made of three layer glass and metal on base; definition initial displacement and stress in large diameter cylindrical shell its.

We suppose that thermal conductivity realizes thermal exchange between inside environment, inside metal layer and other layers for small diameter tube with infinitely long. The tube inner temperature equals environment temperature inside tube at initial moment of time and it equals glass transition temperature inside three layers shell we are speaking about the composite. Heat exchange realizes according to Newton law between outside metal layer and environment. Continuing temperature conditions realize on padding of all layers.
This problem has the view consideration axial symmetry in cylindrical coordinates.

\[ c_k \rho_k \frac{\partial T_k}{\partial t} = \lambda_k \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_k}{\partial r}\right), \]

\[ T_{k|t=0} = T_0, \quad \frac{\partial T_k}{\partial r}|_{r_0} = 0, \]

\[ T_{k|r_0} = T_{k+1|r_0}, \quad \lambda_k \frac{\partial T_k}{\partial r}|_{r_0} = \lambda_{k+1} \frac{\partial T_{k+1}}{\partial r}|_{r_0}, \]

\[ \lambda_4 \frac{\partial T_4}{\partial r}|_{r_4} = -\vartheta_4 (T_4 - T_{en}) |_{r_4}, \]

\[ (k = 1 : r_0 \leq r < r_1, r_0 \to 0, k = 2 : r_1 \leq r < r_2, k = 3 : r_2 \leq r < r_3, k = 4 : r_3 \leq r \leq r_4). \]

Where \( T_k = T_k(r, t) \) is temperature, \( T_{en} \) is temperature of environment, \( c_k(T), \rho_k(T), \lambda_k(T) \) are specific heat, density, thermal conductivity of suitable layers, \( \vartheta_4 \) is heat transfer factor which according to velocity of outside metallic layers blow, \( k = 1, 2, 3, 4 \) is number of medium (1 is air inside tube, 2 is inside metal layer, 3 is glass, 4 is outside metal layer), \( r_k \) are radius of appropriate layers.

The problem was solved numerically finite-difference method. Numerical solution result is shown at the pictures number 1 and 2.

We had supposed that median surface radius is equal to with cylindrical generatrix of all layer when we solved the problem cooling large diameter cylindrical shell.

Moreover thermal conductivity realizes thermal exchange between layers and it realizes according to Newton law between outside metallic layers and environment.

Taking axial symmetry into consideration boundary problem has the view.

\[ c_k \rho_k \frac{\partial T_k}{\partial t} = \lambda_k \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_k}{\partial r}\right), \]

\[ T_{k|t=0} = T_0, \]

\[ \lambda_1 \frac{\partial T_1}{\partial r}|_{r_1} = \vartheta_1 (T_1 - T_{en}) |_{r_1}, \]

\[ T_{1|r_2} = T_{2|r_2}, \quad \lambda_1 \frac{\partial T_1}{\partial r}|_{r_2} = \lambda_2 \frac{\partial T_2}{\partial r}|_{r_2}, \]

\[ T_{2|r_3} = T_{3|r_3}, \quad \lambda_2 \frac{\partial T_2}{\partial r}|_{r_3} = \lambda_3 \frac{\partial T_3}{\partial r}|_{r_3}, \]

\[ \lambda_3 \frac{\partial T_3}{\partial r}|_{r_4} = -\vartheta_3 (T_3 - T_{en}) |_{r_4}, \]

\[ \frac{\partial T_4}{\partial r}|_{s=0} = 0, \]

\[ \lambda_k \frac{\partial T_k}{\partial s}|_{s=1/2} = -\vartheta_k (T_k - T_{en}) |_{s=1/2}, \]

\[ (k = 1 : r_1 \leq r < r_2, k = 2 : r_2 \leq r < r_3, k = 3 : r_3 \leq r \leq r_4). \]

Where \( T_k = T_k(r, s, t) \) is temperature, 1 is generatrix shell, \( k = 1, 2, 3 \) and \( c_k(T), \rho_k(T), \lambda_k(T) \), \( \vartheta_k, r_k \) are as we say.

As the second problem being multivariate difference from the first one so we must use special numerical methods. Economical multivariate difference scheme may be build with locally one-dimensional method. As a result of this method problem reduces to solving consistency of one-dimensional problems easily solved by sweep method. Those schemes have total first time order and second others approximation orders.

Numerical solution result is shown at the picture number 3.

Deformation of three layer cylindrical shell glass and metal on base is made by thermal field symmetrically rotation axis. It causes axisymmetric shell deformation.

Each shell layer deformation is considered in local co-ordinates surfaces with layer median surfaces.

Basic co-ordinate surfaces are surfaces of revolution.
Continuum basic equations have the view for all layers cylindrical shell under such conditions axisymmetric deformation.

Equations of geometry:
\[ \varepsilon_{11}^k = \frac{\partial u_1}{\partial z}, \quad \varepsilon_{22}^k = \frac{\partial u_2}{\partial z}, \quad \varepsilon_{33}^k = \frac{\partial u_3}{\partial z}; \]
\[ 2\varepsilon_{13}^k = 2\varepsilon_{31}^k = \frac{\partial u_1}{\partial s} + \frac{\partial u_3}{\partial s}, \quad \varepsilon_{12}^k = \varepsilon_{23}^k = \varepsilon_{31}^k = 0. \]

Equilibrium equations:
\( (R_k + z_k) \frac{\partial \sigma_{11}^k}{\partial s} + \frac{\partial}{\partial s} \left( (R_k + z_k) \sigma_{13}^k \right) = 0, \)
\( (R_k + z_k) \frac{\partial \sigma_{22}^k}{\partial s} + \frac{\partial}{\partial s} \left( (R_k + z_k) \sigma_{33}^k \right) - \sigma_{33}^k \alpha = 0. \)

State equations for outside metallic layers:
\( \sigma_{11}^k = \frac{E_k}{1-\nu_k^2} \left( \varepsilon_{11}^k + \nu_k \varepsilon_{22}^k \right) - (1 + \nu_k) \alpha \Delta T, \)
\( \sigma_{22}^k = \frac{E_k}{1-\nu_k^2} \left( \varepsilon_{22}^k + \nu_k \varepsilon_{11}^k \right) - (1 + \nu_k) \alpha \Delta T. \)

State equations for glass layer:
\( \sigma_{11}^k = \frac{1}{R_k} \int_0^z \left( \frac{\partial \varepsilon_{11}^k}{\partial z} + \frac{\partial \varepsilon_{22}^k}{\partial z} \right) - (1 + \nu_k) \alpha \Delta T e^{\mu t} \mathrm{d}t, \)
\( \sigma_{22}^k = \frac{1}{R_k} \int_0^z \left( \frac{\partial \varepsilon_{22}^k}{\partial z} + \frac{\partial \varepsilon_{11}^k}{\partial z} \right) - (1 + \nu_k) \alpha \Delta T e^{\mu t} \mathrm{d}t. \)

Where \( \varepsilon_{ij}^k = \varepsilon_{ij}^k(s, z_k) \) is deformation tensor, \( u_i^k = u_i^k(s, z_k) \) is displacement vector, \( \sigma_{ij}^k = \sigma_{ij}^k(s, z_k) \) is stress tensor, \( R_k \) are radiuses of median surface layers, \( r = R_k + z_k, z_k \) is co-ordinates of thickness layers, \( E_k = E_k(T) \) is elastic modulus, \( \alpha_k = \alpha_k(T) \) is thermal broadening factor, \( \nu_k \) is Pearson factor, time derivable shows as upper point, \( \Delta T \) is temperature difference, \( \mu \) is viscous elasticity of glass layer, \( \mu = \frac{x}{\tau}, \eta \) is glass dynamic viscosity.

All stresses in glass initially cooling equal zero, in the result of stress relaxation are as-fired. But glass keeps viscous elasticity properties for some time; however, state equations may be used for glass same as metal.

Front-face-area glass layer edge conditions are geometric and stressing conditions of metallic layers padding:
\( \sigma_{13}^1(s, h_1/2) = \sigma_{13}^2(s, -h_2/2) = \tau_{31}, \quad \sigma_{33}^1(s, h_2/2) = \sigma_{33}^2(s, -h_3/2) = \tau_{33}, \)
\( u_i^1(s, h_1/2) = u_i^2(s, -h_2/2), \quad u_i^1(s, h_2/2) = u_i^2(s, -h_3/2), \quad u_i^1(s, 0) = u_i^2(s, 0). \)

Radian deformations by the way of transverse displacement of padding layer surface are taken into account by padding layers. The displacement include displacement of narrow deformation and thermal change.
\[ u_{3(k)}^k_s = -h_k/2 = w_k + \frac{1}{k} \int_0^{h_k/2} \sigma_{33(k)}^k \mathrm{d}z_k. \]

Where \( w_k \) are median surface layers depressions.

Edge conditions for outside surface metallic layers:
\( \sigma_{13}^1(s, -h_1/2) = \sigma_{13}^2(s, h_3/2) = \sigma_{13}^1(s, h_1/2) = \sigma_{13}^2(s, -h_2/2) = 0. \)

Edge conditions for front surface layers of cylindrical shell are found from conditions of outside force lack:
\[ N_{11}^k(1/2) = 0, \quad Q_{11}^k(1/2) = Q_{11}^1(0) = 0, \quad M_{11}^k(1/2) = 0. \]

Where \( N_{11}(s) \) is inside longitudinal force, \( Q_{11}(s) \) is inside intersecting force, \( M_{11}^k(s) \) is inside bending moment:
\[ N_{11}^k(s) = \int_{-h_k/2}^{h_k/2} (1 + \frac{z_k}{R_k}) \sigma_{11}^k(s, z_k) \mathrm{d}z_k, \]
\[ Q_{11}^k(s) = \int_{-h_k/2}^{h_k/2} (1 + \frac{z_k}{R_k}) \sigma_{13}^k(s, z_k) \mathrm{d}z_k. \]
\[ M_{11}^k(s) = \int_{-h_k/2}^{h_k/2} \left( 1 + \frac{\partial}{\partial s} \right) \sigma_{11}^k(s, z_k) z_k \, dz_k. \]

Median transverse profile edge conditions are found on condition that tangent displacement are symmetrical.

\[ u_1^k(0, z_k) = 0, \quad \frac{\partial u_1^k}{\partial s} |_{s=0} = 0, \quad \varepsilon_{13}^k(0, z_k) = 0. \]

All layer deformations are deduced on base of fine elastic shell theory in compliance with Timoshenko hypothesizes, it has the view taking into account axial symmetry:

\[ \varepsilon_{33}^k = 0, \quad 2\varepsilon_{13}^k = \gamma^k(s). \]

Where \( \gamma^k(s) \) is averaged transverse deformation.

Solutions are presented at the pictures number 4 and 5.

2 Simulation data

Numerically solution bounder problem results are found for technical glass type BB in radius of temperature from glass bath to complete cooling \( \lambda_2 = (0.85 + 0.0142T) \frac{\text{WtC}}{\text{m}}, \rho_2 = (2520 - 2.62T + 0.65 \cdot 10^{-4}T^2) \frac{\text{kg}}{\text{m}^3}, \ c_2 = (820 + 0.64T) \frac{\text{Jl} \cdot \text{C}}{\text{kg}}, \ T_g = 680^\circ \text{C}, \ T_en = 20^\circ \text{C}, \ h_2 = 0.178 \text{m}, \) temperature -averaged elastic modulus is \( E_2 = 0.672 \cdot 10^{11} \text{P}, \ \nu_2 = 0.22, \ \alpha_2 = 8.5 \cdot 10^{-6} \text{at} \).

Steel is taken as a basis for boarding with thermal characteristic \( \lambda_{1,3} = (29 - 0.03T) \frac{\text{WtC}}{\text{m}}, \ \rho_{1,3} = (2700) \frac{\text{kg}}{\text{m}^3}, \ c_{1,3} = (690.8) \frac{\text{Jl} \cdot \text{C}}{\text{kg}}, \ \vartheta_k = (5.6 + 4v) \frac{\text{WtC}}{\text{m}^2}, \ E_{1,3} = 1.851 \cdot 10^{11} \text{P}, \ \gamma_{1,3} = 0.3, \ \alpha_{1,3} = 12.653 \cdot 10^{-6} \text{at}, \ h_1 = 0.002 \text{m}, \ h_3 = 0.01 \text{m}. \)

The pictures number 1 presents temperature distribution of thickness tube with diameters 0.2m, with equal thickness 0.06m. 1 segment is \( 0 \) after 10 seconds, 2 segment is \( C_0 \) after 20 seconds, 3 segment is \( C_0 \) after 100 seconds from the start of outside layers air-cooling at speed 2m/sec.

![Figure 1: Temperature distribution of thickness tube with diameters 0.2m](image)

The picture number 2 presents temperature distribution of thickness cylindrical shell with diameters 3.2m, total thickness 0.189m and length 3.5m after 20 seconds from the start of shell face cooling (1) and on distance 0.1m from shell face (2).

The picture number 3 presents temperature distribution along median surfaces cylindrical shell with total thickness 0.189m and length 3.5m in 30 hours of cooling, 1 segment is \( C_0 \) glass layer, 2 segment is \( C_0 \) inside metallic layer, 3 segment is \( C_0 \) outside metallic layer.
Researching of formation process of cylindrical shell consisting of glass and metal.

Figure 2: Temperature distribution of cylindrical shell with diameters 3.2m.

Figure 3: Temperature distribution along median surfaces cylindrical shell.

Figure 4: Tangent stress distribution along cylindrical shell.
Figure 5: Normal stress distribution along cylindrical shell.

References


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Onset of convection in a liquid with temperature inversion of density

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Abstract

Stability of mechanical equilibrium of plane horizontal layer of liquid with temperature inversion of density is investigated for the case of fixed heat flux at the boundaries. For the long-wave limit the study is carried out analytically, by the stream function, temperature and growth rate perturbations series expansion with respect to wave number; the instability to the perturbations with finite wave length is investigated numerically. As expected, the density inversion prevents convection. On the other hand, parameter range is found where the cellular instability takes place.

1 Introduction

Onset of convection in a plane horizontal liquid layer heated from below, known as the Rayleigh-Benard instability, was comprehensively investigated. Considerable part of works was concentrated on the problem of liquids with temperature inversion of density in view of wide spectrum of applications in many areas of science, like geophysics and astrophysics. Contrary to the classical Rayleigh-Benard instability where the Boussinesq approximation (linear temperature dependence of density in buoyancy term) is used, the density maximum frontier may lay not only on the upper cooled boundary but arbitrarily in the layer. As a consequence, there can be two different layers with stable and unstable stratifications.

Stability of melted ice layer heated from above by radiation flux was investigated in [1] for the case of perfectly conducting lower boundary maintained at temperature equal to 0°C. Experimental and analytical results show that, if \( T_2 < 8^\circ \) than the critical Rayleigh number \( Ra \) depends on temperature of upper border \( T_2 \), otherwise \( Ra \) does not depend on \( T_2 \). Power-low temperature density dependence \( \rho = \rho_m (1 - |T - T_i|^\gamma) \) was used for investigation of convection onset in a horizontal water layer with rigid boundaries near the density maximum temperature [2]. It is
found that the density inversion makes stabilizing effect. The Rayleigh number values appeared to be 10\% less then ones obtained implying the parabolic temperature dependence of the density and are very close to ones obtained using 5th order polynomial. It was also found that the inversion leads to the increase of ware number corresponding to critical Rayleigh number. The influence of the inversion point location on the critical Rayleigh number and amplitude of the arising convective flows in rectangular cavity was studied numerically in [3]. It was noted that amplitude of convection in form of rectangular cells approaches zero when the cavity aspect ratio approaches \( \sqrt{3} \), - the value for which hexagonal convection can be observed.

Onset of convection in a horizontal layer of liquid with temperature dependence of density in the case of constant heat flux at both boundaries was not studied.

2  Problem formulation

Plane horizontal layer of viscous incompressible liquid is considered. Gravity is uniform and directed perpendicular to layer boundaries. Lower boundary is rigid and upper one is free but non-deformable. Constant heat flux is imposed on the boundaries. Temperature dependence of density is taken in form of quadratic polynomial 

\[
\rho(T) = \rho_m (1 - \alpha(T - T_i))^2,
\]

where \( \rho_m \) is maximum density attained at \( T = T_i \). Such dependance with high accuracy describes the water behavior at normal pressure and temperature from \( 0^\circ \) to \( 8^\circ \) C. Unlike Boussinesq approximation this one is characterized by the temperature \( T_i \), called temperature inversion of density. Governing equations are as follows [4]:

\[
\rho \left( \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} \right) = -\nabla P + \eta \Delta \vec{v} + \rho \vec{g},
\]

\[
\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = \chi \Delta T,
\]

\[
\nabla \cdot \vec{v} = 0,
\]

\[
\rho(T) = \rho_m (1 - \alpha(T - T_i))^2,
\]

the boundary conditions read:

\[
z = 0, \vec{v} = 0, \frac{\partial T}{\partial z} = -A,
\]

\[
z = h, \vec{v}_z = 0, \frac{\partial v_x}{\partial z} = 0, \frac{\partial T}{\partial z} = -A.
\]

The problem (1)-(6) has trivial solution which corresponds to the conductive state:

\[
\vec{v} = 0, T = A(z_0 - z), P = \int_0^h \rho dz.
\]

The following quantities are chosen for as scales for time, length, temperature, velocity and pressure: \( h^2/\nu \), \( h \), \( Ah \), \( \nu/h \), \( \rho_m v^2/h^2 \) to formulate the problem in dimensionless form. Temperature is counted from \( T_i \).
Applying curl operation we eliminate the pressure from the Navier-Stokes equations. Stream function $\Psi$ is introduced. Linearized equations for perturbations of stream function and temperature have following form:

$$\lambda \Delta_{zx} \Psi = \Delta^2_{zx} \Psi + 2(z - z_0) \text{Gr} \cdot ikT,$$

$$\lambda T = 1/\text{Pr} \Delta_{zx} T + ik\Psi,$$

The boundary conditions:

$$Z = 0 : T' = \Psi = \Psi' = 0,$$

$$Z = 1 : T' = \Psi = \Psi'' = 0,$$

Where prime denotes the derivative with respect to $z$ and $\Delta_{zx} = \partial^2 / \partial z^2 - k^2$, $\text{Gr} = \alpha g \lambda^2 h^5 / \nu^2$, $\text{Pr} = \nu / \chi$, $z$ is dimensionless coordinate of the inversion point.

### 3 Long-wave stability

For long-wave limit problem can be solved analytically by expansion of stream function $\Psi$, temperature $T$ and growth rate $\lambda$ in series of wave-number $k$ up to 4th order:

$$\Psi = \Psi_0 + \Psi_1 ik - \Psi_2 k^2 - \Psi_3 ik^3 + \Psi_4 k^4,$$

$$T = T_0 + T_1 ik - T_2 k^2 - T_3 ik^3 + T_4 k^4,$$

$$\lambda = \lambda_0 + \lambda_1 ik - \lambda_2 k^2 - \lambda_3 ik^3 + \lambda_4 k^4.$$

Substituting these series (12)-(14) into (8)-(11) we come to following expression for $\lambda = \lambda (\text{Pr}, \text{Gr}, z_0, k)$:

$$\lambda = -\lambda_2 k^2 + \lambda_4 k^4,$$

$$\lambda_2 = \frac{(1440 + 9 \text{Gr} z_0 \text{Pr} - 5 \text{Gr} \text{Pr})}{1440 \text{Pr}},$$

$$\lambda_4 = -\frac{\text{Gr}}{\text{Pr}} \alpha (z_0) + \text{Gr}^2 \beta (z_0) + \text{Gr}^2 \text{Pr} \gamma (z_0) - \text{Gr} \delta (z_0).$$

Where

$$\alpha = (1956240z_0 - 1091376) / 747249600,$$

$$\beta = (336960z_0^2 - 136136z_0 + 37895) / 747249600,$$

$$\gamma = (122265z_0^3 - 460668z_0 + 162300) / 747249600,$$

$$\delta = 4447872z_0 / 74724960.$$
Figure 1: Stability diagram in terms of Rayleigh number $Ra$ and dimensionless coordinate of inversion point $z_0$ in long-wave limit.

It follows from (15) that the critical Rayleigh number is defined by the formula:

$$Ra = 1440/(5 - 9z_0).$$ (19)

For liquids with linear temperature dependence of the density, the density is maximal at the cold boundary and minimal at the hot one, and the density difference is maximal between the boundaries. In other hand for liquids with temperature density inversion density is maximum in inversion point. Obtained Rayleigh number is expressed in modified interpretation through deference between density on borders. It is connected with Rayleigh number in classical interpretation defined through maximum density deference as follows:

$$Ra_{cl} = Ra \begin{cases} 1 - 2z_0 & \text{at } z_0 \leq 0, \\ (1 - z_0)^2 & \text{at } 0 < z_0 \leq 1/2, \\ z_0^2 & \text{at } 1/2 < z_0 \leq 1, \\ 2z_0 - 1 & \text{at } z_0 > 1. \end{cases}$$ (20)

Long-wave perturbations are not the most dangerous ones if $\partial Ra/\partial k < 0$ for $k = 0$. This situation takes place at $\lambda_4 > 0$. Substituting the critical value of Rayleigh number from (19) into $\lambda_4$ we obtain:
\[
\lambda_4 = -124416 \left( 40716z_0^2 - 44317z_0 + 11881 \right) / (9z_0 - 5).
\] (21)

As one can see, \( \lambda_4 < 0 \) for \( z_0 \in (-\infty, z_{01}) \cup (z_{02}, +\infty) \) and \( \lambda_4 > 0 \) for \( z_0 \in (z_{01}, z_{02}) \), where \( z_{01} = 3409/6264 - \sqrt{29009305}/81432 \approx 0.4781 \)

\( z_{02} = 3409/6264 + 81432/\sqrt{29009305} \approx 0.6103. \)

For \( z_0 \in (z_{01}, z_{02}) \) most dangerous perturbations are cell ones. Therefore, the internal \( z_0 \in (z_{01}, z_{02}) \) in stability diagram (Fig. 1) has to be excluded.

4 Stability with respect to perturbations with finite wave-numbers

Further below we consider only neutral monotonous perturbations, in this case \( \lambda = 0 \). Changing the variables as \( T \to \Pr T, \Psi \to i\Psi \) we rewrite the equations (8) - (11) in the following form:

\[
\Psi''' = 2k^2\Psi'' - k^4\Psi - 2(z_0 - z)Ra \cdot k^2T
\] (22)

\[
T'' = k^2T - k^2\Psi
\] (23)

The boundary conditions will take the form

\[
Z = 0 : T' = \Psi = \Psi' = 0
\] (24)

\[
Z = 1 : T' = \Psi = \Psi'' = 0
\] (25)

The problem was solved numerically by the construction of fundamental system of solutions method. Stability map is plotted in Fig. 2 and the dependence of the wave number of most dangerous perturbations on the dimensionless coordinate is presented in Fig. 3.

5 Conclusions

When inversion point is far beyond the layer boundaries \( |z_0| \gg 1 \) the problem reduces to classical Rayleigh problem; in that case there is no Rayleigh number dependence on the dimensionless coordinate of the inversion point. When the difference in temperatures of the boundaries is exceeded, the large-scale motion takes place.

The behavior is changed with the inversion point moving into the layer. The inversion prohibits convection since the part of layer is stratified stably. For \( z_0 = [0.4, 0.7] \) instability type changes, the cellular instability is observed.

Existence of the parameter range when the cellular instability takes place is confirmed numerically (Fig. 2) and analytically in long-wave limit.

One can see singularity (Fig. 2, Fig. 3, and in eq. 15) for \( z_0 \to 5/9 \). Critical Rayleigh number tends to the infinity and the wave number of most dangerous perturbations attains its maximal value, moreover \( \lim_{z_0 \to 5/9 + 0} (k_{cr}) \neq \lim_{z_0 \to 5/9 - 0} (k_{cr}). \)
Figure 2: Stability diagram in terms of Rayleigh number $R_a$ in classical interpretation and dimensionless coordinate of the inversion point $z_0$ for perturbations with finite wave-number.

Figure 3: Wave-number of most dangerous perturbations $k$ versus dimensionless coordinate $z_0$.
References


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Analysis of temporal characteristics of rendezvous algorithms on the orbit

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Abstract

The controlled relative motion of a spacecraft nearby an orbital station is considered. A rendezvous method used on active spacecraft is an algorithm of proportional navigation which is realized with some constant time delay. The coefficient of the guidance law is considered as a control variable. The problem of choice of the mentioned coefficient which provides minimizing of rendezvous time, is analyzed. It is found that the optimal solution includes regular and singular control values both. The results of computer simulation are given.

1 Introduction

Proportional navigation, where the intercepting command acceleration is applied normal to the line of sight (LOS) [1], is one of the most widely used rendezvous algorithms for moving objects of different destination, including space vehicle. It was shown in [2] that this method is optimal in the control problem of linear system with quadratic criterion. In the papers [1], [3] – [5] the influence of parameters of proportional navigation law and its various modifications on the engagement time and closeness characteristics of the rendezvous process was investigated. Those investigations were held in assumption that guidance is realized without delay. In [1] it was shown that in the absence of delay to minimize the rendezvous time the coefficient of proportional navigation law should be chosen maximal. At the same time the delay in realistic guidance systems is inevitable and it neglecting may lead to erroneous results. The analysis of the pursuit-evasion problems taking into account time delay was held in [6]–[9], where linearized kinematics were applied. In [6] the optimal evasion problem against the pursuer which used the proportional navigation strategy with time delay was considered. It was shown that for the case of presence of time delay the evader strategy changes essentially in comparison with the strategy without delay.
The influence of the delay, considered as perturbation parameter on the engagement time was investigated in [10]. A sensitivity analysis with respect to the value of the time delay was also held in the mentioned paper.

In the present paper the terminal phase of plane rendezvous of an active space vehicle and a passive orbital station on the Earth orbit is considered. A rendezvous method used on active spacecraft is an algorithm of proportional navigation which is realized with some minor constant time delay. The objective of this work is to optimize the guidance law taking time delay into account. The coefficient of navigation law is considered as a control variable. The problem is to determine the coefficient which provides minimizing of rendezvous time.

2 Problem Statement

The relative motion is described by the system of nonlinear differential equations in polar coordinates with center point in the center of the station, which is also a center of mass for the whole system. Both objects are considered as point masses, and the distance between them is neglected in comparison with the orbital radius. The equations of relative motion are:

\[
\begin{align*}
\ddot{\rho} - \rho \dot{\phi}^2 - 2\Omega_0 \rho \dot{\phi} &= a_\rho, \\
\rho \ddot{\phi} + 2\dot{\rho} \dot{\phi} + 2\Omega_0 \dot{\rho} &= a_\phi.
\end{align*}
\]

Here \( \rho \) is the range between the spacecraft and the station, \( \phi \) is the angle between the LOS and some constant direction in the chosen polar coordinate system, \( \Omega_0 \) - constant Earth’s rotation frequency, \( a_\rho \) and \( a_\phi \) are the components of control acceleration applied to the active vehicle, directed along and normal to the LOS (Fig. 1).

Assume the commanded acceleration along the LOS is equal to zero, and the acceleration normal to the LOS is programmed with proportional navigation law

\[
a_\phi = k \dot{\phi} (t - \tau),
\]

where \( \tau \) is the constant time delay, \( k \) is the control variable, a piecewise continuous time function bounded by

\[-k \leq k(t) \leq k.\]

(2)

(3)

Figure 1: Relative geometry
The control problem is to minimize the goal function
\[ J = T \rightarrow \min, \]  
which is specified on the trajectories of the system (1), (2) with the corresponding boundary conditions and control limitation (3).
To take into account the time delay we rewrite the acceleration \( a_\phi \) as follows:
\[ a_\phi = k u(t), \]  
where \( u(t) \) is described by the equation
\[ \tau \dot{u}(t) = \dot{\phi}(t) - u(t). \]  
Time delay was taken into account in a similar way for example in [9].
Substituting (5) and (6) into (1) and rewriting it as a Cauchy-type system, the following system of equations is obtained:
\[ \begin{align*}
\dot{\rho} &= \nu, \\
\dot{\nu} &= \rho \omega (\omega + 2 \Omega_0), \\
\dot{\phi} &= \omega, \\
\dot{\omega} &= \frac{k \nu - 2 \nu (\omega + \Omega_0)}{\rho}, \\
\dot{u} &= \theta (\omega - u).
\end{align*} \]  
where \( \theta = \frac{1}{\tau}. \)
The boundary conditions for (7) are:
\[ t = 0 : \quad \rho(0) = \rho_0, \; \nu(0) = \nu_0, \; \phi(0) = \phi_0, \; \omega(0) = \omega_0, \; u(0) = u_0, \]
\[ t = T : \quad \rho(T) = \rho_T. \]  
The problem (3), (4), (7), (8) is Mayer optimal control problem, to analyze it we’ll use Pontryagin maximal principle [2].

3 Optimal Problem Analysis
The Hamiltonian of the problem (3), (4), (7), (8) is
\[ H = \nu \psi_\rho + \rho \omega (\omega + 2 \Omega_0) \psi_\nu + \omega \psi_\phi + \frac{k \nu - 2 \nu (\omega + \Omega_0)}{\rho} \psi_\omega + \theta (\omega - u) \psi_u \]  
and the equations for adjoint variables are
\[ \begin{align*}
\psi_\rho &= -\omega (\omega + 2 \Omega_0) \psi_\nu - \frac{1}{\rho^2} (k \nu - 2 \nu (\omega + \Omega_0)) \psi_\omega, \\
\psi_\nu &= -\psi_\rho + \frac{2}{\rho} (\omega + \Omega_0) \psi_\omega, \\
\psi_\phi &= 0, \\
\psi_\omega &= -2 \rho (\omega + \Omega_0) \psi_\nu - \psi_\phi + \frac{2 \nu}{\rho} \psi_\omega - \theta \psi_u, \\
\psi_u &= -\frac{k}{\rho} \psi_\omega + \theta \psi_u.
\end{align*} \]
Using transversality conditions we obtain the adjoint variables values at the final moment:

$$\psi_v(T) = \psi_\phi(T) = \psi_\omega(T) = \psi_u(T) = 0, \ H(T) = 1. \quad (11)$$

From (10), (11) and the stationary condition for $H$ on the optimal trajectory we get $H(t) = 1$ on $[0; T], \ \psi_\phi \equiv 0$ on $[0; T]$. It follows from the condition for maximum of Hamiltonian (9) that the extremal control satisfies the following criterion:

$$k = \begin{cases} \bar{k}, & H_1 > 0 \\ -\bar{k}, & H_1 < 0, \end{cases} \quad (12)$$

where $H_1 = \frac{u}{\rho} \psi_\omega$ is a switching function.

Clear up whether the singular control can exist in the considered problem. Suppose switching function $H_1$ is identically equal to zero on some time interval $[t_1; t_2] \subseteq [0; T]$. From the condition

$$H_1 = \frac{u}{\rho} \psi_\omega \equiv 0$$

the equality $\psi_\omega \equiv 0$ follows, otherwise $u \equiv 0$, and the system (7) becomes uncontrollable. As far as $H_1 \equiv 0$ on $[t_1; t_2]$, then, differentiating $H_1$ by time by virtue of the systems (7) and (10), we obtain:

$$\dot{H}_1 = \frac{u \psi_\omega + u \dot{\psi}_\omega}{\rho} - \frac{u \psi_\omega}{\rho^2} \dot{\rho} \equiv 0. \quad (13)$$

From the adjoint system and condition $\psi_\omega \equiv 0$ we get:

$$\frac{u \dot{\psi}_\omega}{\rho} = \frac{u}{\rho} \left(-2\rho(\omega + \Omega_0)\psi_v - \theta \psi_u\right) \equiv 0. \quad (14)$$

Therefore

$$\frac{\psi_u}{\psi_v} = -\frac{2\rho}{\theta}(\omega + \Omega_0). \quad (15)$$

Further, $\ddot{H}_1 \equiv 0$ on $[t_1; t_2]$. Equalling second derivative of $H_1$ to zero and using stationary condition $H = 1$ on $[t_1; t_2]$ we can find:

$$v \psi_\rho + \rho \omega(\omega + 2\Omega_0)\psi_v + \theta \psi_u(\omega - u) = 1. \quad (16)$$

From (15) and (16) we find the singular control:

$$k_s = \left(\frac{\rho}{u} \cdot \frac{\psi_\rho}{\psi_v} + \frac{v}{u} + \frac{\theta \rho}{u}\right) (\omega + \Omega_0) \quad (17)$$
Now (12) can be rewritten in the following way:

\[
k = \begin{cases} 
k, & H_1 > 0 \\
\bar{k}, & H_1 \equiv 0 \\
k_s, & H_1 < 0,
\end{cases}
\]  

(18)

Consequently the optimal control problem (3), (4), (7), (8) is formally reduced to the boundary problem for the system of ordinary differential equations (7), (8), (10), (11) with the rule for choosing of control (18). It is generally known that numerical solution of the problems of optimal control with singular paths leads to much difficulties. These difficulties can be overcome if, for example, the structure of the optimal trajectory is known, or the combination of singular and nonsingular arches. To clear up the optimal control structure, let’s consider the auxiliary problem for the reduced dynamic system (7).

4 Auxiliary Problem

Notice that in (7) the control variable \( k(t) \) appears only in one equation. Hence we can pass on to an auxiliary problem for the reduced system releasing the initial conditions for the variable \( \omega(t) \) and to strike off the equation for \( \dot{\omega} \):

\[
\begin{align*}
\dot{\rho} &= \nu, \\
\dot{v} &= \rho\omega(\omega + 2\Omega_0), \\
\dot{\phi} &= \omega, \\
\dot{u} &= \theta(\omega - u).
\end{align*}
\]  

(19)

Consider \( \omega(t) \) as a control in this problem, the control limitation is lacking. The similar procedure in general form is described in [11], [12]. The boundary conditions for the other variables

\[
\begin{align*}
t = 0 : & \quad \rho(0) = \rho_0, \ v(0) = v_0, \ \varphi(0) = \varphi_0, \ u(0) = u_0, \\
t = T : & \quad \rho(T) = \rho_T.
\end{align*}
\]  

(20)

and goal function

\[
k(t) : J = T \rightarrow \min, \\
-\bar{k} \leq k(t) \leq \bar{k}
\]  

(21)

remain the same.

The Hamiltonian of the problem (19) – (21) is:

\[
H = \rho\psi_\rho \omega^2 + (2\rho\Omega_0\psi_v + \psi_\varphi + \theta\psi_u)\omega + (\nu\psi_\rho - \theta u\psi_u).
\]  

(22)

The system for adjoint variables is:

\[
\begin{align*}
\dot{\psi}_\rho &= -\omega(\omega + 2\Omega_0)\psi_v, \\
\dot{\psi}_v &= -\psi_\rho, \\
\dot{\psi}_\varphi &= 0, \\
\dot{\psi}_u &= \theta\psi_u.
\end{align*}
\]  

(23)
By integrating (23) and using boundary values of adjoint variables we obtain:

\[ \psi_{\phi}(t) = \psi_{\phi}(T) \equiv 0 \]
\[ \psi_u(t) = c \cdot e^{\theta t} \equiv 0 \]

To find the optimal control notice that the function \( H \) (22) is quadratic in control \( \omega(t) \), and its maximum is reached when

\[ \omega = -\frac{2 \rho \Omega_0 \psi_v + \psi_\psi + \theta \psi_u}{2 \rho \psi_v} = -\Omega_0 \]

under the condition \( \rho \psi_v < 0 \).

Therefore, the optimal motion in the problem (19) – (21) is motion with constant relative angular velocity.

The auxiliary problem solution corresponds to the singular arch of the optimal trajectory of the problem (3), (4), (7), (8) and is obtained under the assumption that the starting condition \( \omega(0) \) is free, and the limitations (3) are lacking. Hence, if the optimal trajectory of the problem (3), (4), (7), (8) includes the singular arch and \( k_s \) satisfies the condition (3), then this arch adjoins the extremity of the trajectory.

Substituting the auxiliary problem solution \( \omega(t) \equiv -\Omega_0 \) in (17), we find the corresponding singular control value \( k_s \equiv 0 \).

We cleared up the optimal control structure: the coefficient \( k(t) \) of the proportional navigation law should be chosen maximal in absolute value from the allowable class \( k = \bar{k} \) till the angular velocity \( \omega \) decreases to zero, then follows the switching to the singular mode \( k = 0 \) till the reach of the given terminal range \( \rho_T \). Thus, the optimal control synthesis looks like:

\[ k = \begin{cases} 
-\bar{k}, & \omega \neq -\Omega_0 \\
\bar{k}, & \omega \neq -\Omega_0 \\
k_s = 0, & \omega = -\Omega_0.
\end{cases} \]

It follows from the physical meaning of proportional navigation that inclusion of motion path with \( k = -\bar{k} \) in the trajectory is not optimal, it is also confirmed by simulation.

5 Computer Simulation

Consider system (7) with various control modes:

\[ k = \begin{cases} 
\bar{k}, & t < t_s \\
0, & t > t_s
\end{cases} \]

where the switching moment \( t_s \) varies from \( t_s = 0 \) to \( t_s = T \).

The simulation is realized with the constant time delay \( \tau = 0.1 \) and the following boundary conditions:

\[ t = 0: \quad \rho_0 = 1, \quad v_0 = -0.5, \quad \varphi_0 = 1, \quad \omega_0 = 1, \quad u_0 = 1, \]
\[ t = T: \quad \rho_T = 0.4 \]
The system (7) was numerically integrated with chosen limit values of the variables. The plot of rendezvous time (time of reaching terminal range $\rho_T = 0.4$) vs switching point $t_s$ is shown in Fig. 2.

The rightmost point of the plot corresponds to the control mode, on which the proportional navigation law coefficient is chosen constant and maximal $k = \bar{k}$ during the whole approach time. Obviously, this mode is not optimal, because there exists the mode with a switching, on which the required terminal range is reached faster. With the chosen boundary conditions and control limitations minimum of approach time is reached under the control with the switching from $k = \bar{k}$ to $k_s = 0$ at $t_s = 0.325$, which corresponds to the moment when angular velocity reaches value $\omega(t) = -\Omega_0$.

6 Conclusion

The problem of optimization of the proportional navigation law with a constant time delay was considered. To minimize the rendezvous time of a spacecraft and a passive orbital station the guidance law coefficient should be chosen variable: maximal in absolute value till the moment when the LOS angular velocity reaches value $\omega(t) = -\Omega_0$ (regular control) and equal to zero till the end of the process (singular control).

References

Analysis of temporal characteristics of rendezvous algorithms on the orbit


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The Restitution Coefficient of Wet Granules

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Abstract

During the processing and the transportation of granules impacts and mechanical loading and stressing (compression, shearing) in particle-particle and particle-wall contacts often occur. Granules are stressed especially in fluidized beds and during pneumatic transportation. The knowledge of these breakage dynamics is import and has to be investigated.

The normal and tangential coefficients of restitution were examined in the presented work using free fall experiments. The dominant elastic $\gamma-Al_2O_3$, the elastic-plastic zeolite 4A and the dominant plastic sodium benzoate were selected as model granules. The moisture content and the falling height that results in different impact velocities were varied. A free fall apparatus was constructed for this purpose to adjust the falling height. The particle impact velocities are obtained between 0.5 - 5.0 m/s. For higher impact velocities (5.0 - 6.5 m/s) a spring canon was constructed. The impact plate is made of steel and has a thickness of 30mm, so that emerged elastic waves do not affect the impact. A digital high speed camera was used for recording the impact and rebound events. The camera has a frequency of 4.000fps. A video camera was also used to record the rebound height.

1 Granule samples

Three different types of granule samples were chosen: $\gamma-Al_2O_3$, zeolite 4A and sodium benzoate for the investigation (figure 1). The granules are industrially produced and are used for different purposes like drying and cleaning of gas.

These granules were analysed in preliminary tests and were chosen because of their different deformation behaviour from elastic to plastic. $\gamma-Al_2O_3$ shows a dominant elastic, zeolite 4A an elastic-plastic and sodium benzoate a dominant plastic behaviour.

Different physical granule properties were measured. The particle size distribution and sphericity were recorded by digital image analysis (figure 2). The granule density was measured by powder pycnometer and the solid density by He-pycnometer.
The restitution coefficient of wet granules 

\[
\gamma - \text{Al}_2\text{O}_3 \quad \text{zeolite 4A} \quad \text{sodium benzoate} 
\]

dominant elastic \quad \text{elastic-plastic} \quad \text{dominant plastic}

Figure 1: Digital photos of the granule samples [1]

The granules have to be spherical by the free fall and normal impact experiments, so that they rebound perpendicular by the impact plate. The impact events and the rebound height can be recorded. The mean sphericity of sodium benzoate granules is too low (table 1) because of this, only spherical granules of sodium benzoate were hand sorted and used for the experiments.

The porosity \( \varepsilon \) of the granules was calculated with Eq. (1)

\[
\varepsilon = \frac{V_H}{V_g} \frac{V_g - V_s}{V_g} = 1 - \frac{\rho_g}{\rho_s},
\]

with \( V_H \) the volume of voids, \( V_g \) the granule volume, \( V_s \) the solid volume, \( \rho_g \) the granule density and \( \rho_s \) the solid density.

Table 1: Characteristics of the granules [1]

<table>
<thead>
<tr>
<th>characteristics</th>
<th>( \gamma - \text{Al}_2\text{O}_3 )</th>
<th>zeolite 4A</th>
<th>sodium benzoate</th>
<th>sorted</th>
</tr>
</thead>
<tbody>
<tr>
<td>chemical composition</td>
<td>97.9% ( \gamma - \text{Al}_2\text{O}_3 )</td>
<td>85% synthetic zeolite 13X binder: clay</td>
<td>C_6H_5CO_2Na</td>
<td></td>
</tr>
<tr>
<td>granule size in mm</td>
<td>1.5-1.85</td>
<td>1.8-2.5</td>
<td>1.4-1.7</td>
<td></td>
</tr>
<tr>
<td>sphericity</td>
<td>0.95</td>
<td>0.91</td>
<td>0.89</td>
<td>0.92</td>
</tr>
<tr>
<td>granule density ( \rho_g ) in kg/m(^3)</td>
<td>1040</td>
<td>1150</td>
<td>1440</td>
<td></td>
</tr>
<tr>
<td>solid density ( \rho_s ) in kg/m(^3)</td>
<td>3230</td>
<td>3640</td>
<td>1500</td>
<td></td>
</tr>
<tr>
<td>porosity ( \varepsilon )</td>
<td>0.68</td>
<td>0.45</td>
<td>0.04</td>
<td></td>
</tr>
</tbody>
</table>
2 Wetting the granules

To vary the moisture content of the granules an air conditioning chamber was used. The air temperature was set 45°C and the relative air humidity $\varphi = 95\%$. To obtain the largest possible moisture content the granules were temporarily placed in water.

The moisture content $X_w$ is calculated as

$$X_w = \frac{m_{\text{ges}} - m_{\text{TS}}}{m_{\text{TS}}},$$

(2)

with $m_{\text{ges}}$ the total mass and $m_{\text{TS}}$ the mass of the dry probe. The degree of pore saturation is

$$S = \frac{1 - \varepsilon}{\varepsilon} \frac{\rho_s}{\rho_l} X_w,$$

(3)

with $\rho_s$ the solid density and $\rho_l$ the liquid density. The measured values of the moisture content and pore saturation are shown in table 2.

Table 2: Characteristics of the granules

<table>
<thead>
<tr>
<th>materials</th>
<th>moisture content $X_w$ in kg$<em>{\text{water}}$/kg$</em>{\text{TS}}$</th>
<th>pore saturation S</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma - \text{Al}_2\text{O}_3$</td>
<td>0.48 0.69</td>
<td>0.72 1.06</td>
</tr>
<tr>
<td>zeolite 4A</td>
<td>0.23 0.5</td>
<td>0.38 0.82</td>
</tr>
<tr>
<td>sodium benzoate</td>
<td>0.26 soluble</td>
<td>(9.34) soluble</td>
</tr>
</tbody>
</table>
3 Experimental equipment

The free fall experiments were performed by a new fall apparatus figure 4. The granules were released by vacuum tweezers, which are height adjustable, so that the granules can be released at different falling heights. The falling starts without any initial influences of velocity or rotation. The impact takes place on an impact plate (figure 4) made of hardened steel. The impact plate was designed to have a thickness of 30mm, so that emerged elastic waves do not affect the impact. The impact plate offers the possibility to adjust the plate in different angles ($0^\circ - 90^\circ$). The normal and the angular impact are investigated. After the impact the rebound height $h_2$ of the granules was recorded by a video camera.

A digital high speed camera recorded the granules closely before and after the impact. The high speed camera makes 4.000fps and has a resolution of 256*512 pixels. The recorded images were used to calculate the impact and rebound velocities.

A non-high speed video camera was also used to record the complete events of the falling, impact and rebound. The rebound height can be measured by these records and by a scale in the background.

Figure 3: Free fall apparatus
The restitution coefficient $e$ is calculated by Eq. (4)

$$e = \frac{v_R}{v_i} \approx \sqrt{\frac{h_2}{h_1}}$$

and can be written as

$$e = \sqrt{\frac{E_{\text{kin},2}}{E_{\text{kin},1}}} = \sqrt{\frac{E_{\text{kin},1} - E_{\text{diss}}}{E_{\text{kin},1}}} = \sqrt{1 - \frac{E_{\text{diss}}}{E_{\text{kin},1}}}$$  \hspace{1cm} (5)

with $v_R$ the rebound velocity, $v_i$ the impact velocity, $h_2$ the rebound height, $h_1$ the initial height. $E_{\text{kin},2}$ is the kinetic energy of the rebound, $E_{\text{kin},1}$ is the kinetic energy of the impact and $E_{\text{diss}}$ is the energy absorption during the impact.
With the free fall apparatus impact velocities between 0.5 - 5.0 m/s are obtained. A new apparatus was built to extend the impact velocities (figure 5). A spring is used to accelerate the granules. The granules are put in a mount and the spring is loaded by compressing the spring from the equilibrium position. Then the spring is released and the granules move upwards against the impact plate. The velocity of the granules is adjustable by different displacements of the spring. The impact velocities are extending to 6.5 m/s.

![Image of the spring cannon](image-url)

**Figure 5: Spring cannon for accelerating the granules**

4 Results

Some images of the impact of $\gamma - \text{Al}_2\text{O}_3$ recorded with the high speed camera are shown in figure 6. The left picture shows the falling granule before the impact, the central picture the impact and the right picture demonstrates the rebound. The bolt with $h = 9$ mm was used to scale the dimensions. The images were analysed by MATLAB software. A software procedure was written that converts the digital images to binary images and changes the background completely black and makes the entire granule white. The centre of the granule was detected in each image and the program calculated as the velocities differences between the centres of the granule in consecutive images with given frame speed. The impact and rebound velocity was obtained and the restitution coefficient was calculated by Eq. (3).
The normal restitution coefficient is shown versus the impact velocity in Figure 7. All granules show an elastic-plastic impact in the examined velocity range. Furthermore, the following sequence from elastic-plastic to dominantly plastic behaviour (based on the average coefficient of restitution) can be observed: $\gamma - \text{Al}_2\text{O}_3$ ($e = 0.735$), zeolite4A ($e = 0.653$) and sodium benzoate ($e = 0.532$).

The standard deviations of the restitution coefficients measured by 50 repeated tests are relatively large. That was expected because of the inhomogeneity of the granules. For a given particle size, the contact stiffness and the position of the yield point are not constant, since the mechanical characteristics of the primary particles and the bonding agents are randomly distributed within a fraction of granules. The individual granules differ in surface roughness and distribution of pore sizes.

For all examined granules increasing the impact velocity does not change the mean normal coefficient of restitution. In other words, the granules exhibit elastic-plastic behaviour without a viscous effect during the impact in this velocity range.
The granules were wetted up to different moisture contents and then the free fall tests by normal impact were performed. The normal restitution coefficients of wet granules impacted at two different velocities are shown in figure 8 as a function of the moisture content. For sodium benzoate granules, the restitution coefficient decreases with increasing moisture loading. These granules deform more plastically during the impact with increasing moisture because of the granule solubility and softening. The restitution coefficient of zeolite 4A slowly decreases with increasing moisture. During the wetting the liquid removes the solid bridge bonds of the granule. The moisture content has not shown a significant effect on the restitution coefficient of $\gamma - \text{Al}_2\text{O}_3$ granules consisting of stiff ceramic microstructure.

The restitution coefficient of wet granules decreases with increasing impact velocity. Higher impact velocities determine higher impact forces and the contribution of the energy absorption due to plastic deformation increases. This effect has been observed in the examined velocity range only for wet granules.

![Figure 8: Restitution coefficient versus moisture content](image)

**Figure 8** shows a comparison of the two different test methods. The restitution coefficient was determined via the digital high speed camera and the video camera. The video camera was used on former impact experiments to measure the rebound height. With equation (3) the restitution coefficient can be calculated using the initial height and the rebound height. The restitution coefficient is equivalent for zeolite 4A and sodium benzoate in both measurements. Differences occur at larger impact velocities of $\gamma - \text{Al}_2\text{O}_3$ granules. The restitution coefficient obtained by the video camera is much higher than the restitution coefficient calculated with the digital high speed camera. The purpose of the restitution coefficient at large impact velocities becomes more imprecise by the video camera because the determination of the rebound height becomes more difficult by occurring perspective failures.
Figure 9: Comparison of the restitution coefficient versus impact velocity of measurements using the digital high speed camera and a video camera.

The tangential restitution coefficient of $\gamma-Al_2O_3$ was investigated by adjusting the impact plate in different angles. Figure 10 shows schematically the test of the tangential restitution coefficient.

The falling height was $h = 0.3m$ and the impact velocity was $v_i = 2.3m/s$. Figure 11 shows the normal restitution coefficient and the tangential restitution coefficient of $\gamma-Al_2O_3$ at different impact angles. The normal restitution coefficient does not depend on different impact angles. The tangential restitution coefficient decreases with increasing impact angle and reaches a local minimum of $e = 0.65$ close to an impact angle of $30^\circ$. Than the tangential restitution coefficient increases with increasing impact angles and reaches a value of $e = 1$ at above $80^\circ$. The behaviour of the granules on leaving the surface are that it either rolls at near normal angles or slides at huger angles [2].

5 Conclusions

The normal restitution coefficient of $\gamma-Al_2O_3$, zeolite 4A and sodium benzoate were measured successful by a digital high speed camera and a video camera. The
restitution coefficient of examined dry granules is independent of the impact velocity in the range of 0.5 - 4.5m/s. Due to softening the normal restitution coefficients of sodium benzoate and zeolite 4A granules decrease with increasing moisture content. Hence, if the granules are wet then their restitution coefficient decreases with increasing impact velocity. The tangential restitution coefficient of $\gamma - Al_2O_3$ was investigated successful at angles $0^\circ - 80^\circ$. It shows a minimum at an impact angle of $30^\circ$. The coefficient of normal restitution is independent of the impact angle.

References


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Figure 11: Normal and tangential restitution coefficient at different impact angles
Isothermal transition to instability of interface in porous medium

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Abstract

The object of this research is the stability of the phase transition interface in geothermal systems in case when the layer of water overlays the vapor one, their temperatures are equal and time-independent and the capillary effects are important. It is shown that if parameters of the problem are close to their critical values, there are two possible phase transition interfaces which coincide on the margin of stability and cease to exist in the supercritical zone of parameters. A dispersion equation is derived. It is shown that two possible types of transition to instability take place and only one of them is realized (the one with the most unstable mode affiliated with the zero wave number). The nonlinear equation by Kolmogorov-Petrovsky-Piskunov describing the evolution of a narrow band of weakly unstable modes is derived for this type.

1 Introduction

Observations of natural geothermal systems show that for some of them the configuration with water layer (a heavy liquid) overlaying the vapor (a light liquid) is stable [1]. For the first time the stability of such system was studied in [2]. In that work it was assumed that water and vapor are motionless in unperturbed state. In papers [3,4,6] motion in unperturbed state was permitted. The criteria of stability of vertical stationary flows in such systems were derived and possible types of transition to instability were found out [3,4,6]. It was shown that one of possible types of transition to instability is a transition with the most unstable mode according to the zero wave number. For this case the weakly nonlinear Kolmogorov-Petrovsky-Piskunov equation was brought out. It describes the evolution of phase transition interface at the threshold of instability. Several properties of systems which obey this equation were described.

In present work a particular case of the problem described in [3,4,6] is under consideration. We assume that the temperatures of water and vapor are equal
and time-independent. Physically this situation may take place for flows in narrow cracks or porous medium with low permeability [5]. The influence of capillary effects is taken into account.

The linear stability of phase transition interface is explored, possible types of transition to instability are found out. It is shown that only the transition with the most unstable mode affiliated with the zero wave number may be realized. The weakly nonlinear evolution of the system in the neighbourhood of the margin of stability is described.

2 Statement of Problem

The problem of our interest is a geothermal reservoir consisting of two high permeability layers of porous media separated by a low permeability one (Fig. 1). Let’s consider such co-ordinates that x-axis is directed horizontally and z-axis and the vector of gravity are codirectional. The low permeability layer occupies the area \( \{(x, z) | (x, z) \in (-\infty; \infty) \times [0; L]\} \). The upper high permeability layer is saturated by water and the lower does by vapor. We will assume that there is no area with the mixture of two phases. Hence, a phase transition interface takes place in a low permeability layer. Temperatures of water and vapor are equal and do not depend on time or spatial coordinates. Vapor and water are assumed to be incompressible. So, the continuity equations for arias of low permeability layers saturated by water and vapor may be presented in the following form

\[
\text{div} \, \mathbf{v}_j = 0, \quad j = v, w.
\]
Here $v$ is the filtration velocity, indexes: $w$ denotes water, $v$ denotes vapor. The velocity field for flows in porous media or narrow cracks are described by Darcy’s law

$$v_i = -\frac{k}{\mu_j} (\text{grad}P - \rho_j g e_z)$$

Here $k$ is the permeability, $\mu$ is the viscosity, $P$ is the pressure, $g$ is the acceleration of gravity, $\rho$ is the density and $e_z$ is a unit vector directed downwards. The mass conservation law on the boundary between two phases reads:

$$m(1-\frac{\rho_v}{\rho_w})V_n = \frac{k}{\mu_v} \rho_v (\text{grad}P)_n + \frac{k}{\mu_w} (\text{grad}P)_{n-} + \frac{k}{\mu_w} \rho_{wg}(1-\frac{\mu_w \rho_v^2}{\mu_v \rho_w})$$

Here $m$ is the porosity, $V_n$ is the projection of velocity of phase transition interface on the normal to this interphase. Indexes: $n$ is normal to the interface, - and + denote parameters relating to areas saturated by water and vapor respectively. With account for capillary effects, the values of pressure near the phase transition interface in water and vapor areas are connected by the following relation

$$P_+ + P_c = P_-$$

Here $P_c$ is the capillary pressure. If the water wets rock, this pressure is positive. In opposite case it is negative. The pressure of steam near the phase transition interface equals the pressure of saturated vapor.

$$P_+ = P_*$$

The pressure and the temperature of saturated vapor obey the Clapeyron equation

$$\ln \frac{P_*}{P_a} = A_* + B_* \frac{T_*}{P_a}$$

$$A_* = 12.512, \quad B_* = -4611.73, \quad P_a = 10^5\text{Pa}.$$ 

Here $P_a$ is the atmospheric pressure.

Boundary conditions on planes between low and high permeability layers are

$$z = 0 : \quad P = P_0, \quad z = L : \quad P = P^0$$

where the values of $P_0$ and $P^0$ are given and do not depend on time or $x$ coordinate. In Fig. 2 the Clapeyron curve is represented. It illustrates the dependence of vapor pressure saturation on its temperature. Since we assume the system is isothermal, we should consider parameters corresponding to points of the line $T = T_0$. Value of $P_*$ may be explicitly found as an intersection of this line and the Clapeyron curve. The point $F_3 = (T_0, P_*)$ corresponds to values of temperature and pressure on the phase transition interface. The point $F_1 = (T_0, P_0)$ - to values of this parameters on the upper boundary of the layer with low permeability or rock with crack. This interface lays in area saturated by water. Hence point $F_1$ is located above the Clapeyron curve. The point $F_1 = (T_0, P^0)$ lays below this curve. All three points correspond to the line $T = T_0$. So

$$P^0 < P_* < P_0$$
3 Basic flow

We will consider stationary horizontal homogeneous solutions of the system of equations and boundary conditions (1)-(7) as basic flows. Phase transition interface for this flows is a horizontal plane defined by equation $z = h$, where $0 < h < L$. The pressure field for this regimes is described by the following expressions

$$P_w = P_0 + \frac{P_0 + P_c - P_0}{h} z \quad 0 < z < h$$

$$P_v = \frac{P_0 L - P_0 h}{L-h} - \frac{P_v - P_0}{L-h} z \quad h < z < L$$

The location of phase transition plane may be found from equation

$$A - B H + C = 0 \quad (9)$$

$$H = \frac{h}{L}, \quad A = M R_s (P^0 - P_s) < 0, \quad (10)$$

$$B = P_s + P_c - P_0, \quad C = \rho_{w_g} L (1 - M R_s^2) > 0 \quad (11)$$

$$M = \frac{\mu_w}{\mu_v}, \quad R_s = \frac{\rho_v}{\rho_w}$$

Since the phase transition interface locates inside the low permeability layer, the solution of this equation obeys the inequality $0 < H < 1$. Hence (9) leads to the following one:

$$C H^2 - (A + B + C) H + B = 0 \quad (12)$$
Here the value of $H$ also lays between 0 and 1. The number of possible locations of phase transition interface in stationary case is controlled by the sign of the discriminant
\[ D = (A + B + C)^2 - 4BC \] (13)

In Figure 3 the curve $D = 0$ is shown. If the parameters of geothermal system correspond to this curve, only a single solution of equation (12) exists. This solution is
\[ H = \frac{A + B + C}{2C} \] (14)

It satisfies the inequality $0 < H < 1$ on the part of curve between the points $(-C, 0)$ and $(0, C)$. In area 1 parameters of the system correspond to absence of solutions of (12). In another part of plate two solutions of this equation exist
\[ H_1 = \frac{(A + B + C) - \sqrt{D}}{2C}, \quad H_2 = \frac{(A + B + C) + \sqrt{D}}{2C} \] (15)

Both of them simultaneously satisfy the term $0 < H < 1$ only inside the curvilinear triangle marked as area 2 in Fig. 3.

## 4 Linear stability analysis

We will consider small perturbations of these regimes to analyze the linear stability of vertical stationary flows. So phase transition interface may be described in form
\[ z = h + \eta(x, t) \]
where \( h \) is its stationary location and \( \eta(x,t) \) - its perturbation. The pressure field may be presented in a similar form

\[
P_j = (P_j)_{st} + (\delta P_j), \quad j = v, w
\]

Here \((P_j)_{st}\) is stationary pressure field and \((\delta P_j)\) is its perturbation. We assume \(\eta(x,t)\) and \((\delta P_j)\) are of the first order of smallness. Presenting small parameters in the form \(\{(\delta P_j)(z,x,t), \eta(x,t)\} = \{(P_j'(z), \eta'(z))\} \exp(\sigma' t + i\kappa' x)\), where \(\sigma'\) and \(\kappa'\) are the frequency and wave number, one get a dispersion equation using (1)-(7)

\[
m (1 - R_*) \sigma = \frac{k\kappa}{a\mu_w} \left[ \frac{A}{1 - H} \coth[\kappa(1 - H)] + \frac{B}{H} \coth[\kappa H] \right]
\]

\[
\kappa' = \kappa/L, \quad \sigma = \frac{a\sigma'}{L^2}, \quad a = \frac{\mu_w}{\rho_w}
\]

may be derived from(1)-(7). This equation may be also deduced from dispersal equation given in [6] for non-isothermal case by assuming that temperature is constant. It also should be taken into account that, because of the absence of temperature gradients on phase transition interface, specific heat of phase transition vanishes in an isothermal system.

The basic flow is stable if and only if \(\sigma(\kappa) \leq 0\) for all \(\kappa\). If \(\sigma = 0\) the dispersion equation has the form

\[
f(\kappa) = \frac{\coth[\kappa(1 - H)]}{\coth[\kappa H]} \equiv \Delta = -\frac{B(1 - H)}{A H}.
\]

It will be shown below that, if \(f(\kappa) < \Delta\) for any \(\kappa\) then \(\sigma > 0\) for this \(\kappa\). Let \(f(\kappa)\) obey the inequality

\[
f(\kappa) < -\frac{B(1 - H)}{A H}.
\]

The flow obeys the inequalities \(P^2 - P_* < 0\) (see (8)) and \(0 < H < 1\). So multiplying (17) by \(\frac{A\kappa}{1 - H \mu_w} \kappa \coth[\kappa H] < 0\) we’ll get the inequality

\[
\frac{k\kappa}{a\mu_w} \left[ \frac{A}{1 - H} \coth[\kappa(1 - H)] + \frac{B}{H} \coth[\kappa H] \right] > 0
\]

Since \(R_* = \frac{P_c}{P_w} < 1\), \(m > 0\) and \(\sigma\) obeys (16), it is positive for the given value of \(\kappa\). It may be similarly proved that, if \(f(\kappa) > \Delta\) for all \(\kappa\) then \(\sigma \leq 0\) for all values of wave number. Hence, the margin of stability is obtained when \(f(\kappa) = \Delta\).

Let’s use the geometrical interpretation of equality \(f(\kappa) = \Delta\) for clearness. The left-hand side of this formula is strictly positive, tends to 1 when \(\kappa \to \pm \infty\), and has it’s minimum (if \(H < 1/2\) (Fig. 4(a)) or maximum (if \(H > 1/2\))(Fig. 4(d)) when \(\kappa = 0\). The right-hand side of this equation doesn’t depend on wave number and may be presented as a line parallel to \(\kappa\)-axis. Note that for \(\Delta \leq 0\) stationary vertical flow is stable for any location of phase transition interface, because \(f(\kappa) > 0\) for any wave number. The sign of \(\Delta\) is defined by the sign of coefficient \(B\) (see (10),(11) and (16)). Specifically, if \(P_c \leq 0\) (water doesn’t wet the rock), small perturbations can’t
Figure 4: The line $\zeta = \Delta$ and the curve $\zeta = f(\kappa)$ in case $H < 1/2$ for unstable (a) and stable (b) locations of phase transition interface. (c) - dispersal curves for stable (I), unstable (III) and marginal (III) locations. Direction of the narrows illustrates the movement of the line $\zeta = \Delta$ while approaching to the margin of stability. (d) - the line $\zeta = \Delta$ and the curve $\zeta = f(\kappa)$ in case $H > 1/2$. 

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lead the system to instability. We’ll consider only geothermal systems with strictly positive coefficient $B$ bellow.

Let’s show that for $H \geq 1/2$ the basic flow is stable. Let’s assume that it’s not so. Location of phase transition interface which obeys $H \geq 1/2$, may be unstable or neutrally stable only if $\Delta \leq 1$. Hence (see (17))

$$H \leq \frac{1}{2} + \frac{2A - B}{B - A} \quad (18)$$

As it was proved above, for $B \leq 0$ basic state is stable, so we’ll consider the case when $B > 0$. Since $A < 0$, the inequality (18) leads to the condition $H < 1/2$. It contradicts to the assumption $H \geq 1/2$. So the basic flow is stable for the discussed area of parameters.

As opposed to the isothermal problem, the basic state corresponding to $H \geq 1/2$ in case temperature is not constant may be unstable. And the margin of stability is obtained when the line $\zeta = \Delta$ touches the curve $\zeta = f(\kappa)$ at the points $\kappa = \pm \infty$. Thus the most unstable modes correspond to the infinite values of the wave number. This type of transition to instability is not realized in the isothermal problem described in the present work.

Let us consider the case when $H < 1/2$. This location of the phase transition interface is marginally stable if the line $\zeta = \Delta$ touches the curve $\zeta = f(\kappa)$ at zero (see Fig.4(a)(b)). The value of $f(\kappa)$ in the minimum point equals $\frac{H}{(1-H)}$. Hence the criterion of marginal stability is

$$\frac{H}{(1-H)} = \Delta, \quad (19)$$

of stability $- \frac{H}{(1-H)} > \Delta$, of instability $- \frac{H}{(1-H)} < \Delta$.

Let’s show that the criterion of marginal stability and the criterion of coincidence equality solutions for defining location of phase transition interface (12) are equivalent. Substituting $H_1$ from(15) and $\Delta$ from (17) in (19) one may get

$$\left( \frac{A + B + C - \sqrt{D}}{2C - (A + B + C - \sqrt{D})} \right)^2 = \frac{B}{A} \quad (20)$$

If $A + B + C < 0$, then it follows from (10),(11) and (19) that $H_1 < 0$ and $H_2 < 0$. Hence below we’ll assume $A + B + C \geq 0$. One may get the following expression for $A$ from (13)

$$A = -B - C + \sqrt{D_1}, \quad D_1 = D + 4BC$$

Then equation (20) leads to

$$\left( \frac{\xi}{2C - \xi} \right)^2 = \frac{B}{B + C - \sqrt{D_1}}, \quad \xi = \sqrt{D_1} - \sqrt{D} \quad (21)$$

Taking into account that $D_1 = D + 4BC$ after some transformation of (21) the cubic equation for $\xi$, may be obtained

$$\phi(\xi) \equiv -\xi^3 + 2C\xi^2 + 4B\xi + 8BC^2 = 0$$
Isothermal transition to instability of interface in porous medium

Figure 5: Curve $\phi(\xi)$. Points of this curve located above $\xi$-axis correspond to stability of the system, below do to instability. Points laying at this axis correspond to marginal stability.

It has three solutions (fig. 6)

$$\xi_1 = -2\sqrt{BC}, \quad \xi_2 = 2\sqrt{BC}, \quad \xi_3 = 2C$$

Let’s consider only systems with capillary pressure which is small as compared to the water pressure and $P_0 > P_\ast$. Then according to (10), (11) $B$ is small compared to $C$. So $\xi_2 < \xi_3$. It follows from $B > 0$, that $D_1 = D + 4BC > D$ and $\xi = \sqrt{D_1} - \sqrt{D}$. For $\xi \geq \xi_3 = 2C$ one may derive inequality $\sqrt{D} \leq B - C < 0$. This contradicts to the fact that we consider such parameters of the system that at least one real solution of equality (12) exist. The assumption $\xi > \xi_2 = 2\sqrt{BC}$ leads to the same contradiction. So for the domain of parameters under consideration $\phi(\xi) < 0$ (see Fig.5). It means that the location of phase transition interface corresponding the lesser root of (12) is unstable.

It may be similarly proved that the greater root of (12) is stable and for discriminant $D$ tending to zero it obtains the margin of stability.

So for $H < 1/2$ and the values of parameters of the system corresponding to existence of two possible locations of phase transition interface, one of them (corresponding to the lesser $H$) is unstable and the other one is stable. While approaching to the margin of stability the distance between them diminishes and tends to zero when the margin is arrived. After crossing this margin basic state ceases to exist.
5 Derivation of Kolmogorov-Petrovsky-Piskunov (KPP) equation

In this section the transition to instability with the most unstable mode corresponding to the zero wave number is under consideration. Weakly nonlinear unstable perturbation of stationary state in the neighbourhood of the margin of stability are in the center of our attention. Let’s define dimensionless parameters \( \varepsilon_1 = L^2/\nu^2 \) and \( \varepsilon = \eta_a/L \), where \( \nu \) and \( \eta_a \) are the characteristic values of wave length and amplidute. This parameters are small for longwave perturbations. Determine the dimensionless parameters (keeping the old notation)

\[
x \to \nu x, \quad \eta \to \eta_a \eta, \quad z \to Lz, \quad t \to L^2/\alpha t
\]

Performing the expansion of pressure and temperature in vertical coordinate \( z \) in both domains at the location \( z = H \) one gets

\[
P_w = P_c + P_\ast + (\delta P_w)|_{z=H} + \left[ \frac{P_c + P_\ast - P_0}{H} + (\delta P_w)|_{z=H} \right] (z - H) + \frac{1}{2} (\delta P_w)_{zz}|_{z=H} (z - H)^2 + \frac{1}{6} (\delta P_w)_{zzz}|_{z=H} (z - H)^3 + \ldots
\]

\[
P_v = P_\ast + (\delta P_v)|_{z=H} + \left[ \frac{P_0 - P_\ast}{1 - H} + (\delta P_v)|_{z=H} \right] (z - H) + \frac{1}{2} (\delta P_v)_{zz}|_{z=H} (z - H)^2 + \frac{1}{6} (\delta P_v)_{zzz}|_{z=H} (z - H)^3 + \ldots
\]

The equation for \( \eta \) may be deduced by substituting pressure in this form in system (1)-(7) and neglecting all terms of third and higher order of smallness one gets

\[
m(1 - R_\ast) \varepsilon^2 \eta_\tau = \left( \frac{A}{1 - H} - \frac{B}{H} + C \right) + \varepsilon \left( \frac{A}{(1 - H)^2} - \frac{B}{H^2} \right) + \varepsilon \left( \frac{k \varepsilon}{a \mu_w} \left( \frac{A}{(1 - H)^3} - \frac{B}{H^3} \right) \eta^2 - \frac{k \varepsilon_1}{a \mu_w} (A + B) \eta_{xx} \right), \quad \tau = \varepsilon t
\]

Assuming \( \varepsilon_1 = \varepsilon \) and equating terms at \( \varepsilon^0 \) one gets the equation for stationary location of phase transition interface, at \( \varepsilon^1 = 0 \) and at \( \varepsilon^2 \) the following equation

\[
\delta \partial_\tau \eta = \alpha \eta + \beta \partial_{xx} \eta + \gamma \eta^2
\]

\[
\delta = m(1 - R_\ast) > 0, \quad \alpha = \varepsilon^{-1} \frac{k}{a \mu_w} \left( \frac{A}{(1 - H)^3} - \frac{B}{H^3} \right), \quad \beta = - \frac{k}{a \mu_w} (A + B) > 0, \quad \gamma = \frac{k}{a \mu_w} \left( \frac{A}{(1 - H)^3} - \frac{B}{H^3} \right) < 0,
\]

On the margin of stability the coefficient \( \alpha \) is of the first order of magnitude. By using appropriate scaling (the old notations are kept)

\[
\eta \to \frac{|\alpha|}{|\gamma|} \eta, \quad x \to x \sqrt{|\beta|/|\alpha|}, \quad \tau \to \frac{|\delta|}{|\alpha|}
\]
equation (22) may be reduced to the form
\[
\partial_\tau \eta = n' \eta + m' \partial_{xx} \eta - \eta^2, \\
n' = \text{sign}(\alpha), \quad m' = \text{sign}(\beta).
\] (24)

It is KPP equation which describes the evolution of weakly unstable modes in the neighbourhood of the margin of stability. The coefficient \(n\) is negative for stable flow and positive for unstable.

Stationary flows in neighborhood of the threshold of instability are described by equation
\[
\frac{d^2 \eta}{dx^2} = -n' \eta + \eta^2.
\]

It has two points of equilibrium that correspond to stationary vertical flows. For the subcritical case \(\eta = -1\) is unstable and location \(\eta = 0\) is stable. For the supercritical \(- \eta = 0\) is unstable and \(\eta = 1\) is stable. Thus, the transition to instability leads to displacement of the equilibrium points. Nonlinear effects repress exponential growth in time of positive perturbation and perturbations with negative average unboundedly grow\(^7\).

### 6 Conclusions

Vertical stationary flows in isothermal geothermal systems of given type are considered. It is shown that, as opposed to non-isothermal case, the only possible type of transition to instability is a transition with the most unstable mode corresponding to the zero wave number. It is proved that, for values of parameters close to critical two locations of phase transition interface are possible. While approaching to the margin of stability the distance between them decreases and becomes zero for the marginal stability. After crossing this margin basic flow ceases to exist. The influence of weakly nonlinear effects on the growth of perturbation at the threshold of stability is studied. The nonlinear KPP equation is derived. It describes the evolution of a narrow band of weakly unstable modes at the threshold of instability. Perturbations of phase transition interface concentrated between two equilibrium interfaces evolve to the stable one. Perturbations with negative average \(\int_{-\infty}^{\infty} \eta dx < 0\) unboundedly grow in area saturated by water. Thus, a tendency of penetration of vapor in domain occupied by water takes place.

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On Sommerfeld effect attenuation in a non-ideal vibrating system, using a Lugre friction model

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Abstract

In this paper, a non-ideal mechanical system, with LuGre friction model is considered. The mechanical model is an oscillator, not necessarily linear connected to an unbalanced DC motor, of excitation-limited power. The control of motion and the attenuation of the Sommerfeld effect of the considered non-ideal system are analyzed, in this paper. The mathematical model of the system is represented by coupled nonlinear differential equations. The identification of some interesting nonlinear phenomenon, both in the transient and in the steady state motion of the system, during the passage through resonance, under the applied voltages at DC motor (as control parameter) using numerical simulation are investigated, in details.

1 Introduction

The excitation of the vibration systems analyzed here, is taken as always limited; on the one hand by the characteristics of a particular energy source and, by other hand limited by the dependence of the motion of the vibrating system on the motion of the energy source. Note that this connection is expressed by a coupling between the differential equations of motion of the vibrating system and the source. Note, that when the excitation is not influenced by the response of a vibrating system, it is said to be an ideal energy source, or an ideal energy sources. For non-ideal dynamical systems, one must add an equation that describes how the energy source supplies the energy to the equations that govern the corresponding ideal dynamical system. We remarked that in non-ideal systems is present the so-called Sommerfeld effect: steady state frequencies of the DC motor will usually increase as more power (voltage) is given to it in a step-by-step fashion. When a resonance condition with the structure is reached, the better part of this energy is consumed to generate large amplitude vibrations of the foundation without sensible change of the motor frequency. Eventually, enough power is supplied to e motor to initiate the jump, the operating
frequency increases and the foundation amplitude decreases, resulting in lower power consumption by the motor. We mention that for more details on non-ideal systems theory are well described in Refs. [Kononenko, 1969, Balthazar et al., 2003].

We also remember that the LuGre model proposed by Canudas et al. in [Canudas et al., 2005] has become popular itself, because it incorporates many of the observed features of frictional behavior, in the mathematical model. For an example, imbedded within the LuGre model, it is the Striebeck effect. The Striebeck model, exhibits a negative derivative with respect to slip velocity, for small levels of slip velocity. This is one of the key features of friction that contributes to limit-cycle behavior and to stick-slip oscillations in frictional systems. Furthermore, the LuGre model behaves like a linear spring/damper pair, when it is linearized for small motions. At the microscopic level, two surfaces make contact at various asperities. These asperities are represented with bristles, and the bristles deflect like a spring when there is a relative velocity between the two surfaces. The deflection of the springs gives rise to the friction force. If the deflection is sufficiently large, then the bristles will slip in a highly random manner because of the irregular surfaces. Although the deflection of the bristles is random, the LuGre model only considers the average deflection. This was called the LuGre model since it resulted from a collaborative effort of researchers from Lund Institute of Technology, Sweden and Grenoble (Laboratoire d’Automatique de Grenoble), France.

We note that, by one hand, Pontes et al. [Pontes et al., 2000] presented numerical results on dynamic friction applied to a mass block-belt-motor system with limited power supply where the dry friction is between body and belt and by another hand, the initial implementation of vibration control for a non-ideal system, was itself investigated by [Felix et al., 2005, Felix2 et al., 2005], using a tuned liquid column damper and saturation phenomenon through of the numerical simulations. More recently, the nonlinear electromechanical vibration absorber was applied for non-ideal structure [Felix et al., 2008], with success.

We remarked that the main goal of this research is to examine the action of the LuGre friction in the elimination of the Sommerfeld effect, in the vibrations of a non-ideal structure (NIS), by using numerical simulations.

2 Mathematical Modeling

The vibrating system model is composed of an unbalance DC motor, with limited power supply. It contains an oscillatory mass $M$ and DC motor with moment of inertia $J$, unbalance mass $m_0$ and eccentricity $e$, connected to a fixed support by a spring of stiffness $k$, viscous damper $c$ and LuGre Friction $F_L$ applied on the foundation of the DC motor, as shown in Fig.2.

The governing equation of motion, as a set of coupled nonlinear ordinary differential equations, to the vibrating system that is described by Fig.2, with the LuGre friction model) can be written as:
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\[ (m_0 + M)\ddot{x} + c\dot{x} + kx + F_L = m_0e(\dot{\phi}^2 \cos \phi + \ddot{\phi} \sin \phi), \]
\[ (J + m_0e^2)\ddot{\phi} = \Gamma(\dot{\phi}) + m_0e\ddot{x} \sin \phi, \]
\[ \frac{dz}{dt} = \dot{x} - \sigma_0|\dot{z}|Z, \]
\[ F_L = \sigma_0z + \sigma_1\frac{dz}{dt} + \sigma_2\dot{x}, \]
\[ G(\dot{x}) = F_c + (F_s - F_c)e^{-(\phi'/V_s)^2}, \]
\[ \Gamma(\dot{\phi}) = u_1 - u_2\dot{\phi} \]
\[ X'' + c_1X' + X + F_L = q_1(\phi'^2 \cos \phi + \phi'' \sin \phi), \]
\[ \phi'' = \Gamma(\phi') + q_2X'' \sin \phi, \]
\[ \frac{dZ}{d\tau} = X' - \sigma_0^*|\frac{dX'}{d\tau}|Z, \]
\[ F_L = \sigma_0^*Z + \sigma_1^*Z' + \sigma_2^*X', \]
\[ G(X') = \mu_1^* + \mu_2^*e^{-(\phi'/V_s)^2}. \]

Figure 1: Non-ideal system with Lugre Friction
where

\[ \omega_0 = \sqrt{\frac{k}{(m + M)\omega_0}}, \quad c_1 = \frac{c}{(m + M)\omega_0}, \quad q_1 = \frac{m c e}{(m + M)\omega_0}, \quad q_2 = \frac{m_0 c e}{(I + m_0 e^2)} \]

\[ a = \frac{u_1}{\omega_0^2 (J + m_0 e^2)}, \quad b = \frac{u_2}{\omega_0^2 (J + m_0 e^2)}, \quad \sigma_0^* \sigma_0^* = \frac{\sigma_1^*}{k}, \quad \sigma_1^* = \frac{\sigma_1^*}{(m + M)\omega_0}, \]

\[ \sigma_2^* = \frac{\sigma_2^*}{(m + M)\omega_0}, \quad \mu_1^* = \frac{F_x}{k c_0}, \quad \mu_2^* = \frac{F_x - F_e}{k c_0}, \quad V_s = \frac{v_s}{x_0\omega_0}, \quad \Gamma(\phi') = a - b\phi'. \]

In the following case, when the Lure friction is taken into account:

\[ X'' + c_1 X' + X = q_1 (\phi'^2 \cos \phi + \phi'' \sin \phi), \]

\[ \phi'' = \Gamma(\phi') + F_L^* + q_2 X'' \sin \phi, \]

\[ \frac{dZ}{dt} = \phi' - \sigma_0^* \frac{|\phi'|}{Z}, \]

\[ F_L^* = \sigma_0^* Z + \sigma_1^* Z' + \sigma_2^* \phi', \]

\[ G(\phi') = \mu_1^* + \mu_2^* e^{-\frac{(\phi'/V_s)^2}{2}} \]  \hspace{1cm} (4)

the following parameters will be written as:

\[ \sigma_0^* = \frac{\sigma_0 x_0}{\omega_0^2 (I + m_0 e^2)}, \quad \sigma_1^* = \frac{\sigma_1 x_0}{\omega_0^2 (I + m_0 e^2)}, \quad \sigma_2^* = \frac{\sigma_2}{\omega_0^2 (I + m_0 e^2)} \]

\[ \mu_1^* = \frac{F_x}{\omega_0^2 (I + m_0 e^2)}, \quad \mu_2^* = \frac{F_x - F_e}{\omega_0^2 (I + m_0 e^2)}, \quad V_s = \frac{v_s}{\omega_0}. \]  \hspace{1cm} (5)

3 NUMERICAL RESULTS

The numerical simulations for Eq. (3), were carried out, by using Simulink - Matlab™, taken as the numerical integrator the Runge-Kutta fourth order algorithm, with variable time step. The parameters values where selected as being: \( q_1 = 0.4, q_2 = 0.3, b = 1.5, c_1 = 0.01, \sigma_0^* = 0.5, \sigma_1^* = 0.6, \sigma_2^* = 0.004, \mu_1^* = 0.8, \mu_2^* = 0.2, V_s = 0.1 \). The Fig. 2 represents the resonance curve, showing the dynamics of the non-ideal system, during the passage through resonance region (\( \phi' \approx 1 \)). We plotted amplitudes of oscillation of the angular velocity and foundation displacement without Lure friction (star line) and with Lure friction (triangle line), versus the voltage (control parameter) in the range \( 1.2 \leq a \leq 4.0 \), considering variation of increment \( \Delta a = 0.1 \) and over the dimensionless time range \( 0 \leq \tau \leq 1500 \). The initial conditions are taken as being nulls. This graph is estimated by numerical simulations, defining the amplitude for angular velocity of the motor shaft as maximum and minimum value of the oscillations, and the amplitude for the foundation oscillation as (maximum value-minimum value)/2.

The Fig.3 shows the amplitudes of oscillations of the angular velocity and displacement of the foundation of the DC motor. Fig.3(a) shows a predominant interaction, both between the DC motor and the foundation, with large oscillation amplitudes of the angular velocity (without LuGre friction) in the range \( 1.5 \leq a \leq 3.1 \).
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Figure 2: Amplitude-control parameter: a) angular velocity, b) oscillator displacement.

and without sensible change of the DC motor frequency, due to the resonance capture phenomenon, initiating the jump phenomenon in the vicinity $a = 3.2$ while is generating large vibration amplitude of the foundation, as is showed in Fig.3(b) (Sommerfeld effect). Considering the LuGre friction the Sommerfeld effect is then attenuated as it is observed in Fig.3(a), triangle line, while the vibration amplitude of the foundation are reduced drastically as is show in Fig.3(b), triangle line.

Figure 3: Time history: a) angular velocity, b) oscillator displacement for $a = 2.4$.

The Fig.3 shows the action of the LuGre friction force, acting in the elimination of the resonance capture and, in this case the angular velocity tends for $\varphi' = 1.6$ and reducing drastically the foundation oscillations (Fig.3b).

The numerical time traces shown in Fig.3, verify the influence in the reducing of the vibration amplitude of the DC motor foundation, when it is present the synchronization anti-phase, between LuGre friction force $F^*_L$ and the excitation force $q_1(\varphi^2 \cos \varphi + \varphi'' \sin \varphi)$, shown in the equation first of Eq. (3). Fig.3(a) shows the synchronization anti-phase in 100% then the amplitude of $X$ is reduced for 0.56 while Fig.3(b) with 90% of synchronization anti-phase the amplitude of $X$ is reduce.
Figure 4: The relation between the LuGre friction $F^*_L$ (black line) and the excitation force $q_1(\phi'^2 \cos \phi + \phi'' \sin \phi)$ (red line) for a) $a = 1.8$, b) $a = 2.4$.

for 0.73.

Figure 5: Amplitude-control parameter: a) angular velocity, b) oscillator displacement.

The Fig. 5 shows the graph of the resonance curve, that consists of the amplitudes of the angular velocity ($\phi'$) and the foundation displacement (X) versus control parameter ($a$), using the Eq. (4). In this case the LuGre friction is applied in the motor shaft and considering the following parameter values: $\sigma_0^* = 5.0, \sigma_1^* = 2.0, \sigma_2^* = 0.7, \mu_1^* = 2.0, \mu_2^* = 0.5$ and with is condition the resonance capture is then eliminate drastically. Fig. 5(a) shows that the angular velocity no through the vicinity of $\phi' \approx 1$ then the action of LuGre friction force eliminate the Sommerfeld effect while accounts the reduction drastically of the foundation oscillations as it is shown in Fig.3(b).

Numerically simulated, the time history of angular velocity and foundation displacement are presented in Fig.3. With the action of the LuGre friction force the resonance capture to be eliminated drastically and the angular velocity tends to a constant value of $\phi' = 0.17$ shown in the Fig.3(a). In Fig.3(b) one observes that
there is a reduction predominant of the foundation oscillation.

Figure 6: Time history: a) angular velocity, b) oscillator displacement for $a = 2.4$.

Figure 7: Time history: a) angular velocity, b) oscillator displacement for $a = 2.4, \sigma_2^* = 0.2, \mu_1^* = 0.8$.

Fig.3 shows the effect of the parameters $\sigma_2^*, \mu_1^*$ of the LuGre dynamic friction, taken in comparison with the results in Fig.3. One observes the elimination of the resonance capture phenomenon where the angular velocity has small oscillation (Fig.3(a)) and the reduction of the amplitude oscillation of the foundation (Fig.3(b)).

The influence of the LuGre dynamic friction when it is modified the parameters $\sigma_2^*, \mu_1^*$ is then described by the following expression:

$$\varphi'' = a - (b + \sigma_2^* + \sigma_5^*)\varphi' + (\sigma_1\sigma_5^*/\mu_1^* + \mu_2e^{-|\varphi'|/V_1})\varphi - \sigma_0^*Z + q_2X''\sin\varphi. \quad (6)$$

From the coefficient of the second term of Eq. (6) when one modify the value of $\sigma_2^*$ accounts the modification of the frictional torque of the motor shaft and due at the non-ideal phenomenon the angular velocity is influenced in its amplitude oscillation.
in the same proportion of the term fourth. The modification of the parameter $\mu^{*}_{1}$, as the average deflection of the bristles $Z$ tend for constant value, the coefficient of the three term containing nonlinear terms in function of $\varphi'$ influence in the non-ideal system.

4 CONCLUSION

The vibration analysis of a non-ideal system with LuGre dynamic friction is investigated here. The LuGre friction force applied to the DC motor foundation and motor shaft is taken into consideration. The most important results of this paper can be summarized as:

1. In the non-ideal system with LuGre friction force, the Sommerfeld effect is then eliminated.

2. The effect of the resonance capture phenomenon is then reduced.

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On Sommerfeld effect attenuation in a non-ideal vibrating system, using a Lugre friction model


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Concept of vibration damping using piezoelectric actuator systems

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Abstract

The paper deals with vibration damping in flexible structure systems using piezoelectric actuators. The commonly used material for manufacture of piezoelectric actuators lead zirconate titanate (PZT) exhibits strong nonlinear characteristic. So non unique magnitude - phase relationship can cause instability of complex MIMO system. The purpose and contribution of this paper consist in the discussion of a hybrid structural control architecture which combines feedback-based transient suppression and robust narrow band disturbance compensation using adaptive filtering method.

1 Introduction

Piezoelectric materials and systems have been constantly developed and improved for last 30 years. Among materials applied for manufacture of piezoelectric actuators and sensors polycrystalline piezoelectric ceramic materials such as lead zirconate titanate (PZT) are mainly used. Application of additives allows to obtain materials with sufficiently wide spectrum of characteristics (piezoelectric constant, Curie temperature, dielectric losses etc.). In particular piezoelectric actuators on the basis of PZT have successfully been used in systems of micro positioning. However all polycrystalline piezoelectric ceramics exhibit non-linear response to an electric field or mechanical stress.

For active control of sound and vibration, two types of control strategies have been widely applied - feedforward and feedback. The first one was adopted from the area of noise suppression. Basically such regulation system consists of a controller which, using correlated to disturbance signal, minimizes measured vibration. For both approaches at least a nonparametric model of the control object - mechanical structure with electronic equipment - is needed. During operation in most cases only the controller is changed. Because of model uncertainties the feedforward arrangement is preferable. The difficulty in developing feedback controller is frequently
caused by the fact that most flexible structures on the one hand are characterized by the presence of numerous natural vibration modes within the control bandwidth and on the other hand are subjected to parameter variations. Hence, these structural systems require robust control algorithms such as $H_2$, $H_{\infty}$ control with frequency shaped cost functions [1], [2] or sliding mode control (SMC) [3], [4].

The purpose and contribution of this paper consist in the discussion of a hybrid structural control architecture which combines feedback-based transient suppression and robust narrowband disturbance compensation using adaptive filtering method. It was shown in [5] that inclusion of a feedback loop in addition to adaptive feedforward one leads to faster convergence times of the adaptive compensator. A frequency estimator based on adaptive notch filter with constrained poles and zeros is used to identify the dominant frequencies in disturbance. The reference signal for feedforward compensator is than generated for each disturbance frequency separately and therefore each harmonic component can be processed independently using an adaptive filter with only two coefficients. SMC for feedback loop is used in this study to achieve robust stability in the presence of uncertainties.

2 Impact of actuator nonlinearities

The most commonly used material for manufacture of piezoelectric actuators is lead zirconate titanate (PZT) solution. Due to its polycrystalline structure the spontaneous polarisation by cooling PZT material below Curie temperature will be first oriented randomly. So in this state ceramic does not exhibit the piezoelectric effect. To align ferroelectric domains and consequently to make the material piezoelectrically active a sufficiently high electric field (up to 3.5 kV/mm) must be applied. This process is called poling. However when the electrical field is removed some of crystallographic axes due to mechanical stress in crystals change their previous orientations. This reversible domain switching results in strong non-linear behaviour of ceramics (Fig. 1). On the one hand if a piezoelectric actuator is driven by a periodic voltage with constant amplitude the actuator strain $x(t)$ can be approximated by a cubic function of applied voltage $U_a(t)$

$$x(t) = aU_a(t) + bU_a^2(t) + cU_a^3(t) \quad (1)$$

The coefficients $a$, $b$, $c$ in (1) are different for increasing and decreasing curves and depend on the voltage amplitude. When the voltage $U_a(t)$ is sinusoidal than according to (1) the actuator displacement contains both fundamental harmonic and higher harmonics.

The higher harmonic components are usually very small. But it can lead by high modal density to very strong excitation of resonance frequencies in mechanical structure and thereof to degradation of control effect in feedforward narrowband control architecture.

On the other hand the effective piezoelectric strain coefficient can increase by up to 50% compared to its small-signal value. Also due to electromechanical coupling the nonlinear effect will be enhanced, if the actuator is driven in resonance. At small electrical excitation the transfer function behaves typically for lightly damped
Figure 1: Strain versus applied voltage
mechanical systems. But when the excitation is increased there is an unstable region near the resonance frequency where the amplitude and the phase of transfer function are not unique defined [6].

Because of the practical significance of the nonlinear behaviour of piezoelectric ceramics it is desirable to include the piezoelectric hysteresis into model of considered mechanical structure. During last 10 years a lot of successful attempts to model the piezoelectric nonlinearities have been made. However many of these models have no strong physical interpretation. So for our purposes we chose the model (Fig. 2) presented by Goldfarb and Celanovic [7].

\[ \begin{align*}
\ddot{q} + \dot{b} \dot{x} + kx &= F_t + F_{ext} \\
q &= nx + C_a U_t \\
F_t &= nU_t \\
U_t &= U_a - U_{rc} \\
U_{rc} &= f(q)
\end{align*} \]

Equations (3), (4) present the interaction between electrical and mechanical domains. The nonlinearities are introduced through (6). The parameters of the model can be identified experimentally. Further this model was extended and transformed into state space by Adriaens [8]. Also the identification procedure was described [9].

In contrast with positioning systems, where collocated actuator-sensor pairs are often used so that every pair can be usually considered as SISO arrangement, smart structures are in general represented by MIMO systems with essential crosscoupling terms. So non unique magnitude - phase relationship due to nonlinear behaviour of piezoelectric material can cause instability of the control system.
3 Hybrid control architecture

Feedforward control systems on the basis of finite impulse response (FIR) filters are widely applied for both broadband and narrowband vibration suppression of flexible mechanical structures when a reference to disturbance can be obtained. However, it is necessary to take into account, that the needed amount of filter coefficients in a broadband control system is proportional to the length of the impulse response of the system. Application of an infinite impulse response filter (IIR) instead of FIR filter can lead to instability. In many practical applications there are dominant harmonics in disturbances acting on mechanical structures. Therefore it is preferable to use a feedforward compensator with only two coefficients for every harmonic component of disturbance. If both harmonic and impulse disturbances are simultaneously acting on the mechanical structure, the estimated gradient will be disturbed. So it leads to degradation of performance of adaptive algorithm [10]. The proposed controller architecture combines feedback-based transient suppression and robust narrowband disturbance compensation using adaptive filtering method (Fig. 3) [10].

First, the robust feedback control is designed to suppress impulse disturbances. Second, the dominant frequencies of harmonic excitations are estimated from a noised reference signal using adaptive frequency estimator and one harmonic signal is than generated at each frequency. Third, adaptive FIR filters with two coefficients are used to suppress vibrations at each excitation frequency separately.

Figure 3: Hybrid control structure

4 Narrowband adaptive vibration control

To obtain the reference signal a frequency estimation method (Fig. 4(a)) that uses adaptive notch filter with constrained poles and zeros is chosen because of its low
computational burden and fast convergence rate [12]. The reference signal is generated for each disturbance frequency separately and therefore each frequency component is processed independently.

Many of the adaptive active structural vibration control systems utilize the least-mean-square (LMS) control algorithm, which has been proved successful for applications where the disturbance is stationary or with slowly varying statistics [13], [14]. To ensure convergence of the conventional LMS algorithm in presence of secondary path transfer function, which describes the signal path between actuator and sensor, the modification of LMS known as filtered least-mean-square algorithms (FxLMS) has to be used (Fig. 4(b)) [13]. To obtain the model of the secondary path there are a lot of different methods [14]. The simplest one is to use the similar FIR filter.

![Figure 4: Adaptive frequency estimator (a); Narrowband adaptive filter (b)](image)

5 Sliding mode control

Flexible structure as object of regulation represents often systems with some zeros in the right part of the complex plane that conducts to a significant phase shift between control and measurement signals. In consequence, even at insignificant deviations of parameters loss of stability is possible. Therefore it is necessary to construct a robust feedback, which guarantees stability of the system in presence of uncertain parameters [1]. On the other hand model reduction also results in model uncertainties.

For further discussion the system must be transformed into state space form

\[
\dot{x} = Ax + B_1d + B_2u \tag{7}
\]

\[
y = Cx \tag{8}
\]

with \( u \) - control inputs and \( d \) - disturbances.

Sliding mode control or variable structure control is naturally robust with respect to uncertainties in the structural parameters [15]. Basically it is a control law that switches with theoretically infinite frequency between two values [15], with the objective to bring the system’s states onto the sliding surface (hyperplane) given by

\[
s_i = \{x \in \mathbb{R}_m ||S_i x = 0\} \tag{9}
\]
with the switching function

\[ s_i(t) = S_i x \quad (10) \]

In the MIMO case with \( p \) measured signals there are \( p \) sliding surfaces. Also \( s \) is not longer a scalar function but a vector consisting from \( s_i \) [15]. Utilizing the equivalent control method under assumption that the disturbance \( d \) can be replaced by its estimated value the equivalent linear control action is found as

\[ u_{eq} = -(SB_2)^{-1}(SAx + SB_1\hat{d}) \quad (11) \]

The equivalent control corresponds to the slow component of the real control which may be derived by filtering out the high-frequency components using a low pass. This opportunity is used to keep the nonlinear control gain within small bound. To make the system robust versus parameter deviations the nonlinear control signal should be added [15], [4]

\[ u_n = -\rho \text{ sign}(s) \quad (12) \]

A positive variable \( \rho_i \) in the simplest case can be set as a scalar. Its value must be chosen sufficiently large to ensure the reachability condition, which is derived from analyzing the Lyapunov’s function [15]

\[ V = \frac{1}{2}s^2 \quad (13) \]

and leads to

\[ ss < 0 \text{ or } s\dot{s} < \eta \quad (14) \]

If equation (14) is satisfied then a stable sliding motion exists on the hyperplane (9). The derivation of stability conditions in presence of structured and unstructured uncertainties can be found in [15], [3]. Here we state that a sufficient large positive scalar \( \rho_i \) exists to stabilize the system (7), (8) whose value can be tuned during experimental verification. To avoid the chattering problem due to discontinuous control the signum function in (12) is replaced by a smoothing function as in [15].

Equations (7), (8) excluding for simplification the disturbance \( d \) can be transformed with non-singular orthogonal transformation matrix \( T_c \) in the regulator canonical form

\[ \dot{\tilde{x}}_1 = A_{11}\tilde{x}_1 + A_{12}\tilde{x}_2 \quad (15) \]

\[ \dot{\tilde{x}}_2 = A_{21}\tilde{x}_1 + A_{22}\tilde{x}_2 + \tilde{B}_2 u \quad (16) \]

and correspondingly the switching function in new coordinates may be expressed as

\[ s(t) = \left[ \tilde{S}_1\tilde{x}_1 + \tilde{S}_2\tilde{x}_2 \right] \quad (17) \]

During sliding motion the switching function will be identically to zero. Thus gives

\[ \tilde{x}_2 = - (\tilde{S}_2)^{-1}\tilde{S}_1\tilde{x}_1 = -M\tilde{x}_1 \quad (18) \]

Substituting equation (18) into (15) gives the equations of motion of the system in sliding mode

\[ \dot{\tilde{x}}_1 = A_{11}\tilde{x}_1 - A_{12}M\tilde{x}_1 \quad (19) \]
\[ \ddot{x}_2 = -M \ddot{x}_1 \] (20)

The properties of the system in sliding motion can be changed by appropriate choice of \( M \). The sliding surface can be designed in different ways, for example using standard linear feedback design techniques [15], [4]. In this work with the feedback term \( M \) the poles of the closed loop were located nearly dominant poles of the system with \( H_\infty \) state feedback [5]. Then the sliding surface is transformed in the original coordinates (10). To realize the control signals according to (11) and (12) the states of the system must be known. Implementation of feedback output control on the basis of SMC theory is restricted to systems without zeros in the right plane [15]. So a state observer has to be designed. In [4] a Kalman filter as state estimator was used. However, its performance is often insufficient to prevent the observation spillover in the control system. So we looked for a more robust observer. One proposition was to use the controller/observer representation of \( H_\infty \) controller to reconstruct states of the system [5]. In \( H_\infty \) filtering in comparison with Kalman theory white noise disturbances are replaced by deterministic disturbances of finite energy that is specified with weighting functions. So the robust states reconstruction is possible.

6 Results and discussions

The experimental set-up (Fig. 5) considered in this paper consists of two flexible beams, that are joined through a pair of piezoelectric actuators with each other. The aim consists in isolating the lower beam from vibration of the upper beam.

![Figure 5: Scheme of the experimental set-up](image-url)
It is assumed that the velocity can be obtained by integration of the acceleration signal. The beams are clamped fully on their edges by a strong steel frame. The frame in turn is rigidly fixed to the foundation via four fastening angles. The active isolation system is controlled to suppress transmitted forces from the upper to the bottom beam.

In the considered system the upper beam represents a structure on which disturbance forces act. In consequence the structure connected to it (the bottom beam), on which for example may be located a sensitive equipment, will be also subjected to vibration even if some passive isolators are used. Application of active isolation system should increase quality of isolation in particular in the field of frequencies up to 500 Hz.

For testing of the hybrid control structure the system was excited with periodic and impulse signals. In Fig. 6 the results for the case of transient vibration are shown. The theoretical and experimental results have proved that hybrid control offers good possibilities for improving active control effectiveness in industrial noise and vibration control problems characterized by mixed impulsive and persistent disturbances. However piezoelectric materials are highly nonlinear. On the one hand it can lead to excitation of higher harmonics in mechanical structures, when the actuator is driven with a sinusoidal voltage. And on the other hand due to the actuator nonlinearities the transfer function of system is not unique defined. So by designing the hybrid controller a robust stability of feedback loop must be guaranteed. For this purpose the nonlinear controller - Sliding Mode Controller - was used.

Figure 6: Control performance of SMC

References


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Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

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1 Introduction

If you open any book or fundamental article on elastoplasticity [1], [2] for large strains you meet immediately Liu multiplicative decomposition for deformation gradient $F$, namely

$$ F = F_e \cdot F_p $$

This decomposition represents full deformation gradient as the product of elastic $F_e$ and plastic $F_p$ deformation gradients. So this decomposition is well known and
widespread. In motivations which lead to this decomposition authors use so called elastic and plastic displacements. But it is well known that these displacements don’t exist even in the case of small strains. Are they exist for large strains? It is the question for thinking. The second question is as follows. This decomposition is in strong contradiction to the method of rheological models which delivers thermodynamically consistent constitutive equations in every cases of application. Has Liu decomposition the same quality? I had started to discuss these contradictions with eminent German scientists: H. Lippman, E. Stein, Besdo, F. Ziegler, C. Miehe and others. Why German ones but not Russian? First reason for it was the fact that Russian scientists didn’t like to use multiplicative decomposition: they preferred to use functionals as A. Ilushin. The second reason for this was the fact that I had visited GAMM-meetings regularly. I tried to convince German scientists that multiplicative decomposition is wrong. I had bright success in discussions with H. Lippman and F. Ziegler: they agreed with me from the first discussions. But E. Stein, Besdo and C. Miehe were strongly against my position. Then E. Stein and Besdo changed their position. They started to say: may be you are right. C. Miehe continuous to be against my position up to now. I am seeing my main task in this presentation to convince the participants that classical multiplicative decomposition is wrong and that we should use multiplicative decomposition of slightly different form, namely modified form

\[ F = F_e \cdot F_p \]

It is valid for elastoplastic materials without kinematical hardening and is wrong for materials with kinematical hardening. I intend to prove that only additive decomposition for strain rate

\[ D = D_e \cdot D_p \]

is valid in any case.

\section{Denotations. Reminescenses. Conclusions.}

We use standard denotations. They are shown on the Fig 1. We see there initial and actual configurations of some material body. Initial coordinate of material particle M is denoted by \( \mathbf{R} \), while actual one by \( \mathbf{r} \). We describe motion of the particle M by the mapping

\[ \mathbf{r} = \mathbf{r}(\mathbf{R}, t) \],

where \( t \) is time. When we say deformation, we have in mind the motion (1). We introduce so called deformation gradient by the equation

\[ F = (\nabla \mathbf{r})^T \],

where \( \nabla \) is nabla operator, and \((\cdot)^T\) is the operation of transposition. Multiplicative decomposition of deformation gradient we introduce by the following equation

\[ F = F_e \cdot F_p \]
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

This formula is the main subject of our discussion. Now we recall the well known equations of mechanics of deformable body. Time-derivative of deformation gradient has following expression

$$\dot{\mathbf{F}} = (\mathbf{D} - \mathbf{\Omega}) \cdot \mathbf{F}$$

(4)

where \(\mathbf{D}\) is strain rate tensor and \(\mathbf{\Omega}\) is spin tensor. They have following expressions

$$\mathbf{D} = \left(\dot{\mathbf{F}} \cdot \mathbf{F}^{-1}\right)^{S}, \quad \mathbf{\Omega} = -\left(\dot{\mathbf{F}} \cdot \mathbf{F}^{-1}\right)^{A}$$

(5)

Cauchy-Green measure of strain has following expression [3]

$$\mathbf{C} = (\mathbf{F}^{T} \cdot \mathbf{F})$$

(6)

We present time-derivative of Cauchy-Green measure of strain

$$\dot{\mathbf{C}} = 2\mathbf{F}^{T} \cdot \mathbf{D} \cdot \mathbf{F}$$

(7)

Cauchy-Green strain is traditionally introduced by the formula

$$\varepsilon = \frac{1}{2} (\mathbf{C} - \mathbf{E})$$

(8)

where \(\mathbf{E}\) is tensoral unity At last we should note that we shall use in our considerations Cauchy stress tensor \(\tau\) and free energy of Helmholtz \(\psi\). As usually we suppose that it depends on only measure of strain \(\mathbf{C}\). So we have

$$\psi = \psi(\mathbf{C})$$

(9)

Let us introduce new qualities by will. For the description of pure elastic strains we introduce following quantities

$$\mathbf{F}_{e}, \mathbf{C}_{e} = \mathbf{F}_{e}^{T} \cdot \mathbf{F}, \varepsilon_{e} = \frac{1}{2} (\mathbf{C}_{e} - \mathbf{E})$$

(10)

We suppose that they satisfy to the equations

$$\dot{\mathbf{C}}_{e} = 2\mathbf{F}_{e}^{T} \cdot \mathbf{D}_{e} \cdot \mathbf{F}_{e},$$

(11)

where

$$\mathbf{D}_{e} = \left(\dot{\mathbf{F}}_{e} \cdot \mathbf{F}_{e}^{-1}\right)^{S}, \quad \mathbf{\Omega} = -\left(\dot{\mathbf{F}}_{e} \cdot \mathbf{F}_{e}^{-1}\right)^{A}$$

(12)

Elastic stress we denote \(\tau_{e}\), and free energy of elastic strain by \(\psi_{e}\). We have

$$\psi = \psi_{e}(\mathbf{C}_{e})$$

(13)

For the description of pure plastic strains we introduce following quantities

$$\mathbf{F}_{p}, \quad \mathbf{C}_{p} = \mathbf{F}_{p}^{T} \cdot \mathbf{F}, \varepsilon_{p} = \frac{1}{2} (\mathbf{C}_{p} - \mathbf{E})$$

(14)
We suppose that they satisfy to the equations

\[ \mathbf{D}_p = \left( \mathbf{F}_p \cdot \mathbf{F}_p^{-1} \right)^S, \quad \Omega_p = - \left( \mathbf{F}_p \cdot \mathbf{F}_p^{-1} \right)^A \]

(15)

At last we note that for description of plastic stresses we use denotation \( \tau_p \), and suppose that free energy of plasticity is equal to zero

\[ \psi_p = 0. \]

(16)

Now we present the main conclusions which we shall prove in consequence.

1. Modified Liu multiplicative decomposition (3) is not only one way in elastoplasticity for material without kinematical hardening.

2. For any elastoplastic material without kinematical hardening we can use any another decompositions of elastoplastic strain on elastic and plastic parts.

3. Theorem. Only additive decomposition of strain rate delivers thermodynamically consistent constitutive equation for elastoplastic material with kinematical hardening

3 Structure of constitutive equation of Prandtl elastoplastic material

Rheological model of this material is shown on Fig.2. It consists on two reological element: elastic and plastic. Elastic rheological element we describe by equation

\[ \tau_e = 2\rho \mathbf{F}_e \cdot \frac{\partial \psi_e}{\partial \mathbf{C}_e} \cdot \mathbf{F}_e^T, \]

(17)

where \( \rho \) is density. Rheological model of this material is shown on Fig.2. It consists on two reological element: elastic and plastic. Elastic rheological element we describe by equation

\[
\begin{cases}
N(S_p) < \tau_s, & \mathbf{D}_p^* = 0 \\
N(S_p) = \tau_s, & \mathbf{S}_p = \frac{\tau_s}{N(\mathbf{D}_p)} \mathbf{D}_p^* 
\end{cases}
\]

(18)

where \( \mathbf{S}_p \) is deviator of plastic stress, \( \tau_s \) is plastic limit, and \( N(\mathbf{S}_p) \) is the norm of \( \mathbf{S}_p \). For instance, Mises norm can be used

\[ N(\mathbf{S}_p) = \sqrt{\frac{1}{2} \mathbf{S}_p \cdot \mathbf{S}_p} \]

(19)

Equation (18) is traditional equation of rigid-plastic material which connects only deviators. So spherical part of \( \mathbf{D}_p^* \) is equal to zero. We didn’t define exactly the strain rate \( \mathbf{D}_p^* \). We will do it latter. At last we should say something about the connection of elastic and plastic elements in Prandtl model. It is the main problem
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

we should discuss. It is the problem of decomposition of strain. It will be the subject of future consideration. But something is possible to formulate now. Because elastic and plastic elements are connected in series, we can write force condition

$$\tau = \tau_e = \tau_p$$  \hspace{1cm} (20)

Now we pay attention to the thermodynamics of Prandtl material. Second law of thermodynamics for isothermal process has the form

$$\tau \cdot \cdot D - \rho \psi \geq 0$$  \hspace{1cm} (21)

We suppose that free energy of the model is the sum of free energy of elements, e.g.

$$\psi = \psi_e + \psi_p$$

But the last term here is equal to zero, so we have

$$\psi = \psi_e(C_e)$$  \hspace{1cm} (22)

Evaluating time-derivates of $\psi$, we get

$$\dot{\psi} = \frac{\partial \psi_e(C_e)}{\partial C_e} \cdot \dot{C}_e$$

Due to equation (11) it can be transformed to the form

$$\dot{\psi} = \frac{\partial \psi_e(C_e)}{\partial C_e} \cdot (2F_e^T \cdot D_e \cdot F_e) = \left( 2F_e \cdot \frac{\partial \psi_e(C_e)}{\partial C_e} \cdot F_e^T \right) \cdot \cdot D_e$$

Thus taking in account equation (17), we get following result

$$\dot{\psi} = \frac{\tau_e}{\rho} \cdot \cdot D$$  \hspace{1cm} (23)

Substitution of equation (23) in (21) renders following equation

$$\tau \cdot \cdot D - \tau_e \cdot \cdot D_e \geq 0$$  \hspace{1cm} (24)

or due to equation (20) —

$$\tau_p \cdot \cdot (D - D_e) \geq 0$$  \hspace{1cm} (25)

Now we divide plastic strain on two parts: spherical $\sigma E$ and deviatoric $S_p$.

$$\tau_p = \sigma E + S_p$$  \hspace{1cm} (26)

and substitute this result in (25). We get

$$\sigma E \cdot \cdot (D - D_e) + S_p \cdot \cdot (D - D_e) \geq 0$$  \hspace{1cm} (27)

Quantities $\sigma$ and $S_p$ are independent and can take arbitrary value. But inequality (27) should be fulfilled. Let us put $S_p = 0$. Then we get following equation from (27)

$$\sigma E \cdot \cdot (D - D_e) \geq 0$$
It is linear inequality. So we should have
\[ E \cdot (D - D_e) \geq 0 \] (28)

It means that spherical part of \((D - D_e)\) is equal to zero. As the result of (28) the inequality (27) takes the form
\[ S_p \cdot (D - D_e) \geq 0 \] (29)

Now we intend to put (29) in (18)
\[
\begin{bmatrix}
N(S_p) < \tau_s, & D_p = 0, & S_p \cdot (D - D_e) \geq 0 \\
N(S_p) = \tau_s,
\end{bmatrix}
\]
\[
\frac{\tau_s}{N(D_p^*)} D_p \cdot (D - D_e) \geq 0
\] (30)

Now we should select \(D_p^*\) in that manner, in order to satisfy (30) without any conditions. Let us introduce first proposition
\[ D_p^* = D_p \]

Then equation (30) will take the form
\[
\begin{bmatrix}
N(S_p) < \tau_s, & D_p = 0, & S_p \cdot (D - D_e) \geq 0 \\
N(S_p) = \tau_s,
\end{bmatrix}
\]
\[
\frac{\tau_s}{N(D_p^*)} D_p \cdot (D - D_e) \geq 0
\] (31)

So we didn’t get solution of thermodynamical problem. We must involve in considerations the decomposition of strain rate
\[ D = D_e + D_p \] (32)

We can easily find
\[ D - D_e = D_p \] (33)

Substitution of (33) in (31) delivers the inequalities
\[
\begin{bmatrix}
N(S_p) < \tau_s, & D_p = 0, & S_p \cdot D_p \geq 0 \\
N(S_p) = \tau_s,
\end{bmatrix}
\]
\[
\frac{\tau_s}{N(D_p^*)} D_p \cdot D_p \geq 0
\] (34)

We see that second law of thermodynamics is satisfied unconditionally! It is possible to see that second law of thermodynamics was satisfied without usage of the Liu multiplicative decomposition. May be we should refuse to apply Liu multiplicative decomposition and use only additive decomposition for strain rate (32)? We shall discuss this question in next two sections.
4 Why do the researches like to use Liu multiplicative decomposition in the theory of elastoplasticity for large strains?

a. They like to use Liu decomposition, because they believe to the Fair-tale about intermediate plastic configuration of the elastoplastic body.

Let us inspect this fair-tale. According to this Fair-tale three configurations are introduced: initial, actual and intermediate (Fig.3). We recall that we used only two configurations in section 1: initial and actual. As in section 1 we denote initial position by \( \mathbf{R} \) and actual one by \( \mathbf{r} \). We denote the position of material point \( \mathbf{M} \) in the intermediate configuration by \( \mathbf{p} \). The motion of material particle from initial configuration can be given by mapping (1)

\[
\mathbf{r} = \mathbf{r} (\mathbf{R}, t)
\]

But this motion can be considered as motion, having to stages: motion from initial configuration in intermediate one

\[
\mathbf{p} = \mathbf{p} (\mathbf{R}, t)
\]  
(35)

and then motion from intermediate configuration to actual

\[
\mathbf{r} = \mathbf{I} (\mathbf{p}, t)
\]  
(36)

The researches who use multiplicative decomposition usually call the motion (35) by pure plastic motion, while the motion (36) by pure elastic one. Substitution of equation (35) in (36) leads to the mapping

\[
\mathbf{r} = \mathbf{I} (\mathbf{p} (\mathbf{R}, t), t)
\]  
(37)

We can consider eqn (37) as complex function of \( \mathbf{R} \): \( \mathbf{p} \) depends from \( \mathbf{R} \), and \( \mathbf{I} \) depends from \( \mathbf{p} \). Applying nabla operator to (37), we get

\[
(\nabla \mathbf{r}) = (\nabla \mathbf{p}) \cdot \nabla_p (\mathbf{I}),
\]  
(38)

where \( \nabla_p \) is nabla operator with respect to coordinates \( p_1, p_2 \) and \( p_3 \). Substituting equation (38) in equation (2) we get

\[
\mathbf{F} = (\nabla \mathbf{r})^T = (\nabla_p \mathbf{I})^T \cdot (\nabla \mathbf{p})^T
\]  
(39)

Then researches usually introduce denotations

\[
(\nabla_p \mathbf{I})^T = \mathbf{F}_e, \quad (\nabla \mathbf{p})^T = \mathbf{F}_p
\]  
(40)

and get desirable result

\[
\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p
\]
They call this result as fundamental base for introduction of Liu decomposition. But can we agree with them? No! We can not consider this motivation as fundamental base for introduction multiplicative decomposition for deformation gradient! Why? *.

We don’t believe in existence of pure plastic (36) and pure elastic (37) motions. Geometrically linear theory of elastoplasticity delivers huge bright examples of nonexistence of plastic and elastic fields of displacement separately! **. We can present direct proof of nonexistence of separate motions. We know (40) and can get by transposition following formulae

\[
\nabla p I = F_e^T, \quad \nabla p = F_p^T \tag{41}
\]

Conditions of existence of motions (36) and (37) are

\[
\nabla p \times F_e^T = 0, \quad \nabla \times F_p^T = 0 \tag{42}
\]

By multiplying first equation on \(\nabla p\) we can transform it to the new form

\[
(\nabla p) \cdot (\nabla_p \times D_e^T) = \nabla \times F_e^T = 0
\]

So the conditions (42) take the form

\[
\nabla \times F_e^T = 0, \quad \nabla \times F_p^T = 0, \tag{43}
\]

We can’t find anywhere the proof of satisfaction of these equations! Our main statement is : we can’t accept decomposition (2)

\[
F = F_e \cdot F_p
\]

But without any consciousness we can accept multiplicative decompositions of another sort

\[
F = F_e \cdot F_{lp} \tag{44}
\]

\[
F = F_{pe} \cdot F_e \tag{45}
\]

In comparison with equation (2) we use here not \(F_p\) but \(F_{lp}\) - gradient of elastoplastic motion or \(F_{pe}\) gradient of plasto-elastic motion. These gradients can be calculated from (44), (45) by equations.

b. The researchers like to use Liu multiplicative decomposition because it is easy to compute difference \(D - D_e\), which we meet in thermodynamics condition (3) .

\[
F_{lp} = F_e^{-1} \cdot F, \quad F_{pe} = F \cdot F_e^{-1}
\]

We shall use decomposition (44) and will have

\[
F = F_e \cdot F_{lp}, \quad F^{-1} = F_{lp}^{-1} \cdot F_e^{-1} \tag{46}
\]

Differentiation of first equation gives the result

\[
\dot{F} = \dot{F}_e \cdot F_{lp} + F_e \cdot \dot{F}_{lp}
\]
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

Multiplying the both sides of last equation on $\mathbf{F}^{-1}$ we get

$$
\dot{\mathbf{F}} \cdot \mathbf{F}^{-1} = \dot{\mathbf{F}}_e \cdot \mathbf{F}_{lp} \cdot \mathbf{F}^{-1}_{ep} \cdot \mathbf{F}_e^{-1} + \mathbf{F}_e \cdot \dot{\mathbf{F}}_{ep} \cdot \mathbf{F}^{-1}_{ep} \cdot \mathbf{F}_e^{-1}
$$

or

$$
\mathbf{D} + \Omega = \mathbf{D}_e + \Omega_e + \mathbf{\tilde{D}}_p + \mathbf{\tilde{\Omega}}_p
$$

(47)

where we have denoted

$$
\mathbf{\tilde{D}}_p = \left( \mathbf{F}_e \cdot \dot{\mathbf{F}}_{ep} \cdot \mathbf{F}^{-1}_{ep} \cdot \mathbf{F}_e^{-1} \right)^S
$$

$$
\mathbf{\tilde{\Omega}}_p = \left( \mathbf{F}_e \cdot \dot{\mathbf{F}}_{ep} \cdot \mathbf{F}^{-1}_{ep} \cdot \mathbf{F}_e^{-1} \right)^A
$$

Following significant equations we can get from equation (47)

$$
\mathbf{D} - \mathbf{D}_e = \mathbf{\tilde{D}}_p
$$

(48)

$$
\Omega - \Omega_e = \mathbf{\tilde{\Omega}}_p
$$

(49)

c. Researchers like to use Liu decomposition, because it is easy to satisfy the thermodynamical inequality (30) Indeed if we use second proposition

$$
\mathbf{D}_p^* = \mathbf{\tilde{D}}_p
$$

(50)

and put this result in equation (30) and take in account (48) we get

$$
\begin{cases}
\mathbf{N} (\mathbf{S}_p) < \tau_s, & \mathbf{\tilde{D}}_p = 0, \quad \mathbf{S}_p \cdot \mathbf{\tilde{D}}_p \geq 0 \\
\mathbf{N} (\mathbf{S}_p) = \tau_s, & \frac{\tau_s}{\mathbf{N} (\mathbf{D}_p)} \mathbf{\tilde{D}}_p \cdot \mathbf{\tilde{D}}_p \geq 0
\end{cases}
$$

(51)

This equation is satisfied unconditionally! Our main statement is as follows. Theory of plastic intermediate configuration is not fundamental base for introduction of the most popular multiplicative decomposition.

$$
\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p
$$

So it don’t exist! But instead of this decomposition we can use another decomposition

$$
\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_{ep}
$$

(52)

We should consider this decomposition as an invention of mind. So this decomposition has equal rights with another decompositions invented by another minds. One of these decompositions - namely (32) was presented above. The question arises: may be we can invent another decompositions in addition to presented two. The answer is positive. Next section is devoted to this problem.
5 New reasoning. What is the result of new reasoning?

Let us return to the equation (48) and let us write it inverse form

$$D^* = \tilde{D}_p = D - D_e$$

Then the equations of plasticity (18) will take the form

$$\begin{cases} N\left(S_p\right) < \tau_s, & D - D_e = 0 \\ N\left(S_p\right) = \tau_s, & S_p = \frac{\tau_s}{N\left[D - D_e\right] (D - D_e)} \end{cases}$$

and we will have thermodynamical restrictions in following form

$$\begin{cases} N\left(S_p\right) < \tau_s, & D - D_e = 0, \ S_p \cdot (D - D_e) \geq 0 \\ N\left(S_p\right) = \tau_s, & \frac{\tau_s}{N\left[D - D_e\right] (D - D_e) \cdot (D - D_e)} \geq 0 \end{cases}$$

We see that they are satisfied! This is the general solution of thermodynamics problem for Prandtl material with arbitrary decomposition. Indeed, we can consider different decompositions of strain and for any of them we can evaluate the difference $D - D_e$. For instance, we have

- $D - D_e = D_p$ for additive decomposition $D = D_e + D_p$
- $D - D_e = \tilde{D}_p$ for multiplicative decomposition $F = F_e \cdot F_{ep}$
- $D - D_e = D_0^p$ for multiplicative decomposition $F = F_{pe} \cdot F_e$

We can continue our evaluations for new and new decompositions

- $D - D_e = D_{oo}^p$ for ...
- $D - D_e = D_{poo}^p$ for ...

And so on, and so on.

Then we can accept

- $D^* = D_p$ for decomposition $D = D_e + D_p$
- $D^* = \tilde{D}_p$ for decomposition $F = F_e \cdot F_{ep}$
- $D^* = D_0^p$ for decomposition $F = F_{pe} \cdot F_e$
- $D^* = D_{oo}^p$

And so on. In any case we have unique result

$$D^* = D - D_e$$

If we put equation (56) in (18) we get unique equation (54) of plasticity for any decomposition. If we put equation (54) in thermodynamical inequality (29), we get equation (30). Again we see that the second law of thermodynamics is satisfied.
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

But it is not the main result of new reasoning! Playing the words, we changed the constitutive equation of plasticity! New equation has the form of equation (54)

\[
\begin{bmatrix}
N(S) < \tau_s, & D - D_e = 0 \\
N(S) = \tau_s, & S_p = \frac{\tau_s}{N(D - D_e)}(D - D_e)
\end{bmatrix}
\]

(57)

We should add standard equation of elasticity (17)

\[
\tau_e = 2\rho F_e \cdot \frac{\partial \psi_e(C_e)}{\partial C_e} \cdot F_e^T
\]

(58)

Writing (57) and (58) we took in account force condition (20). It is the system of equations for calculation only kinematical parameters of elasticity: \(F_e, C_e, D_e\). It don’t contents parameters of plasticity \(F_p, C_p, D_p\). It is applicable for any decompositions of strain, because it don’t depend from decomposition of strain at all. We got two significant results:

1. Liu multiplicative decomposition of strain gradient is not only one way in elastoplasticity.

Now we present example of possible decompositions of strain in elastoplasticity

\[
D = D_e + D_p
\]

(59)

\[
F = F_e \cdot F_{ep}
\]

\[
F = F_{pe} \cdot F_e
\]

(60)

\[
\varepsilon = \varepsilon_e + \varepsilon_p
\]

\\

If you use Liu decomposition, with the same success you can use any another decomposition of elastoplastic strain on two parts: elastic and plastic, or elastic and elastoplastic.

2. We can use equation of decomposition for calculating parameters of plasticity \(F_p, C_p, D_p\). We get different result for different decompositions. We see that plastic strain depends from our will. It is very dangerous situation. We should make so called regularization.

All these statements are valid only for elastoplastic material without kinematical hardening. Next section is devoted to the elastoplastic material with kinematical hardening. We think that it is the way to make above mentioned regularization.

\section{Structure of constitutive equation of Prandtl material with kinematical hardening}

Rheological model of this material is shown on Fig. 4. As on Fig.2 we have again elastic element and plastic one. But in parallel to plastic element we have second
elastic element which describes so called kinematical hardening. We describe this element by additional equation of elasticity similar to (17)

\[ \tau_h = 2\rho F_p \cdot \frac{\partial \psi_h (C_p)}{\partial C_p} \cdot F_p^T \]  

(61)

Remaining element we describe as before: elastic one - by equation (17), and plastic one by equation (54). Force condition of connection of elements are as follows

\[ \tau = \tau_e = \tau_p + \tau_h \]  

(62)

We suppose that free energy of material is equal to the sum of free energies of elements, e.g.

\[ \psi = \psi_e (C_e) + \psi_h (C_p) \]  

(63)

It is possible to generalize equation (63) and use more general equation

\[ \psi = \psi (C_e, C_p) \]  

(64)

We should add to the system of equations (61), (62), (17) and (54) additional one, which describes decomposition of strain on two parts elastic and plastic. This last equation should connect \( F_e \) a \( F_p \) and \( F \). What decomposition should be selected? We intend to solve this last problem with the help of second law of thermodynamics.

### 7 Thermodynamical analysis of Prandtl material with kinematical hardening

The second law of thermodynamics for isotermic processes has the form of equation (21)

\[ \tau \cdot \dot{D} - \rho \dot{\psi} \geq 0 \]

But now we have more complex free energy. It is given by equations (63) or (64). Differentiation of (63) gives following result

\[ \dot{\psi} = \frac{\partial \psi_e (C_e)}{\partial C_e} \cdot \dot{C}_e + \frac{\partial \psi_h (C_p)}{\partial C_p} \cdot \dot{C}_p \]  

(65)

Now we use equation (7) for \( \dot{C}_e \) and \( \dot{C}_p \)

\[ \dot{C}_e = 2F_e^T \cdot D_e \cdot F_e \]  

(66)

\[ \dot{C}_p = 2F_p^T \cdot D_p \cdot F_p \]  

(67)

Substituting these expressions in equation (65) and rearranging result we get

\[ \dot{\psi} = \frac{1}{\rho} (\tau_e \cdot \dot{D}_e + \tau_h \cdot \dot{D}_p) \]
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?

At last we substitute this result in (21) and get following equation

\[ \tau \cdot D - \tau_e \cdot D_e + \tau_h \cdot D_p \geq 0 \]  

(68)

At last we rearrange equation (68) with the help of force condition (62) to the following form

\[ \tau_p \cdot (D - D_e) + \tau_h \cdot (D - D_e - D_p) \geq 0 \]  

(69)

This inequality is very convenient for extracting significant conclusions. Left hand side of this inequality is linear function of stress of hardening \( \tau_h \). Tensor \( \tau_h \) depends on only plastic strain \( C_p \). Another values of (69) e.g. \( \tau_p \cdot (D - D_e) \) and \( (D - D_e - D_p) \) depend only on strain rates. These strain rates \( D, D_e \) and \( D_p \) can have values, which are independent from \( C_p \) and \( \tau_h \). We can say in another manner: \( \tau_h \) can take values, which are independent from another members of equation (69).

We see that left hand side of equation (69) is linear function of \( \tau_h \). So according to the well-known theorem about linear inequalities [4] the necessary and sufficient condition for satisfaction inequality (69) are as follows

\[ D - D_e - D_p = 0 \]  

(70)

\[ \tau_p \cdot (D - D_e) \geq 0 \]  

(71)

First equation (70) represents the well-known additive decomposition (32)

\[ D = D_e + D_p \]

Due to plastic incompressibility (28) eqn (71) can be transformed to the form (29). After substituting there eqn (54) we get eqn (55). Latter is satisfied without any conditions. The main result of previous reasoning can be formulated by the theorem.

**Theorem 1.** Only additive decomposition of strain rate (32) delivers thermodynamically consistent constitutive equation for Prandtl elastoplastic material with kinematical hardening.

This theorem gives us the desired determinacy in calculation of plastic strain. Now we write down constitutive equation of Prandtl elastoplastic material with kinematical hardening. This system of equations consists of equation of elasticity

\[ \tau = 2 \rho F_e \cdot \frac{\partial \psi_e}{\partial C_e} \cdot F_e^T, \]  

(72)

equation of plasticity

\[
\begin{bmatrix}
N(S_p) < \tau_s, \quad D_p = 0 \\
N(S_p) = \tau_s, \quad S_p = \frac{\tau_s}{N(D_p)} D_p
\end{bmatrix}
\]  

(73)

force condition

\[ \tau = \tau_p + \tau_h \]  

(74)
equation of hardening

\[ \tau_h = 2\rho \mathbf{F}_p \cdot \frac{\partial \psi_p (C_p)}{\partial C_p} \cdot \mathbf{F}_p^T, \quad (75) \]

and at last - decomposition for strain rate

\[ \mathbf{D} = \mathbf{D}_e + \mathbf{D}_p \quad (76) \]

The system (72)-(76) delivers unique measure of plastic strain

\[ C_p = \mathbf{F}_p^T \cdot \mathbf{F}_p \quad (77) \]

So we had avoided indeterminacy in calculating plastic strain.

8 Conclusions

1. The theory of plastic intermediate configuration is not fundamental base for introduction of the most popular multiplicative decomposition (Liu decomposition).

\[ \mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p \]

2. Modified Liu decomposition

\[ \mathbf{F} = \mathbf{F} \cdot \mathbf{F}_{ep} \]

is acceptable, but is not only one way in elastoplasticity for materials without kinematical hardening. It is possible to use any another decomposition.

3. Only additive decomposition of strain rate (76) delivers thermodynamically consistent constitutive equation for elastoplastic Prandtl material with kinematical hardening.

![Diagram](image-url)
Is the multiplicative decomposition of deformation gradient the only one way in elastoplasticity for large strains?
References


On influence of non-linear damping on whirling of a rigid rotor with four degrees of freedom

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Abstract

The cylindrical precession of a rigid unbalanced rotor in non-linear elastic bearings with non-linear external friction is investigated. It is assumed that the rotor has four degrees of freedom. It is shown that the limit value of the precession amplitude depends on the external friction coefficient and self-centering of the rotor does not occur. It is established, using the elementary catastrophe theory, that the loss of stability of cylindrical precession on passing through a zero root can be accompanied by excitation of a hyperboloidal precession. The boundary for the onset of self-excited oscillation is obtained and it is shown by means of numerical modelling that supercritical Hopf bifurcation and a strange attractor can occur.

1 Introduction

Analysis of influence of non-linear external friction on free oscillations of the linear system with one degree of freedom was carried out in [1]. It was established in case of square law that a logarithmic decrement decreases with the amplitude decay. Mutual action of linear internal friction and non-linear external friction on a Jeffcott rotor with two degrees of freedom was studied in [2]. It was observed that self-centering of the rotor does not occur and square non-linear external friction produces a certain balancing effect. In this paper, using methods and results of [4] the precessional motion of a rigid statically unbalanced rotor mounted in non-linear elastic bearings with non-linearity of Duffing’s type has been studied. Linear internal friction and square external friction are taken into account.

2 Equations of motion and direct synchronous precessions

We consider a dynamically symmetrical rigid rotor of mass $M$, length $L_r$ and moments of inertia $J_p$ (axial) and $J_t$ (equatorial). The rotor is supported vertically in
two immovable non-linearly elastic with bearing-spacing equal to \( L \). The distance apart the center of mass and the \( j \)-th end of the axis of the rotor (of the pivot) is equal to \( e_j L \), so that \( e_1 + e_2 = 1 \). The quantity \( e_j \) can be negative, if the center of mass is on the outside of \( j \)-th bearing. The rotor is statically unbalanced with the static eccentricity equal to \( e \). We assume that the spin speed \( \Omega \) is constant. By neglecting the displacement of the rotor along the axis of rotation, it can be treated as a mechanical system with four degrees of freedom. The Cartesian coordinates \( u_j, v_j (j = 1, 2) \) of the rotation axis’ point in a plane which is perpendicular to the axes of the bearings are selected as the generalized coordinates. The elastic bearings are assumed to possess central symmetry. In this case, the reaction of a bearing only has a radial component, which is equal to \( F_{j} = -F_{j}(|S_{j}|)u_{j} \). Here, \( S_{j} = u_{j} + v_{j} \) is the displacement from the equilibrium position (in complex form) and \( n_{j} \) is a unit vector in the direction of \( S_{j} \). We consider the non-linearity of the Duffing’s type, i.e. \( F_{j} = -(a_{0}^{(j)} + a_{1}^{(j)}|S_{j}|^{2})S_{j} \) \((j = 1, 2)\). Coefficients \( a_{0}, a_{1} \) characterize elastic properties of the bearings. The non-linear forces of external friction are proportional to the square of the absolute rotation rate \( R_{j}^{(e)} = -\mu_e |S_{j}| S_{j} \). The forces due to internal friction, which are proportional to the relative velocity \( R_{j}^{(i)} = -\mu_i (\dot{S}_{j} - i\Omega S_{j}) \) are taken into account [3].

The equations of motion of the rotor can be obtained using theorems on the motion of the center of mass and the change in the angular momentum with respect to the center of mass. We now introduce a characteristic angular velocity \( \omega_0 \), the choice of which depends on the function \( F_{j} \). After changing to the dimensionless variables \( s_{j} = S_{j}/e \), \( \tau = \omega_{0} t \) and dimensionless angular velocity \( \Omega = \Omega/\omega_{0} \), the equations of motion take the form

\[
\sum_{j=1,2}(e_{3-j}\dot{s}_{j} + \mu_{e}|s_{j}|\dot{s}_{j} + \mu_{i}(s_{j} - i\Omega s_{j}) + \nu_{j}(1 + c_{j}|s_{j}|^{2})s_{j}) = \Omega^{2}\exp(i\Omega\tau),
\]

\[
\sum_{j=1,2}(-1)^{j}[\dot{s}_{j} - i\Omega\lambda\dot{s}_{j} + kle_{j}|s_{j}|\dot{s}_{j} + \mu_{i}(\dot{s}_{j} - i\Omega s_{j}) + \nu_{j}(1 + c_{j}|s_{j}|^{2})s_{j}] = 0.
\]

Differentiation is carried out with respect to the dimensionless time \( \tau \). The parameters have the following meaning

\[
k = \frac{M L^{2}}{(J_{t} - J_{b})}, \quad \lambda = \frac{J_{b}}{J_{t}}, \quad \nu_{j} = \frac{a_{0}^{(j)}}{a_{0}^{(T)}}, \quad \mu_{e} = \frac{\tilde{\mu}_{e}}{M}, \quad \mu_{i} = \frac{\tilde{\mu}_{i}}{M \omega_{0}}.
\]

In the case of a dynamically prolate body \((\lambda < 1)\), the parameter \( k > 0 \), and in the case of a dynamically oblate body \((\lambda > 1)\), we have \( k < 0 \).

System (1) admits of a solution of the form (see [4])

\[
s_{j} = R_{j}\exp(i\psi_{j})\exp(i\Omega\tau), \quad j = 1, 2
\]

where \( R_{j}, \psi_{j} \) are real constants and \( R_{j} > 0 \). The solution (3) represents a direct synchronous circle precession or in other words, a circle forward whirling motion. This precession can be cylindrical, conic or hyperboloidal according to the surface
traced by rotation axis in 3D space. If \( \psi_1 = \psi_2 \) and \( R_1 = R_2 \), then (3) represents a cylindrical precession. If \( \psi_1 = \psi_2 \) or \( \psi_1 = \psi_2 + \pi \) for \( \forall R_1, R_2 \), it is a conic precession and if \( \psi_1 \neq \psi_2 \) for \( \forall R_1, R_2 \), it is a hyperboloidal one.

Substituting solution (3) into system (1) we obtain a linear inhomogeneous system of algebraic equations in the quantities \( \exp(i \psi_j) (j = 1, 2) \) and, solving this system, we obtain

\[
\exp(i \psi_j) = \frac{X(2B_{3-j} + i k \mu_e X \sqrt{Y_j})}{2 \sqrt{Y_j} \Delta_{\text{res}}}. 
\]

Here \( X = \Omega^2, Y_j = R_j^2, \Delta_{\text{res}} = 2 \Delta - 2 k \mu_e^2 X^2 \sqrt{Y_1 Y_2} + i \mu_e \sqrt{X} \sum_{j=1,2} (k A_{3-j} + 2 B_{3-j}) \), \( \Delta = A_1 B_2 + A_2 B_1, \quad A_j = 1 + c_1 Y_j - \frac{X}{2}, \quad B_j = \frac{k}{2} (1 + c_1 Y_j) - X \).

The set \( \Delta = 0 \) defines the set of non-linear resonances in the space \( \{X, Y_1, Y_2\} \) (see [4]). It will be shown that instability in the cylindrical precession arises close to this set.

The property \( |\exp(i \psi_j)| = 1 \) enables us to exclude the quantities \( \psi_j \) and obtain the system with respect to \( Y_j \) and it is then also possible to find the phases \( \psi_j \). We note that all of the quantities \( \exp(i \psi_j), \Delta \) and \( \Delta_{\text{res}} \) are independent of the internal friction coefficient \( \mu_i \).

Let us suppose that the bearings are identical, i.e. \( c_1 = c_2 = c \). Then among the solutions (3), it is possible to pick out the solutions \( s_1 = s_2 \) corresponding to a cylindrical precession. But, among the solutions (3), there are also some such that \( s_1 \neq s_2 \). Henceforth, we shall study cylindrical direct synchronous precession (CyP).

### 3 Bifurcation of a cylindrical precession

We consider \( \psi_1 = \psi_2 = \psi \) and \( Y_1 = Y_2 = Y \). The set of non-linear resonances degenerates into \( AB = 0 \) with \( A = 1 + c Y - X/2, \quad B = k (1 + c Y^2)/2 - X \) and is represented by the two straight lines. By using the property \( |\exp(i \psi)| = 1 \), we obtain from formula (4) the amplitude-frequency and phase-frequency characteristics in the form

\[
\sqrt{Y(A^2 + \mu_e^2 X^2 Y)} - \frac{X}{2} = 0, \quad \tan(\psi) = -\frac{\mu_e X \sqrt{Y}}{A}.
\]

The limit value \( Y_\infty = \lim_{X \to \infty} Y \) can be determined as the positive root of the equation \( 4 \mu_e^2 Y_\infty^2 + Y_\infty - 1 = 0 \) and written as

\[
Y_\infty = \frac{1}{8} \left( -1 + \sqrt{1 + 16 \mu_e^2} \right) \frac{1}{\mu_e^2}.
\]

It depends on the external friction coefficient \( \mu_e \) and tends to zero with \( \mu_e \to \infty \), which means that self-centering of the rotor does not occur as in case of the rotor with 2 d.o.f. (see in accordance). Influence of quadratic external friction results in certain balancing effect.
We can see that the point of intersection of the amplitude-frequency characteristic (AFC) and non-linear resonance $A = 0$ is determined by coordinates

$$X_\ast = \frac{2 \mu_e + c}{\mu_e}, \quad Y_\ast = \frac{1}{2} \mu_e. \quad (7)$$

In case of linear external friction the similar point has coordinates (see [5])

$$X_{\ast{\text{lin}}} = \frac{4 \mu_e^2}{2 \mu_e^2 - c}, \quad Y_{\ast{\text{lin}}} = \frac{1}{2} \mu_e^2 - c. \quad (8)$$

These results are in accordance with the conclusions by [1].

In Figure 1a there are AFC for a dynamically prolate rotor ($\lambda < 1, k > 0$) and the following values for parameters $\lambda = 0.7, k = 2.4, c = 0.0625$. In Figure 1b the AFC is shown for the same values of the constructive parameters and $\mu = 0.02$.

To solve a stability problem we apply standard linear analysis. In linear approximation the system (1) of the eights order splits up into two independent sub-systems of the fourth order. Therefore, the characteristic polynomial of the eights order also splits up into two polynomials of the fourth order. The coefficients of the characteristic polynomial $P_2$ for the second equation of the system (1) have the form

$$b_0 = 1, \quad b_1 = \frac{1}{2} k l (3 \mu_e \sqrt{XY} + 2 \mu_i),$$

$$b_2 = lB + lD + (1 + l)^2 X + \frac{1}{4} k^2 l^2 (\mu_i^2 + 3 \mu_i \mu_e \sqrt{XY} + 2 \mu_e^2 X Y),$$

$$b_3 = \frac{1}{2} kl(3(1 + l) \mu_e X \sqrt{XY} + lD(2 \mu_e \sqrt{XY} + \mu_i) + lB(\mu_e \sqrt{XY} + \mu_i)), $$

$$b_4 = \frac{1}{2} l^2(2BD + k^2 \mu_e^2 X^2 Y), \quad D = \frac{k}{2} (1 + 3 c Y) - X. \quad (9)$$

The coefficients $a_0, a_1, ..., a_4$ of the polynomial $P_1$ for the first equation are determined using the corresponding formulae (9) when $k = 4, l = 1$.

The conditions for a transition through zero roots

$$a_4 = 0 \quad \text{or} \quad \left(1 + c Y - \frac{X}{2}\right) \left(1 + 3 c Y - \frac{X}{2}\right) + 2 \mu_e^2 X^2 Y = 0,$$

$$b_4 = 0 \quad \text{or} \quad \left(\frac{k}{2}(1 + c Y) - X\right) \left(\frac{k}{2}(1 + 3 c Y) - X\right) + \frac{k^2}{2} \mu_e^2 X^2 Y = 0 \quad (10)$$
are independent on the internal friction coefficient \( \mu_c \) as is also the AFC (5). It can be seen from conditions (10) that instability occurs close to the non-linear resonances \( A = 0 \) and \( B = 0 \). The curves \( a_4 = 0 \) and \( b_4 = 0 \) are shown in the Figure 1b with thin lines as the unstable parts of the AFC.

When the internal friction coefficient \( \mu_i \) is fairly large, the quantities \( a_3 \) and \( b_3 \) can become negative for fairly large values of \( X \) and bounded values of \( Y \). Moreover, when \( a_4 > 0 \) and \( b_4 > 0 \), the inequalities \( a_3 < 0 \), \( b_3 < 0 \) imply the the inequalities \( \Delta_3(P_1) < 0 \), \( \Delta_3(P_2) < 0 \), that is, at the high angular velocity the CyP of the rotor becomes unstable. For the chosen parameter \( \lambda = 0.7 \) the inequalities \( b_3 > 0 \), \( \Delta_3(P_2) > 0 \) hold for all \( X \) and the boundary of the transition through pure imaginary roots has the form \( \Delta_3(P_1) = 0 \). The expression of \( \Delta_3(P_1) \) is ponderous, but it can be obtained easily using mathematical packages. The curve \( \Delta_3(P_2) = 0 \) is also shown in Figure 1b.

**Bifurcation of a CyP on passing through a zero root.** System (1) will be autonomous in a rotating system of coordinates, and the elementary catastrophe theory can be used to study the behavior of the system in the segment \( \{a_4 \leq 0\} \cup \{b_4 \leq 0\} \) (see [6]). The curves \( a_4 = 0 \) and \( b_4 = 0 \) in the \( \{X,Y\}\)-plane form a bifurcation set, and points I – IV of the intersection of the curves and AFC are degenerate critical points. A change in a parameter causes a qualitative change in the behavior of the system in the neighborhood of a degenerate critical point.

It is easy to follow how the loss of stability of a CyP occurs over the range of frequencies from point I to point IV. When the frequency increases, the degenerate point I splits into three non-degenerate points, the CyP becomes unstable and two stable states of direct synchronous precession appear. These precessions are no longer cylindrical but hyperboloidal. In case of a fixed frequency the radii of the pivots can be found by solving system \( |\exp(i\psi_1)| = 1 \), \( |\exp(i\psi_2)| = 1 \). Then, it can be verified that \( \tan(\psi_1 - \psi_2) \neq 0 \), that is, the phases are not identical and do not differ by \( \pi \). When the frequency increases further and on passing through the critical point II, it, in turn, also splits into three non-degenerate points. The number of different cylindrical precessions increases up to three, two of them are unstable, and one with the minimum amplitude is asymptotically stable. Finally, on passing through the point IV, the number of non-degenerate points falls to two. There is a single cylindrical precession process and it is asymptotically stable. The rest direct synchronous precessions are hyperboloidal.

**Hopf bifurcation. Limit cycles and strange attractors.** The equation \( \Delta_3(P_1) = 0 \) also defines a bifurcation set in the \( \{X,Y\}\)-plane. At the point \( V \) of intersection of this curve and the AFC, the characteristic polynomial \( P_1 = 0 \) has a single pair of pure imaginary roots. Numerical integration of the system (5) shows that in the case of structural parameters (see p. 508) the bifurcation is of the "soft" type, that is, the loss of stability is accompanied by the evolution of a stable limit cycle (see [7]). In other words, in this case there is a supercritical Hopf bifurcation (see [6]).

For the chosen structural parameters and \( \mu_e = 0.02 \), \( v\mu_e = 0.2 \) the coordinates of the point \( V \) are \( X_V = 6.582 \), \( Y_V = 2.333 \). The limit cycle in the \( \{R_1, \tilde{R}_1\}\)-plane of the phase space \( \{R_1, \tilde{R}_1, R_2, \tilde{R}_2, \psi_1 - \tilde{\psi}_2, \psi_1 - \tilde{\psi}_2\} \) is shown in Figure 2a for the value \( X = 9.5 \) (\( \Omega = 3.08 \)). The initial position of the axis of rotation is parallel with the bearings line.
This graph corresponds to 300 revolutions of the rotor after 100 revolutions. The periodic motion, which is parameterized by this limit cycle, is a CyP, since at the same time $\psi_1 - \psi_2 = 0$. The limit cycle for the second pivot (in the $\{R_1, \dot{R}_1\}$-plane) has the same form.

The frequency response of this periodic motion is shown in the Figure 2b. To obtain the frequency response we take the total time period $T = 100T_{\text{rot}}$, where $T_{\text{rot}} = 2\pi/\Omega = 198.69$. Number of samples is equal to $n = 3200$. So interval between samples $\Delta \tau = T/n = 0.0621$ and sample rate $f_s = 1/\Delta \tau = 16.105$. Dimensionless circular frequency, corresponding to $N$-th harmonic, can be calculated as $\omega_N = N\Omega/100$. We can see that the resonance harmonics have numbers 43, 86 and 128, which is typical for periodic motion. Therefore, the frequency spectrum will be $\{1.36; 2.72; 4.05\}$. The period of autovibration is approximately determined as $T_a = 2\pi/\omega_{\text{min}} = 4.62$, that is, The period of autovibration is almost two times greater than the period of rotation ($T_a/T_{\text{rot}} = 2.325$).

Strange attractor. Numerical integration of system (1) was carried out over the range of frequencies $X \in [7, 20] (\Omega \in [2.65, 4.47])$ which showed, that stable self-excited oscillations exist for all frequencies from this range but, for certain frequency values, their attraction domain is extremely restricted. For instance, in the range $X \in (7.5, 12) (\Omega \in (2.74, 3.46))$ the self-excited oscillations became sensitive to a change in the initial data and, together with stable limit cycle, the existence of other attractors was revealed.

The numerical experiment showed that, for the frequencies in the range $X \in (7.5, 12)$ a further $2T_a$-periodic limit cycle exists which parameterizes a hyperboloidal precession of complex structure. A typical implementation of the process $R_1(\tau)$ looks as follows. In the initial stage (apart from the very first revolutions) the trajectory in the $\{R_1, \dot{R}_1\}$-plane is close to a $T_a$-periodic limit cycle. A doubling of the period then occurs and the trajectory splits into two branches (one within the limit cycle and the other outside it). Then the motion "slides down" unto chaotic motion (a "strange attractor" is observed) after which synchronization occurs and a $2T_a$-periodic limit cycle is established. A strange attractor in the $\{R_1, R_2\}$-plane ($\tau = 0 [\mod (2\pi/\Omega)]$) for $X = 9.5$ and initial values $R_1 = 1.5, R_2 = 1.0, \psi_1 = 0.2$ (the rest values are equal to zero) is shown in Figure 3a. Synchronization is distinctly visible, that is, the existence of a two-loop limit cycle.
On influence of non-linear damping on whirling of a rigid rotor with four degrees of freedom

The phase trajectory in the \( \{ R_1, \dot{R}_1 \} \)-plane for different periods of time is shown in Figure 3b, c. The initial stage, corresponding to the time interval of 40 to 100 revolutions of rotor, is presented in Figure 3b with one-loop limit cycle. The stage of a chaotic motion, corresponding to the time interval of 100 to 200 revolutions of rotor is presented in Figure 3c. And finally, the two-loop limit cycle, corresponding to the time interval of 500 to 700 revolutions of rotor, is shown in Figure 3b.

References


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Mechanics of the equal channel angular extrusion

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Abstract

The mechanics of equal channel angular extrusion (ECAE) of rigid perfectly plastic material was investigated by upper bound theory and finite element method. The obtained dependencies of punch pressure, total shear from die angle and frictional conditions were compared with results of Segal’s slip line analysis. The good agreement was found. All analyses show that an increase in friction leads to a relative increase of punch pressure, decrease of total shear and deformation inhomogeneity. Increase in die angle results to the decrease of both punch pressure and total shear. The deformation inhomogeneity also becomes more pronounced. The combination of upper bound and FEM analyses is recommended for the further investigation of ECAE mechanics.

1 Introduction

In recent years, significant progress has been made in many fields of modern technique related to the production of ultra fine grained and nanostructured materials. A wide range of technologies for manufacturing of materials with submicrometer grain size have been developed. For the production of bulk parts with ultra fine or nanosize structure the severe plastic deformation (SPD) is usually applied. Among the several SPD methods the equal channel angular extrusion (ECAE) is the most widely used for grain refinement. This method was proposed by V. M. Segal research group in the early 80’s [1]. The general concept lies in the deformation of a billet in a die with two equal channels intersecting at an angle $2\theta$ (Fig. 1a). A very large resulting shear deformation of the billet can be obtained by using several consecutive extrusion passes.

Recently ECAE was intensively studied mostly in respect to structure characterization of obtained products. The ECAE mechanics was also investigated. V. M. Segal obtained the relationships for calculation of ECAP pressure and resulting shear
Figure 1: ECAE setup (a) and slip line field (b) proposed by V. M. Segal [2]-[3]: 1, 4 - intersecting channels; 2 - punch; 3 - sample.

strain by the slip line theory [2]-[3]. B. S. Altan et al. [4] used for this aim the upper bound analysis and continuous velocity field. A. Laptev and co-workers applied within the upper bound approach a discontinuous velocity field for a right-angled die, when \(2\theta = 90^\circ\) [5]. S. Li et al. simulated metal flow at ECAP by the finite element method [6]. J. Alkorta and co-workers compared the results obtained by the upper bound theory and the finite element simulation [7].

The goal of the present work is the generalization of our previous upper bound solution [5] for the ECAE die with an obtuse angle i.e. \(2\theta > 90^\circ\) and verification of obtained results by finite element analysis. The plane strain state and 2D geometry was discussed. The rigid-perfectly plastic behavior of the extruded material was assumed. The Tresca friction law was used by Segal’s slip line solution and present upper bound analyses. The Coulomb friction law was applied in finite element calculations because Tresca law is not incorporated into the herein used commercial FE software.

2 Segal’s slip line analysis

The slip line field proposed by V. M. Segal is presented in Fig. 1b [2]-[3]. The appearance of a dead zone is assumed. The slip line analysis gives the formula for relative punch pressure in the form [2]

\[
\frac{p}{2k} = \left[ \cot \eta + 2(\eta - \theta) \right] + m/[(\sin(\eta) \cdot (\sin \eta + \cos \eta))],
\]

where \(p\) is a punch pressure; the plasticity constant \(k\) is a yield shear stress of extruded material and for a 2D problem \(k = \sigma_S/\sqrt{3}\);

\[
\eta = (\pi/2) - (1/2) \cdot \arccos(2m);
\]

\(m \in [0, 0.5]\) is a friction factor in Tresca law expressed by equation

\[
\tau_F = 2mk;
\]
\( \tau_g \) is a friction stress.

ECAE is a technique used for the grains refinement. Therefore the estimation of the resulting plastic deformation is of great importance. Corresponding to the V. M. Segal solution the total shear is the sum of the shears on the lines OA and OB and the shear appearing by passing through the sector AOB. The summary shear is [3]

\[ \gamma = 2 \cdot \cot \eta + 2 \cdot (\eta - \theta). \quad (4) \]

### 3 Upper bound analysis

According to the upper bound approach we have to introduce a trial velocity field which can be continuous, discontinuous or mixed. In the present work the discontinuous velocity field was used. The plastic region was divided into 4 rigid triangular sections as shown in Fig. 2a. The appearance of a dead zone numbered by 4 was also assumed. The length \( h \) characterizes the dead zone dimension. The friction only along the segments AG and BF was taken into account. Corresponding hodograph is shown in Fig. 2b. The influence of a back pressure was not discussed in this study.

![Figure 2: Triangular rigid sections (a) and velocity hodograph (b) used in upper bound analysis](image)

The balance of external and internal power at plastic deformation was expressed by equation

\[ p a V_1 = k (l_{1-2}[V_{1-2}] + l_{2-3}[V_{2-3}] + l_{2-4}[V_{2-4}]) + 4m k (a \cdot \cot \theta - h) \cdot V_1, \quad (5) \]

where \( p, V_1 \) are the punch pressure and velocity; \( a \) is a the channel width; \( l_{i-j} \) is the length of the sliding interfaces between the blocks \( i \) and \( j \); \([V_{i-j}]\) is velocity of relative sliding of these blocks; \( i, j = 1, 2, 3 \). The terms in equation (5) were expressed as functions of velocity \( V_1 \) and relative height of the dead zone \( x = h/a \). After substitution obtained relationships in equation (5) and algebraic transformation, the formula for calculation of relative punch pressure was obtained

\[ (p/2k) = \left[ (1 + x \tan \theta + (\cot \theta - x)^2) / (\tan \theta + \cot \theta - x) \right] + 2m(\cot \theta - x), \quad (6) \]
In the case of right-angled die this relationship coincides with corresponding equation in our previous paper [5]. According to the upper bound theory the best approximation of the real \( p/2k \) value corresponds to the minimum of (6) when

\[
x = \frac{(1 + 2m)(1 + \tan^2 \theta) - \tan \theta \sqrt{2(1 + 2m)(1 + \tan^2 \theta)}}{[(1 + 2m)\tan \theta]}.
\]  

(7)

By using (6) and (7) it is possible to calculate both the relative punch pressure \( p/2k \) and the relative height of the dead metal zone \( x \).

The total ECAE shear strain \( \gamma \) is the sum of the shear strains on the velocity discontinuity lines AC and BC in Fig. 2a, i.e.

\[
\gamma = \gamma_{1-2} + \gamma_{2-3}.
\]  

(8)

It is known that

\[
\gamma_{i-j} = \frac{[V_{i-j}]}{V_{i-j}^n},
\]  

(9)

where \( V_{i-j}^n \) is the velocity vector component orthogonal to the discontinuity line \( l_{ij} \).

Using hodograph in Fig. 2b the following relationship was obtained

\[
\gamma = 2 \left(1 + (\cot \theta - x)^2 \right) / (\tan \theta + \cot \theta - x)\right).
\]  

(10)

For rectangular die this relationship coincides with corresponding equation in our earlier paper [5].

The results of slip line and upper bound analysis were compared in Fig.3. The good agreement especially for shear strain was found. As expected the values of relative punch pressure obtained by upper bound theory are slightly higher than corresponding values derived by slip line theory.

[Figure 3: Dependence of relative punch pressure (a) and shear strain (b) from angle of channels intersection 2\( \theta \) and friction factor \( m \). \( \bullet, \square, \triangle - \) upper bound solution with \( m = 0; 0.15 \) and 0.25. Lines \(-, - - -, - - - - -\) - slip line solution with \( m = 0; 0.15 \) and 0.25]

Both theories predict sufficient decrease of \( p/2k \) and \( \gamma \) with increasing of angle \( 2\theta \) between intersecting ECAE die channels from \( 90^\circ \) to \( 120^\circ \). The increase of friction factor from \( 0 \) to 0.25 leads to rise of the punch pressure and to remarkable decrease of shear. In both cases the strain field was assumed as a homogeneous one. This may be in reality not true. Also the postulated appearance of the dead zone should be verified. To investigate these issues the finite element analysis was carried out.
4 FEM analysis

The commercial finite element software LsDyna v.11 was utilized for ECAE simulations. The ECAE die was simulated as a perfectly rigid body with no motion along all 3 degrees of freedom in accordance with applied static boundary conditions. The billet cross-section was modeled with 1249 elements. The elements used were 4-node PLANE162 Explicit 2D Structural Solids. The sample was loaded with a prescribed displacement with a rate of $V = 2.5 \text{mm/s}$ accordingly to applied kinematic boundary conditions. Hourglassing control (0.15) was used in the formulation to prevent element Hourglassing eigenmodes. Friction stress was limited according to shear strength of billet material $k$. The analysis incorporated a rigid ideal plastic material model. The calculation were provided for Coulomb friction coefficients of 0; 0.15 and 0.25. The channel intersection angle was $90^\circ$, $105^\circ$ and $120^\circ$.

![Finite elements mesh and shear strain contours](image)

Figure 4: Finite elements mesh and shear strain contours obtained by FEM analysis at different friction coefficients $f$

The results of simulation of ECAE in a right-angled die are presented in Fig. 4. The first drawing illustrates the finite element mesh used in analysis. The next three pictures show the shear strain distribution in the billet extruded at different friction conditions. The thin shear band is observed at the absence of friction $f = 0$. The dead zone does not appear. When the friction increase the shear band becomes wider. The shear strains are not concentrated anymore and distributed in inhomogeneous manner. The triangular dead zone appears near the die corner and becomes larger when friction increases.

The influence of the angle between channels on the shear band is illustrated in Fig. 5 for ECAE with Coulomb friction coefficient of 0.15. No presence of a dead zone
was observed at 2θ = 105° and 2θ = 120°. In both cases the shear band is wide. The shear strain distribution through the billet cross-sections is inhomogeneous. Similar trends were found in absence of friction f = 0 and at friction with f = 0.25.

Figure 5: Influence of die angle and friction coefficient on shear distribution at ECAE

5 Discussion

The calculated by FEM dependencies of relative punch pressure from the die angle and Coulomb friction coefficient are shown in Fig.6a.

Figure 6: Dependence of relative punch pressure (a) and shear strain (b) from the angle of channels intersection 2θ, friction coefficient f and friction factor m. – , ■ , ▲ - FEM analysis with f = 0; 0.15 and 0.25. Lines – , – – – , – – – – slip line solution with m = 0; 0.15 and 0.25

The corresponding data of slip line analysis are also presented. Despite the different friction laws were used the results of FEM and slip line calculations are in quite good agreement. The same is true for the dependencies of average shear strain from die angle presented in Fig.6b. The low influence of the friction law can be explained by normal stress distribution on straight lines of channels. In the upper channel it is near zero and in the lower one is near to 2k [3]. In both cases Tresca and Coulomb friction laws have the similar form.
The influence of die angle and friction coefficient on punch pressure and total shear obtained by FEM analysis is similar to discussed for upper bound and slip line solution above. In contrast to assumption used at upper bound analysis FEM modeling does not predict appearance of dead zone at $2\theta = 105^\circ$ and $2\theta = 120^\circ$. Moreover a small gap between the billet and the die wall in the corner was found by FEM. The FEM simulation predicts the appearance of a dead zone only in right-angled die, Fig. 4. The relative height of this zone was computed as a function of friction coefficient and compared with results of upper bound analysis in Fig. 7. A good agreement was found despite the using of different friction laws.

![Graph](image.png)

Figure 7: Frictional effect on relative height of dead zone calculated by upper bound theory and FEM at ECAE in right-angled die

Upper bound modeling is in general much simpler comparing to the slip line analysis. Nevertheless, as it is shown in this paper, it provides the similar results. Therefore together with FEM analysis it can be used for further ECAE mechanics investigation. The interesting point for example is an influence of geometry of the die corner on ECAE pressure, shear and deformation homogeneity. This work is in progress.

6 Conclusions

The equal channel angular extrusion of rigid ideal plastic material was investigated by upper bound theory and finite element method. Both obtained results are in good agreement with results of Segal’s slip line analysis in respect to punch pressure, total shear and size of dead zone. Thus used in this work upper bound method based on discontinuous velocity field can be applied for further investigation of ECAE.

Both analytical and numerical analyses show a sufficient increase in punch pressure and a decrease in total shear strain with increasing friction. The FEM analysis predicts an increase in deformation inhomogeneity at friction growing. Therefore, friction should be minimized as much as possible for practical applications of ECAE.

An increase in die angle leads to a sufficient decrease in both punch pressure and total shear strain. Thus more ECAE passes may be needed to achieve the same grain refinement at using a die with an obtuse angle. Also the deformation inhomogeneity grows with increase of the die angle. Therefore, the use of an obtuse die angle would be a reasonable choice only if lower punch pressure is required.

Further investigations of influence of right-angled die corner geometry on punch pressure, resulting shear and deformation inhomogeneity are in progress.
References


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DEM based numerical investigations of stirred media mills

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Abstract

Stirred media mills are commonly used in various industries for fine and ultra fine grinding. Stress energy and number of stress events or specific energy, respectively, are the most important influencing variables on the comminution result in stirred media mills. Former numerical investigations of Blecher [4] and Theuerkauf [5] had shown that the stress energy and the number of stress events are not constant over the grinding chamber volume. Caused by different tangential velocities of the grinding beads areas with high energy density and high stress energies, respectively, as well as areas with low stress energies exist. Thus, for an exact description of the mill performance the frequency distribution of stress energy must be known. Up to now it is not possible to quantify the stress energy distribution of mills with different operating and geometry conditions experimentally, although the knowledge of grinding media motion is very important for optimization of the grinding chamber geometry with regard to the comminution result, wear and grinding media separation.

At the Institute for Particle Technology, Technische Universität Braunschweig, the Discrete Element Method (DEM) is successfully used for investigations of dry operated stirred media mills [8, 9]. Aim of this work is to extend this existing model to investigate wet operated stirred media mills as well. For this the influence of fluid on the grinding bead motion was investigated and a Stokes number dependent restitution coefficient was implemented into the model. The extended DEM model was validated by comparing the simulated results of grinding bead velocity distribution and stirrer shaft torque with those measured from a same-scale laboratory mill. Thereby the simulation results show a good correlation with the measured results. Moreover, simulated grinding media velocities, stress energy distributions and stress frequency distributions are investigated and discussed for different operating conditions.

1 Introduction

Stress energy and number of stress events or specific energy, respectively, are the most important influencing variables on the comminution result in stirred media
Figure 1: Qualitative frequency distribution of stress energy

mills. Based on these variables Kwade [1] has developed a so-called mill related stress model for a better description of the physical processes in stirred media mills. Thereby the stress energy SE is defined as the energy transferred to the product particles at one stress event. The stress energy per contact is usually referred to the kinetic energy of the grinding beads [2, 3] and is given as

$$SE \propto E_{\text{kin}} = \frac{1}{2}m_{GB}v_{\text{rel}}^2 \quad (1)$$

where $v_{\text{rel}}$ is the relative velocity of two grinding beads and $m_{GB}$ is the mass of a single grinding bead. The stress frequency is defined as the number of stress events per second. Numeric investigations of Blecher [4] and Theuerkauf [5] had shown that the stress energy and the number of stress events are not constant over the grinding chamber volume. Thus, for an exact description of the mill the frequency distribution of stress energy must be known.

A frequency distribution like shown in Figure 1 describes which relative frequency belongs to a certain stress energy and, thus, how often a certain stress energy takes place per unit time. The reason for this stress energy distribution is the grinding bead motion inside the grinding chamber. Caused by different tangential velocities of the grinding beads areas with high relative contact velocities and high stress energies, respectively, as well as areas with low stress energies exist. Up to now it was not possible to quantify the stress energy distribution for mills with different operating and geometry conditions experimentally. Therefore in this numerical work a Discrete Element Method (DEM) based approach is used to determine the stress energy distribution by tracing the motion of a single grinding bead and its interactions with others and walls.

2 Discrete Element Method (DEM)

The DEM-Approach used in this work was introduced by Cundall and Strack [6]. It is a time stepping algorithm that requires the repeated application of the Newton’s second law of motion to each particle (grinding bead) inside the considered
DEM based numerical investigations of stirred media mills

Figure 2: DEM calculation cycle

system (grinding chamber), a force-displacement law to each contact and a constant updating of wall (agitator, grinding chamber) positions. The calculation cycle is illustrated in Figure 2.

According to this model the translational and rotational motion of a single grinding bead can be described by Newton’s second law of motion

\[ m_{GB} \frac{dv_{GB}}{dt} = \sum F_{GB} \]  
\[ I_{GB} \frac{d\omega_{GB}}{dt} = \sum M_{GB} \]  

where \( m_{GB}, v_{GB}, \omega_{GB} \) and \( I_{GB} \) are the mass, translational velocity, angular velocity and moment of inertia of every single grinding bead inside the grinding chamber. \( F_{GB} \) and \( M_{GB} \) are the sum of forces and moments, respectively acting on the grinding bead. The most important force acting on a grinding bead inside a stirred media mill is the contact force. The contact force can be generally modeled by a spring-dash pot system with friction element as shown in Figure 2. In this work a nonlinear contact model based upon the work of Mindlin and Deresiewicz [7] was used.

The resulting normal contact force is given by

\[ F = F^n + F^t + F^n_d + F^t_d \]  

were \( F^n \) and \( F^t \) are the contact force, \( F^n_d \) and \( F^t_d \) are the damping force in normal and tangential direction with

\[ F^n = \frac{4}{3} E^* \sqrt{R^*} \delta^{n\frac{1}{2}} \]  
\[ F^n_d = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S^n m^* \nu_{rel}^n} \]

\[ S^n = 2E^* \sqrt{R^* \delta^n} \]  

(7)

\[ F^t = -S^t \delta^t \]  

(8)

and

\[ F_{\text{max}}^t = \mu F^n \]  

(9)

\[ S^t = 8G^* \sqrt{R^* \delta^n} \]  

(10)

\[ F_d^t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S^t m^s v_{\text{rel}}^t} \]  

(11)

where \( R^*, m^*, E^*, G^* \) are the reduced radius, mass, Young’s modulus and shear modulus of a single grinding bead. \( S^n \) and \( S^t \) is the stiffness, \( v_{\text{rel}}^n \) and \( v_{\text{rel}}^t \) the relative contact velocity in normal and tangential direction. \( \delta^n \) is the total overlap, \( \mu \) the static friction coefficient and \( \beta \) the damping coefficient with

\[ \beta = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \]  

(12)

The restitution coefficient \( e \) and the friction coefficient \( \mu \) can be modeled or determined experimentally.

### 3 Interaction between fluid and grinding beads

Inside the grinding chamber of wet operated stirred media mills three different phases exists: Grinding beads, fluid and product particles. In the following the suspension out of fluid and product particles is considered as one phase with an inherent viscosity. Thus, in the following only to phases fluid and grinding beads are considered. The grinding beads are not equally distributed inside the grinding chamber. There are areas with a high concentration of grinding beads near the grinding chamber wall (see area 2 in figure 3) as well as areas with low grinding bead concentration near the stirrer shaft (see area 1 in figure 3). Scott [10] measured the bead concentration and found a significant gradient in bead concentration from the grinding chamber wall to the stirrer shaft (see fig. 4).

Near the grinding chamber wall a grinding bead volume concentration of 50% can be found. According to Scott the grinding bead volume concentration near the stirrer shaft ranges between 30-40 %. Whether the grinding bead motion inside the grinding
chamber is fluid or contact controlled, can be investigated by comparing the ratio of momentum response time of a grinding bead to the time between collisions [11]. Thus, the two-phase flow inside the grinding chamber can be considered dense if

\[
\frac{\tau}{\tau_C} = \frac{n \pi \rho_{\text{GB}} d_{\text{GB}}^4 v_{\text{rel}}}{18 \eta} > 1
\]  

(13)

where \(\tau_C\) is the average time between bead-bead collisions and the momentum response time \(\tau\) which corresponds to the time a grinding bead requires to respond to a change in fluid velocity. \(n\) is the number density of grinding beads \(\rho_{\text{GB}}\) is the density and \(d_{\text{GB}}\) the diameter of a single grinding bead. \(\eta\) is the fluid viscosity and \(v_{\text{rel}}\) the relative velocity of grinding beads.

Applying equation 13 it follows that the flow inside the grinding chamber of wet operated stirred media mills can be considered usually as dense. Therefore, the grinding bead motion is primary controlled by collisions (contact forces) and marginal by fluid forces (drag and lift). Under this condition the fluid primarily damps the collisions and lubricates the contact surfaces. Thus, for calculation of stress energy distributions it is sufficient to regard the fluid by an adjusted restitution and friction coefficient in the formerly described DEM model for dry operated stirred media mills.
4 Simulation conditions

A wet and dry operated laboratory mill with a horizontal orientated grinding chamber having a volume of 1 liter was studied in this work. The mill was equipped with a disk stirrer which consists out of four perforated discs with a diameter of 70 mm (see fig. 5).

The free volume of the grinding chamber was filled up to 80 % with 3 mm mono sized glass beads corresponding to a bead filling ratio of 80 %. The tip speed was varied from 6 m/s to 12 m/s.

Based on restitution coefficients $e_{dry}$ measured by drop tests for glass grinding beads in dry environment the wet restitution coefficient which depends on the Stokes number can be calculated according to Barnocky and Davis as follows [12]:

$$e_{wet} = e_{dry} + \frac{1 + e_{dry}}{St} \ln \frac{x_c}{x_0}$$

(14)

with

$$St = \frac{m_{GB} v_{rel}}{6 \pi \eta d_{GB}^2}$$

(15)

<table>
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<th>Parameter</th>
<th>Value</th>
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</tbody>
</table>

Table 1: Physical parameters of the simulation
$m_{\text{GB}}$ is a coefficient based on the surface roughness and the distance of the grinding beads, $m_{\text{GB}}$ is the mass and $d_{\text{GB}}$ the diameter of a single grinding bead. $v_{\text{rel}}$ is the relative contact velocity and $\eta$ is the viscosity of the surrounding fluid. The dry static friction coefficient was measured by shear tests. The wet static friction coefficient was taken from the literature for water lubricated glass beads [13]. In most cases only the marked area (see fig. 5) with periodic boundaries was used for simulations to reduce the number of particles and therewith the simulation time. The simulations were performed using the commercial software package EDEM™ by DEM solutions.

5 Model validation

The simulation results were validated by measuring the distribution of grinding bead velocities (see fig. 6) and the torque of the stirrer shaft (see fig. 7). For measurement of the grinding bead velocity distribution a laboratory stirred media mill with glass grinding chamber was used. The laboratory mill had the same scale and geometry conditions as used for the simulations. 80 % of the grinding chamber volume was filled with a bulk of 3 mm mono sized glass beads. The tip speed of the disc agitator was 6 m/s. For measurement of the grinding media velocity 5 % colored glass beads were used as tracer for the Particle Tracking Velocimetry (PTV). A high speed camera system was used to record the grinding bead motion near the grinding chamber wall.

Figure 6 shows the simulated and measured grinding bead velocity distributions. One can see that the simulated and the measured median values of the grinding bead velocity distribution show a good agreement. The deviation of simulation and measurement is caused by the relative little number of measured tracer grinding beads (26 grinding beads) in comparison to the high number of simulated grinding beads (884 grinding beads). For model validation using the stirrer shaft torque the laboratory mill was equipped with a torque meter. As shown in figure 7 the calculated stirrer shaft torque show a good agreement with the measured net stirrer shaft torque. The net torque is the gross torque (including friction in seal and

![Figure 6: Measured and simulated grinding bead velocity distribution](image-url)
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Figure 7: Stirrer shaft torque

bearing) reduced by the so-called no-load torque (measured without grinding beads and fluid). The fluctuations of the simulated torque results from a higher time scale resolution of the simulation in comparison to the measurement equipment.

In summary, it can be concluded that the simulation results show a good agreement with corresponding measurement results. Therefore, the model is appropriate to deliver informations about variables and operation conditions not measured before.

6 Simulation results

Based on the model described above a lot of information about different processes and parameters inside the grinding chamber can be generated.

Figure 8: Single grinding bead trajectory

Figure 8 presents a single grinding bead trajectory showing that the tangential movement of the grinding bead is influenced by a secondary movement in radial and axial direction. Figure 9 shows the grinding beads colored according to their
velocity. Significant differences in the velocity inside the grinding chamber can be seen. Therefore, areas with high relative grinding bead contact velocities as well as areas with low relative contact velocities exist inside the grinding chamber. Areas with high contact velocities are near stirrer disk outer edges and holes. Areas with low contact velocities can be found near the stirrer shaft.

Figure 10, presenting the frequencies of relative contact velocity, shows that high relative contact velocities occur low frequencies as well as medium relative contact velocities with high frequencies. As shown in equation 1 the contact stress energy is proportional to the kinetic energy and therewith to the square of the relative contact velocity of the grinding beads. From this follows a stress energy distribution inside the grinding chamber as shown in figure 11.

Figure 11 shows the cumulative stress energy distribution calculated for the laboratory mill for three different operating conditions (two wet and one dry operation). One can see, that the medium value of stress energy increases with tip speed. Caused by the fluid damping the mean stress energy in wet operated mills is not as high as in dry operated mills. However, the total number of collisions per time is significantly
Figure 11: Stress energy distribution of the mill with disk agitator and various operating conditions

<table>
<thead>
<tr>
<th>Operation condition [filling ratio, tip speed]</th>
<th>Stress frequency $[10^8 \text{s}^{-1}]$</th>
<th>SE$_{50}$ $[10^{-3}]$</th>
<th>SE$_{95}$ $[10^{-3}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>80 %, wet 6 m/s</td>
<td>86</td>
<td>$5.1 \cdot 10^{-03}$</td>
<td>0.1</td>
</tr>
<tr>
<td>80 %, wet 12 m/s</td>
<td>123</td>
<td>$2.8 \cdot 10^{-03}$</td>
<td>0.6</td>
</tr>
<tr>
<td>80 %, dry 6 m/s</td>
<td>48</td>
<td>$1.2 \cdot 10^{-02}$</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 2: Stress energy of the mill with disk agitator and various operating conditions

Figure 12 compares the stress frequency for distribution of wet and dry operating conditions. Caused by reduced friction conditions inside wet operated mills, the grinding bead mobility in wet operation is higher than in dry operation. Especially a significantly higher frequency of collision with medium stress energy can be found in wet mode, whereas the frequency of collisions with high stress energies in the vicinity of the disc holes is similar. If the medium stress energies are sufficient to break the particles wet milling is much more efficient than dry milling. From this it follows that the total stress frequency in wet operated stirred media mills is higher than in dry operated mills (see figure 12 and table 2). Based on the dependence of stress energy, stress number and specific energy one can find in wet operated stirred media mills a higher specific energy input per time as in dry operated mills.

7 Conclusion

Aim of this work was to extend an existing discrete element model in an economic way for investigations of wet operated stirred media mills. Firstly, the effect of the fluid on the grinding bead motion was investigated. It could be shown that inside the grinding chamber a dense multiphase flow exists and, therefore, the influence of fluid forces is small compared to contact forces. Hence it is possible to describe the fluid effect by a Stokes number dependent restitution coefficient and an adjusted friction coefficient in a discrete element model used up to now for dry operated stirred media mills.
Figure 12: Stress frequency distribution for dry and wet operated stirred media mills

The extended model was validated with experimental results, in terms of grinding bead velocity distribution and stirrer shaft torque, showing a good agreement of simulated and measured results. Therefore, the derived model is appropriate to deliver informations about processes and not measurable parameters inside the grinding chamber. It could be shown by simulations that the median value of stress energy increases with the tip speed. Caused by the damping features of the fluid, the median value of stress energy in dry operated stirred media mills is higher than in wet operated mills. On the other side the reduced friction in wet operated mills results in a higher grinding bead mobility and, therewith, in a higher stress frequency. Thereby the specific energy input per unit time in wet operated stirred media mills is higher than in dry operated mills.

References


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Modeling of hexagonal close-packed crystal lattices

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Abstract

This work is devoted to modeling of ideal hexagonal close-packed (HCP) crystal lattices. Two models are proposed, on the base of which a formula for tensor of stiffness is derived. If we know the components of this tensor, we can calculate the elastic modules of the material. The aim of this work is to link macro characteristics with micro ones for HCP metals. With regard to the experimental data stiffness of interatomic bonds is estimated. Elastic characteristics are calculated in both models and compared to their experimental values for a range of HCP metals. It is shown that coincidence depends on the place occupied by this or that metal in the periodic table. The best coincidence was obtained for Zn and Cd by means of anisotropic model.

1 Introduction

Modeling of crystal lattices is one of the important steps on the way from macro world to micro world, where the internal structure, which can not be described by means of continuity hypothesis, becomes essential. Nowadays, there exist several rather complex models of hexagonal close-packed (HCP) crystal lattices [1]. However, they do not provide an adequate agreement with experiment. In this work modeling based on methods of molecular and particle dynamics [2], according to which the medium is represented by a set of material points interacting through a pair potential, is proposed.

A crystal lattice is close-packed if it is characterized by maximum concentration of units in elementary volume with the given minimum distance between the units. It can be represented in observable form as a union of solid spheres (figure 1). Each sphere, or a unit, has 12 “closest neighbours” which form a so-called first coordination sphere. Most metals have a close-packed lattice. It can be either FCC (face-centered cubic), or BCC (body-centered cubic), which are “simple” lattices, or HCP (hexagonal close-packed), which is a “complex” one. Analytical formulae for the components of stiffness tensor can be easily obtained only for “simple” lattices.
As for “complex” ones, some difficulties can be encountered. Nevertheless, in the work [5] an explicit expression for the stiffness tensor of HCP lattice was obtained

\[
4\mathbf{C} = 4\mathbf{C}^* - 2 (3\mathbf{C} - 2\mathbf{C}^{-T} \cdot 3\mathbf{C}^{T})
\]  

(1)

In this formula \(2\mathbf{C}, 3\mathbf{C}, 4\mathbf{C}^*\) are determined by vectors of first coordination sphere of a reference unit, stiffness and length of interatomic bonds and also by elementary cell volume. The main problem was to get explicit expressions for nonzero components of stiffness tensor as functions of micro parameters of the material (stiffness and length of interatomic bonds). This difficulty was overcome by creating of quite simple models which consider only the first coordination sphere. It has been shown in [2] that such models are stable and provide the necessary accuracy for “simple” lattices when calculating elastic characteristics.

2 Isotropic model

Let us consider an isotropic model. Elementary cell of HCP lattice is represented by a triangular prism with the basis in the form of a regular hexagon, and in the center of volume of each second prism the additional unit is placed. Each unit (atom) has exactly 12 “closest neighbours”, and the cell consists of tetrahedrons which tops lay in units of a lattice. Here \(a_0\) is length of a bond between two atoms in a plane (its stiffness is \(c_0\)), \(a\) is length of a bond between two atoms leaving a plane (its stiffness is \(c\)), \(h\) is distance between layers (height of a tetrahedron). Let us also introduce \(\eta = \frac{2h}{a_0}\). Let \(\eta = \eta_0\), where \(\eta_0 = 2\sqrt{\frac{2}{3}}\). In this case \(a = a_0\) (and \(c = c_0\)) and so the tetrahedron is regular. Having introduced a suitable coordinate system, one can get the expressions for vectors \(\mathbf{a}_\alpha\) of the first coordination sphere. Assuming \(\mathbf{e}_\alpha = \frac{\mathbf{a}_\alpha}{|\mathbf{a}_\alpha|}, |\mathbf{a}_\alpha| = a_0, \alpha = 1 \div 12\), the following is obtained
Figure 2: HCP lattice’s elementary cell and its typical part

\[ \begin{align*}
\varepsilon_1 &= \frac{1}{2} i, & \varepsilon_2 &= \frac{1}{2} i + \frac{\sqrt{3}}{2} j, & \varepsilon_3 &= -\frac{1}{2} i + \frac{\sqrt{3}}{2} j, \\
\varepsilon_4 &= -\frac{1}{2} i, & \varepsilon_5 &= -\frac{1}{2} i - \frac{\sqrt{3}}{2} j, & \varepsilon_6 &= \frac{1}{2} i - \frac{\sqrt{3}}{2} j, \\
\varepsilon_7 &= \frac{1}{2} i - \frac{1}{2 \sqrt{3}} j + \sqrt{\frac{2}{3}} k, & \varepsilon_8 &= \frac{1}{2} j + \sqrt{\frac{2}{3}} k, & \varepsilon_9 &= -\frac{1}{2} i - \frac{1}{2 \sqrt{3}} j + \sqrt{\frac{2}{3}} k, \\
\varepsilon_{10} &= \frac{1}{2} i - \frac{1}{2 \sqrt{3}} j - \sqrt{\frac{2}{3}} k, & \varepsilon_{11} &= \frac{1}{2} j - \sqrt{\frac{2}{3}} k, & \varepsilon_{12} &= -\frac{1}{2} i - \frac{1}{2 \sqrt{3}} j - \sqrt{\frac{2}{3}} k
\end{align*} \]

Elementary cell volume is \( V_0 = \sqrt{2} \frac{c a^3}{2} \). Taking into account, that

\[ \begin{align*}
4C & = \frac{ca^2}{2 V_0} \sum_{\alpha=1}^{12} \varepsilon_\alpha \varepsilon_\alpha \varepsilon_\alpha \varepsilon_\alpha, & 3C & = \frac{ca}{4 V_0} \sum_{\alpha=1}^{12} \varepsilon_\alpha \varepsilon_\alpha \varepsilon_\alpha, & 2C & = \frac{c}{4 V_0} \sum_{\alpha=1}^{12} \varepsilon_\alpha \varepsilon_\alpha \varepsilon_\alpha
\end{align*} \]

and substituting (2) to (3) and then to (1), explicit expressions for nonzero components of stiffness tensor are

\[ \begin{align*}
C_{11} &= \frac{119}{48 \sqrt{2}} \frac{c}{a_0}, & C_{12} &= \frac{37}{48 \sqrt{2}} \frac{c}{a_0}, & C_{13} &= \frac{2}{3 \sqrt{2}} \frac{c}{a_0}, \\
C_{33} &= \frac{8}{3 \sqrt{2}} \frac{c}{a_0}, & C_{44} &= \frac{13}{16 \sqrt{2}} \frac{c}{a_0}
\end{align*} \]

Bulk modulus is

\[ K = \frac{11}{9} \frac{E}{\varepsilon^2} \cdot 4C \cdot E = \frac{4}{3 \sqrt{2}} \frac{c}{a_0} \]

Being aware of \( a_0 \) for particular metal and at least one \( C_{kn} \) from experiment, it is not difficult to calculate the other \( C_{kn} \), \( c \) and bulk modulus \( K \).
3 Anisotropic model

Obviously, the closer is a lattice of a real metal to regular one, the higher is the accuracy of the formulae above. Actually, the following three cases are realized: \( \eta > \eta_0 \), \( \eta \approx \eta_0 \), \( \eta < \eta_0 \). To be able to describe all three cases, a more complex model is necessary.

Let us consider an anisotropic model \( (\eta \neq \eta_0) \). In this case \( |a_\alpha| = a_0 \) for \( \alpha = 1 \div 6 \) and \( |a_\alpha| = a \) for \( \alpha = 7 \div 12 \). It is obvious that \( a = \frac{a_0}{2\sqrt{3}} \sqrt{4 + 3\eta^2} \). So the following is obtained for vectors of the first coordination sphere

\[
\begin{align*}
e_1 &= i, & e_2 &= \frac{1}{2}i + \frac{\sqrt{3}}{2}j, & e_3 &= -\frac{1}{2}i + \frac{\sqrt{3}}{2}j, \\
e_4 &= -i, & e_5 &= -\frac{1}{2}i - \frac{\sqrt{3}}{2}j, & e_6 &= \frac{1}{2}i - \frac{\sqrt{3}}{2}j, \\
e_7 &= \frac{1}{2}i - \frac{1}{2}\sqrt{3}j + \frac{\eta}{2}k, & e_8 &= \frac{1}{\sqrt{3}}j + \frac{\eta}{2}k, & e_9 &= -\frac{1}{2}i - \frac{1}{2}\sqrt{3}j + \frac{\eta}{2}k, \\
e_{10} &= \frac{1}{2}i - \frac{1}{2}\sqrt{3}j - \frac{\eta}{2}k, & e_{11} &= \frac{1}{\sqrt{3}}j - \frac{\eta}{2}k, & e_{12} &= -\frac{1}{2}i - \frac{1}{2}\sqrt{3}j - \frac{\eta}{2}k & (6)
\end{align*}
\]

Considering, that stiffness of interatomic bonds in a plane \( c_0 \) is not equal to stiffness of interatomic bonds leaving a plane \( c \), and substituting (6) to (3) and then to (1), we receive nonzero components of stiffness tensor and bulk modulus

\[
\begin{align*}
C_{11} &= \frac{1296c_0 + 11 (4 + 3\eta^2) c}{288\sqrt{3}a_0\eta}, & C_{12} &= \frac{432c_0 + (4 + 3\eta^2) c}{288\sqrt{3}a_0\eta}, \\
C_{13} &= \frac{(4 + 3\eta^2) \eta c}{24\sqrt{3}a_0}, & C_{33} &= \frac{(4 + 3\eta^2) \eta^3 c}{16\sqrt{3}a_0}, \\
C_{44} &= \frac{432c_0 + 3 (4 + 3\eta^2) c}{288\sqrt{3}a_0\eta}, & K &= \frac{1728c_0 + (4 + 3\eta^2)^2 c}{1296\sqrt{3}a_0\eta} & (7)
\end{align*}
\]

Being aware of \( a_0 \) and \( \eta \) for particular metal and at least two \( C_{kn} \) from experiment, it is not difficult to calculate the other \( C_{kn} \), c, \( c_0 \) and bulk modulus \( K \).

4 Results and conclusions

1. One-parametrical (isotropic) and two-parametrical (anisotropic) models of HCP metals’ lattices (“complex” lattices) were created.

2. For both models stiffness tensors were made up and simple analytical expressions connecting their nonzero components and microscopic stiffness of interatomic bonds were received.

3. Basing on experimental data from work [1] stiffness of interatomic bonds was calculated for some metals.
4. Verification on the bulk modulus, which showed a good agreement (divergence less than 10 %) with experimental data was carried out: more than for 75 % of the considered metals in isotropic model and more than for 85 % of metals in anisotropic model (figure 3).

5. Some connection between position of HCP metals in the periodic table and quality of the description of their lattice by means of the first and second model was noticed.

<table>
<thead>
<tr>
<th>Type</th>
<th>Element</th>
<th>$\eta/\eta_0$</th>
<th>$c/c_0$</th>
<th>$c$(Isotr), eV/Å²</th>
<th>$c_0$, eV/Å²</th>
<th>$K$(exp), eV/Å³</th>
<th>$K$(Isotr), eV/Å³</th>
<th>$K$(Anisotr), eV/Å³</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Cd</td>
<td>1,1545</td>
<td>0,1760</td>
<td>0,9119</td>
<td>1,5268</td>
<td>0,2915</td>
<td>0,4496</td>
<td>0,2771</td>
</tr>
<tr>
<td>I</td>
<td>Zn</td>
<td>1,1367</td>
<td>0,1635</td>
<td>1,0812</td>
<td>1,8762</td>
<td>0,3733</td>
<td>0,5287</td>
<td>0,3734</td>
</tr>
<tr>
<td>II</td>
<td>Mg</td>
<td>1,0055</td>
<td>1,0188</td>
<td>0,6675</td>
<td>0,6801</td>
<td>0,2210</td>
<td>0,2159</td>
<td>0,1974</td>
</tr>
<tr>
<td>II</td>
<td>Co</td>
<td>0,9999</td>
<td>1,0942</td>
<td>2,8637</td>
<td>2,7238</td>
<td>1,1948</td>
<td>1,1780</td>
<td>1,0696</td>
</tr>
<tr>
<td>II</td>
<td>Re</td>
<td>0,9889</td>
<td>1,1097</td>
<td>6,1081</td>
<td>5,9032</td>
<td>2,3221</td>
<td>2,2491</td>
<td>2,1009</td>
</tr>
<tr>
<td>III</td>
<td>Zr</td>
<td>0,9752</td>
<td>1,2448</td>
<td>1,6928</td>
<td>1,5793</td>
<td>0,5200</td>
<td>0,4800</td>
<td>0,5024</td>
</tr>
<tr>
<td>III</td>
<td>Ti</td>
<td>0,9728</td>
<td>1,2172</td>
<td>1,7198</td>
<td>1,6336</td>
<td>0,6561</td>
<td>0,6031</td>
<td>0,5611</td>
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<td>III</td>
<td>Hf</td>
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<td>2,0499</td>
<td>1,9669</td>
<td>0,6804</td>
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<td>0,6199</td>
</tr>
<tr>
<td>III</td>
<td>Be</td>
<td>0,9675</td>
<td>1,3056</td>
<td>2,4325</td>
<td>2,2463</td>
<td>0,6261</td>
<td>0,5744</td>
<td>1,2086</td>
</tr>
</tbody>
</table>

Table 1: Results’ set

Figure 3: Results’ set

It is seen from table 1 that if a metal’s lattice is close to regular ($\eta \approx \eta_0$), which is true for Mg, Co, Re, isotropic model provides better coincidence. It is also obvious that isotropic model does not work properly in case of Cd and Zn, as in their lattices the distance between layers is much bigger than in the regular one. That is why, when a metal’s lattice is close to regular, there is no need to use complex models (e.g. anisotropic model), as the accuracy decreases. The reason is that in anisotropic model more experimental data should be employed in comparison with isotropic one, and so computational error might be accumulated because of the initial data error.

According to figure 3, considered metals can be divided into three groups. For Cd and Zn $\eta > \eta_0$, and stiffness of a bond between two atoms leaving a plane has much smaller value than stiffness of a bond in a plane. For Mg, Co and Re $\eta \approx \eta_0$, and the difference between $c$ and $c_0$ is not more than 10%. For Zr, Ti, Hf and Be $\eta < \eta_0$, and the difference between $c$ and $c_0$ ascends to 30%.
It has been noticed, that the majority of elements in each group occupy neighbouring positions in the periodic table, e.g. Ti, Zr and Hf belong to group 4. What is more, Zr and Hf occur mostly together. So, it can be concluded, that they should have more or less the same properties, which is proved by calculations and is successfully reflected in this work.

Let us note, that most considered HCP metals are referred to as “d-elements”. There are only one or two electrons in these elements’ external electronic layer, and other valence electrons are located in preexternal layer [3]. Besides, most considered metals’ oxides and hydro-oxides behave amphoterically. Taking into account the results obtained and also chemical properties of HCP metals, it may be possible to improve the existing models and create better ones, especially when strength characteristics are dealt with.

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References


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Influence of internal fine structure on propagation of strain solitary waves in crystals

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Abstract  
The nature of dispersion and nonlinearity in solids with complex internal structure is studied. It is shown, that the essential nonlinearity may be described by only one additional cubic nonlinear term in the equation for longitudinal strain waves. It is found that the influence of internal structure makes provides an importance of the wave velocity in the existence of one or another kind of localized strain waves is revealed. Also it is shown that similar profiles of the macro-strain solitary waves may be accompanied by distinct profiles of the micro-strain waves.

Introduction  
Among non-linear strain waves of special interest are those that propagate keeping their shape and velocity. One of them is the bell-shaped solitary wave arising as a result of a balance between nonlinearity and dispersion. It is important to find the conditions required for the existence of the solitary wave in order to know when localization of the strain field is possible. On the other hand, existence of such localized strain waves allows us to estimate the unknown material parameters measuring the wave amplitude and velocity since the relationships between the wave and the material parameters may be found in an explicit form.

To describe the strain solitary waves, it is necessary to reveal the sources of nonlinearity and dispersion. The classic elastic theory admits two main kinds of nonlinearity. The first one is the geometrical nonlinearity following from the exact relationship for the tensor of finite strains. An anharmonicity in interatomic interaction gives rise to the so-called physical nonlinearity. Contrary to the geometrical nonlinearity, it is not described by an exact analytical formula but is modeled using hypothesis about deformations. Of most popular are the weakly non-linear models based on the power series expansion of the energy density in small strains or strain tensor invariants. The Murnaghan model [1] may be noted among them since it...
is valid for isotropic materials like metals, polymers etc. In particular, the series truncated by the fourth order term is called the nine-constants Murnaghan model, and the energy density $\Pi$ reads

$$\Pi = \frac{\lambda + 2\mu}{2} I_1^2 - 2\mu I_2 + \frac{l + 2m}{3} I_1^3 - 2m I_1 I_2 + n I_3 + \nu_1 I_1^4 + \nu_2 I_1^2 I_2 + \nu_3 I_1 I_3 + \nu_4 I_2^2,$$  \hspace{1cm} (1)$$

where $I_k, k = 1, 2, 3$ - are the invariants of the Cauchy-Green strain tensor, the fourth order elastic moduli ($\nu_1, \nu_2, \nu_3, \nu_4$), as well as the third order ones, $l, m, n$, may be of either sign contrary to the positive second order moduli $\lambda, \mu$. One can obtain the stress-strain relationship from Eq.(1) in the 1D case, $P = E U_x + C_1 U_x^2 + C_2 U_x^3$, ($U_x$ is longitudinal strain, $E$ is the Young modulus), where the second term describes the quadratic nonlinearity, and $C_1 = C_1(l, m, n)$. The last term accounts for the cubic nonlinearity, and its coefficient depends on both the third and the fourth order moduli. Usually, only quadratic nonlinearity is used (the so-called five-constants Murnaghan model, $\nu_i = 0$ in Eq.(1)) to describe longitudinal strain waves since relative contribution $C_2 U_x/C_1$ of the last term in the stress-strain relationship is negligibly small for usual elastic materials [2, 3, 4, 5, 6].

Another source of nonlinearity is caused by the presence of the components with contrasting elastic features including cracks intergranular contacts, dislocations at the boundaries of the grains of poly-crystals. It was found in Refs. [16, 17, 18] that this nonlinearity is essential, and weakly nonlinear models in the form power series truncation like (1) cannot be applied in a strict sense. Nevertheless, they are used already as exact expressions in the framework of a phenomenological approach [16, 17, 18, 19]. An analysis and experimental observations show that the contribution of the quadratic and cubic nonlinearities turns out of the same order for materials with essentially non linear features.

Finally, one can note the works dealing with materials having complex internal structure. Thus, the rotatory molecular groups were added to the usual one atomic chain in Refs. [3, 20, 21], and large rotations were considered. A more complicated internal motion is modeled in Refs. [22, 23], where translational internal motion is considered together with rotations. In both models this essential nonlinearity has not been modeled by any power series expansion, instead, the trigonometric functions were used.

Dispersion in classic elastic bodies is caused by finite transverse sizes of a waveguide. To see how strong this dispersion may be one can note experimental observations of the strain solitary wave of the amplitude of order $10^{-4}$ and the width $33\text{mm}$ in a rod of the radius $R = 5\text{mm}$ [5]. Also dispersion appears as a result of an internal complex structure of material [7, 8, 9, 10, 11]. Some estimations have been done for materials with grains and for sandstones [12, 13]. According to them the solitary waves may exist in such media with anticipated typical width $0.1 - 100\text{m}$. Finally, one can note phonon dispersion arising in crystals due to the finite atomic sizes. It gives rise to the strain solitary wave of the amplitude of order $10^{-4}$ and the width of $100\text{Å}$ observed in experiments [14, 15]. One can note that all above mentioned experiments were described by the solitary wave solutions obtained using Eq.(1) [5, 14].
In this paper, the solitary wave solutions are studied for the model taking into account internal structural deviations in a crystal. First, the 1D case of the model developed in [22] is transformed to the equation for the travelling macro-strain waves. An analysis of this equation reveals strong dependence of the solitary wave solutions on their velocity. It is also found that similar macro-strain waves give rise to completely distinct micro-strain waves, thus to the different variations in the internal structure of the material.

1 Model for media with essentially nonlinear translational internal structure

The model in [22, 23] considers a complex lattice of a crystal consisting of two sub-lattices generalizing linear analog developed by Born & Kun [24]. Besides interatomic forces between atoms, the relative sub-lattices motion is taken into account in the model, hence it generalizes the well-known Frenkel-Kontorova model for the simple lattice to describe structural deviations in the bi-atomic lattice.

According to [22, 23] the governing equations are obtained using a continuum approach without making a continuum limit of a discrete model similar to Refs. [3, 21]. The equations are derived for the vectors of macro-displacement \( \mathbf{U} \) and relative micro-displacement \( \mathbf{u} \) for the pair of atoms with masses \( m_1, m_2 \),

\[
\mathbf{U} = \frac{m_1 \mathbf{U}_1 + m_2 \mathbf{U}_2}{m_1 + m_2}, \quad \mathbf{u} = \frac{\mathbf{U}_1 - \mathbf{U}_2}{\alpha}
\]

where \( \alpha \) is a period of sub-lattice. In general, it allows us to describe both translational and rotational motions of the internal structure. In the one-dimensional case, only translational motion is considered, and the Hamilton principle is employed with kinetic energy density \( K \)

\[
K = \frac{\rho \mathbf{U}_t^2 + \mu \mathbf{u}_t^2}{2}
\]

and the internal density energy \( \Pi \) -

\[
\Pi = \frac{E \mathbf{U}_{xx}^2 + \kappa \mathbf{u}_t^2}{2} + (p - S \mathbf{U}_x)(1 - \cos(u))
\]

Comparing it with the Murnaghan model (1), one can see the absence of the terms describing physical nonlinearity at the macro level. Instead, the last term in Eq. (2) accounts for the sub-lattices interaction. In the absence of coupling at \( S = 0 \), the Frenkel-Kontorova model is revealed. Trigonometric functions allow us to describe an indentity of the complex lattice after displacement proportional to to the period of the sub-lattice.

Then the following coupled equations are obtained,

\[
\rho \mathbf{U}_{tt} - E \mathbf{U}_{xx} = S(\cos(u) - 1)_x,
\]

\[
\mu \mathbf{u}_{tt} - \kappa \mathbf{u}_{xx} = (SU_x - p) \sin(u).
\]
For wave processes the r.h.s. in Eqs. (3), (4) should be of lower order in comparison with those in the l.h.s. The function \( u \) may be of order one, the macro-strain \( v = U_x \) is of order \( 10^{-4} \div 10^{-5} \), and the Young modulus is of order \( 10^{10} \) for most of materials. Therefore, the value of the parameter \( S \) is of order \( 10^6 \) as follows from Eq. (3) while \( p - 10^3 \) follows from Eq. (4).

One can obtain from Eqs. (3), (4) the single equation for the macro-strain considering travelling wave solutions depending only on the phase variable, \( \theta = x - V t \). In this case Eq. (3) reads

\[
\cos(u) = 1 - \frac{(E - \rho V^2)U_x - \sigma}{S},
\]

where \( \sigma \) is constant of integration. Then it follows from Eq.(4) that

\[
v_0^2 = a_1 v + a_2 v^2 + a_3 v^3 + a_4 v^4.
\]

where the coefficients \( a_i \) depend on the velocity \( V \),

\[
a_1 = \frac{2p \sigma (2S + \sigma)}{S(E - \rho V^2)(\mu V^2 - \kappa)}, \quad a_2 = \frac{p(4p(E - \rho V^2)(S + \sigma) + S \sigma (2S + \sigma))}{S(E - \rho V^2)(\kappa - \mu V^2)},
\]
\[
a_3 = \frac{2p(E - \rho V^2) + S(S + \sigma)}{S(\mu V^2 - \kappa)}, \quad a_4 = \frac{E - \rho V^2}{\kappa - \mu V^2}.
\]

The term \( v_0^2 \) reflects dispersion that is caused by coupling like nonlinearity. The quadratic and cubic nonlinear term arise for the macro-strain, hence the weakly nonlinear case is generalized by adding one non-linear term since the ODE with only quadratic nonlinear term is obtained for longitudinal strain waves [6]. Also, in the weakly nonlinear case the non-linear term coefficient of the governing ODE does not depend on the phase velocity [6].

The equation (6) is similar to the ODE reduction of the Gardner equation that accounts for internal shear waves in two-layer fluids [28]. It possesses solutions vanishing at infinity, \( |\theta| \to \infty \), provided that \( a_1 = 0 \) that happens for \( \sigma = 0 \) or \( \sigma = -2S \). The non-linear term coefficients ratio \( a_3/a_4 = \max p/S, S/E \), turns out of order \( 10^{-3} \), that yields almost equal contribution of quadratic and cubic nonlinearities for typical elastic strains of order \( 10^{-4} \). In fluids this equality happens for very special ratio between the width of the layers and their densities (this is weakly nonlinear problem!) [28].

## 2 Essentially nonlinear localized strain waves

The equation (6) at \( a_1 = 0 \) possesses known exact solutions of two types [28],

\[
v_1 = \frac{A}{Q \cosh(k \theta) + 1}, \quad (7)
\]
\[
v_2 = -\frac{A}{Q \cosh(k \theta) - 1}. \quad (8)
\]
Influence of internal fine structure on propagation of strain solitary waves in crystals

\[ V^2 \left( 0; c_1^2 - c_0^2 \right) \]

<table>
<thead>
<tr>
<th>( A )</th>
<th>( Q_+ )</th>
<th>( Q_- )</th>
<th>wave</th>
</tr>
</thead>
<tbody>
<tr>
<td>( &gt; 0 )</td>
<td>( &gt; 0 )</td>
<td>( - )</td>
<td>tensile (7)</td>
</tr>
<tr>
<td>( &gt; 0 )</td>
<td>( -1; 0 )</td>
<td>( &gt; 0 )</td>
<td>tensile (7)</td>
</tr>
<tr>
<td>( &gt; 0 )</td>
<td>( &gt; 0 )</td>
<td>( - )</td>
<td>compression (8)</td>
</tr>
<tr>
<td>( &gt; c_1^2 + c_0^2 )</td>
<td>( &lt; 1 )</td>
<td>( &gt; 0 )</td>
<td>compression (7)</td>
</tr>
</tbody>
</table>

Table 1: Signs of the wave parameters and types of the waves for \( \sigma = 0 \).

where for \( \sigma = 0 \)

\[ A = \frac{4 S}{\rho(c_0^2 + c_0^2 - V^2)}, \quad Q_{\pm} = \pm \frac{c_1^2 - V^2 - c_0^2}{c_1^2 - V^2 + c_0^2}, \quad k = 2 \sqrt{\frac{p}{\mu(c_1^2 - V^2)}} \]  

(9)

and for \( \sigma = -2S \)

\[ A = \frac{4 S}{\rho(c_0^2 + V^2 - c_1^2)}, \quad Q_{\pm} = \pm \frac{V^2 - c_1^2 - c_0^2}{V^2 - c_1^2 + c_0^2}, \quad k = 2 \sqrt{\frac{p}{\mu(V^2 - c_1^2)}} \]  

(10)

where \( c_1^2 = E/\rho \), \( c_0^2 = S^2/(p \rho) \), \( c_1^2 = m/\mu \). Hence, in the first case \( V^2 < c_1^2 \), and in the second one \( V^2 > c_1^2 \). In both cases the solution of the first kind (7) is realized for \( Q_{\pm} > 0 \), while bounded solution of the second kind (8) appears at \( Q_{\pm} < -1 \). The sign of the amplitude of the wave \( A/(Q_{\pm} + 1) \) depends on the relation between \( V \), \( c_1 \), \( c_0 \). The variation of the value of the amplitude of the wave \( A/(Q_{\pm} + 1) \) does not depend on the variation of velocity \( V \) while \( A/(Q_{\pm} + 1) \) does.

However, the variations are different for different values of \( \sigma \). Thus, for \( \sigma = 0 \) the amplitude of the tensile wave increases with increase in the velocity, while that of the compression wave decreases. For \( \sigma = -2S \) all is conversely. Possible types of the solitary waves also depend upon both the velocity and \( \sigma \). These results are summarized in Tables 1 and 2. Special case corresponds to the so-called "fat" wave that appears as \( Q_{\pm} \) tends to zero. In this case the width of the wave increases without limit while its amplitude tends to the finite value equal to \( A \).

An analysis of the exact solutions should take into account the coupling governed by Eq. (5). Depending upon the value of the first derivative at \( \theta = 0 \), one can express it in a different way. Thus for \( \sigma = 0 \) corresponding to initially undisturbed internal structure of the crystal one has either

\[ u = \arccos \left( \frac{(\rho V^2 - E)U_x}{S} + 1 \right), \]  

(11)

if the derivative is zero, while for non-zero derivative a more complex representation holds

\[ u = \arccos \left( \frac{(\rho V^2 - E)U_x}{S} + 1 \right) \] for \( \theta \leq 0 \),  

(12)

\[ u = 2\pi - \arccos \left( \frac{(\rho V^2 - E)U_x}{S} + 1 \right) \] for \( \theta > 0 \),  

(13)
Table 2: Signs of the wave parameters and types of the waves for $\sigma = -2S$.

<table>
<thead>
<tr>
<th>$V^2$</th>
<th>$0; c_L^2 - c_0^2$</th>
<th>$(c_L^2 - c_0^2; c_L^2)$</th>
<th>$(c_L^2; c_L^2 + c_0^2)$</th>
<th>$&gt; c_L^2 + c_0^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$&lt; 0$</td>
<td>$&gt; 0$</td>
<td>$&gt; 0$</td>
<td>$&gt; 0$</td>
</tr>
<tr>
<td>$Q_+^-$</td>
<td>$&gt; 0$</td>
<td>$&lt; -1$</td>
<td>$(-1; 0)$</td>
<td>$&gt; 0$</td>
</tr>
<tr>
<td>wave</td>
<td>compression (7)</td>
<td>compression (8)</td>
<td>tensile (7)</td>
<td>tensile (7)</td>
</tr>
</tbody>
</table>

Then it follows that simultaneous existence of the compression and tensile waves is impossible that differs from the case of abnormal nonlinearity studied in [25, 26, 27] and suitable for seismic media [16, 17, 18, 19]. Also different micro deviations correspond to the similar bell-shaped profiles of the macro-strain wave. Indeed, the wave (11) has the shape of a kink while Eqs.(12), (13) account for the bell-shaped profile. Similar distinctions in the micro-filed profiles are observed for the case $\sigma = -2S$ that corresponds to the internal structure of the crystal initially disturbed by static loading.

3 Conclusions

To sum up, both dispersion and nonlinearity for the macro-strain wave may be caused by variations in the internal structure of a crystal. It gives rise to a balance required for existence of the bell-shaped solitary waves. The study of the wave behaviour allows us to establish analytically the relationships between the velocity of the wave and the parameters of the material needed for the existence of one or another kind of localized strain wave. This may help us to estimate the nonlinear and dispersive properties of the material caused by coupling of the macro- and micro- fields using, e.g., the values found in [14]. Also structural deviations might be predicted by observation of macro-strain solitary waves. It is important that the governing equation turns out similar to that of obtained in the framework of the phenomenological approach when the weakly nonlinear model (1) is formally used [25, 26, 27]. In the last papers numerical simulations are performed to demonstrate that the profiles of the exact travelling wave solutions arise even in a more general unsteady processes as a result of an evolution of rather arbitrary initial perturbation. Similar technique will be employed in the following to show an appearance of the solitary waves in the framework of the model considered.

Acknowledgements

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Influence of internal fine structure on propagation of strain solitary waves in crystals


Self-synchronization of four mechanical vibroexciters at various variants of kinematical connection

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Abstract

Nowadays unbalanced vibroexciters self-synchronization theory is rather well-studied [1, 2]. At the same time application opportunities of this phenomenon are not exhausted yet. In the present work we consider one of arrangements with self-synchronized vibroexciters which can be used in various cases when both horizontal and vertical oscillations of working tool are required. Installations used in foundry manufacture can exemplify this fact.

The system in question includes two pairs of coaxial unbalanced vibroexciters, installed on a softly vibroinsulated platform which performs planar oscillations. These pairs of exciters are placed at the end faces of the platform located at right angles to each other.

Object of the work is a definition of conditions at which rotor phasings in synchronous modes of rotation are steady at various variants of vibrators connection in pairs. The research was executed with the use of integral test of stability. In each case the character of platform oscillations was determined.

Another case of system with four vibroexciters was considered by [3].

1 The system scheme

The system scheme is shown in Fig.1. The rigid platform 1 of mass M is in-stalled on vibroinsulated springs 2 of rather small rigidity C. Two pairs of coaxial mechanical vibroexciters are installed on the end faces of the platform. Eccentricities of the exciter rotors ε and unbalanced masses m in each pair are considered to be identical (εh and εh, m_h and m_v correspondingly). All vibroexciters are considered possessing identical positive partial angular speeds ω. Intervals of rotors axes from the center of platform masses are denoted by b and h. For the generalized coordinates we’ll take horizontal displacement x and vertical displacement y of the platform from the position corresponding to the unstrained elastic elements, rotation angle of the platform φ, read anticlock-wise from the line of horizon, and also rotation angles of the rotors φ_s, read according to Fig.1.
2 The task solution with using integral test of stability. Potential energy of system

For the task solution we’ll take integral test of stability [1, 2]. If, as in the considered case, partial angular speeds of unbalanced vibroexciters are positive and identical or not strongly differ from each other, the platform is softly vibroinsulated, and oscillation part of the system is linear, then the averaged kinetic energy of the platform can be taken for the potential function $D$

$$D = \langle T_0 \rangle = \frac{M}{2} \left( x^2 + y^2 \right) + \frac{I}{2} \dot{\varphi}^2 \rangle \quad (1)$$

Here brackets $\langle \rangle$ denote averaging for the period of oscillations $T = \frac{2\pi}{\omega}$, and coordinates $x$, $y$ and $\varphi$ correspond to the set forced platform oscillations on conditions that the rotors uniformly rotate with identical frequency $\omega$ with arbitrary initial phases $\alpha_s$. Rough minima of function $D$ on phase difference $\alpha_3 - \alpha_4$ correspond to the steady stationary modes of synchronous rotation of the rotors.

The equations of small oscillations of the platform under the specified conditions have the form:

$$\begin{cases}
M\ddot{x} = m_h\dot{\varepsilon}_h \omega^2 (\sin \varphi_1 + \sin \varphi_2) + m_v\dot{\varepsilon}_v \omega^2 (\sin \varphi_3 + \sin \varphi_4) \\
M\ddot{y} = m_h\dot{\varepsilon}_h \omega^2 (\cos \varphi_1 + \cos \varphi_2) + m_v\dot{\varepsilon}_v \omega^2 (\cos \varphi_3 + \cos \varphi_4) \\
I\ddot{\varphi} = m_h\dot{\varepsilon}_h \omega^2 h (\sin \varphi_1 + \sin \varphi_2) + m_v\dot{\varepsilon}_v \omega^2 b (\cos \varphi_3 + \cos \varphi_4)
\end{cases} \quad (2)$$

where

$$\varphi_s = \sigma_s(\omega t + \alpha_s), \quad s = 1, ..., 4 \quad (3)$$

and values $\sigma_s$ assume the directions of rotor rotation: $\sigma_i = 1$ anticlockwise, $\sigma_i = -1$ clockwise.

Solving equations (2) under conditions (3), we find:

$$\begin{align*}
x &= -\frac{m_v\dot{\varepsilon}_v}{M} \sin[\sigma_1(\omega t + \alpha_1)] - \frac{m_h\dot{\varepsilon}_h}{M} \sin[\sigma_2(\omega t + \alpha_2)] - \\
&- \frac{m_v\dot{\varepsilon}_v}{M} \sin[\sigma_3(\omega t + \alpha_3)] - \frac{m_h\dot{\varepsilon}_h}{M} \sin[\sigma_4(\omega t + \alpha_4)] \\
y &= -\frac{m_v\dot{\varepsilon}_v}{M} \cos[\sigma_1(\omega t + \alpha_1)] - \frac{m_h\dot{\varepsilon}_h}{M} \cos[\sigma_2(\omega t + \alpha_2)] - \\
&- \frac{m_v\dot{\varepsilon}_v}{M} \cos[\sigma_3(\omega t + \alpha_3)] - \frac{m_h\dot{\varepsilon}_h}{M} \cos[\sigma_4(\omega t + \alpha_4)] \\
\varphi &= -\frac{m_v\dot{\varepsilon}_v}{M} \sin[\sigma_1(\omega t + \alpha_1)] - \frac{m_h\dot{\varepsilon}_h}{M} \sin[\sigma_2(\omega t + \alpha_2)] - \\
&- \frac{m_v\dot{\varepsilon}_v}{M} \cos[\sigma_3(\omega t + \alpha_3)] - \frac{m_h\dot{\varepsilon}_h}{M} \cos[\sigma_4(\omega t + \alpha_4)]
\end{align*} \quad (4)$$

Considering the formulas of averaging,

$$< \cos[\sigma_1(\omega t + \alpha_1)] \cos[\sigma_2(\omega t + \alpha_2)] > = \frac{1}{2} \cos[\sigma_1(\omega t + \alpha_1) - \sigma_2(\omega t + \alpha_2)]$$

$$< \sin[\sigma_3(\omega t + \alpha_3)] \cos[\sigma_1(\omega t + \alpha_1)] > = \frac{\sigma_3}{2} \sin[\sigma_3(\omega t + \alpha_3) - \sigma_1(\omega t + \alpha_1)]$$
We obtain:

\[ D = \sigma_1 \sigma_2 m^2 \varepsilon_1 \varepsilon_2 \Omega^2 \cos(\alpha_1 - \alpha_2) \left[ \frac{1}{M} + \frac{h^2}{2I} \right] - \sigma_3 \sigma_4 m^2 \varepsilon_3 \varepsilon_4 \Omega^2 \cos(\alpha_3 - \alpha_4) \left[ \frac{1}{M} + \frac{b^2}{2I} \right] + \]

\[ + m_3 m_v \varepsilon_3 \varepsilon_v \Omega^2 \left( \frac{\sigma_1 \sigma_3}{M} \cos(\alpha_1 - \alpha_3) + \frac{\sigma_1 \sigma_4}{M} \cos(\alpha_1 - \alpha_4) + \frac{\sigma_2 \sigma_3}{M} \cos(\alpha_2 - \alpha_3) + \right) \]

\[ + \frac{\sigma_2 \sigma_4}{M} \cos(\alpha_2 - \alpha_4) - \sigma_1 \frac{b h}{2I} \sin(\alpha_3 - \alpha_1) - \sigma_1 \frac{b h}{2I} \sin(\alpha_4 - \alpha_1) - \]

\[ - \sigma_2 \frac{b h}{2I} \sin(\alpha_3 - \alpha_2) - \sigma_2 \frac{b h}{2I} \sin(\alpha_4 - \alpha_2) \right) + C \]

(5)

where C - a constant insignificant further.

3 The cases of kinematical connection of the rotors in pairs

Let’s consider some cases of kinematical connection of the rotors in pairs:

1. The upper and side rotors are connected in such a manner that each pair provides rectilinear driving force in vertical and horizontal directions correspondingly (Fig.2). The following values of parameters correspond to this case:

\[ \sigma_1 = -\sigma_2 = 1; \quad \alpha_1 = \alpha_2; \quad \sigma_3 = -\sigma_4 = 1; \quad \alpha_3 = \alpha_4 + \pi \]

2. The upper and side rotors are connected in such a manner that both pairs raise vertical driving force. In this case

\[ \sigma_1 = -\sigma_2 = 1; \quad \alpha_1 = \alpha_2; \quad \sigma_3 = -\sigma_4 = 1; \quad \alpha_3 = \alpha_4 \]

It is easy to see, that in both cases functions D do not depend on angles $\alpha_s$, i.e. the pairs of vibrators are not dynamically connected. Neither self-synchronization, nor self-phasing in this case does occur.

In the first case oscillations occur under the law:

\[
\begin{align*}
    x &= -\frac{2m_v \varepsilon_v}{M} \sin(\omega_v t + \alpha_3) \\
    y &= -\frac{2m_h \varepsilon_h}{M} \cos(\omega_h t + \alpha_1) \\
    \varphi &= 0
\end{align*}
\]

(6)

and in the second

\[
\begin{align*}
    x &= 0 \\
    y &= \frac{2m_h \varepsilon_h}{M} \cos(\omega_h t + \alpha_1) - \frac{2m_v \varepsilon_v}{M} \cos(\omega_v t + \alpha_3) \\
    \varphi &= -\frac{2m_v \varepsilon_v}{M} b \cos(\omega_v t + \alpha_3)
\end{align*}
\]

(7)

It is easy to notice, that in the first case for providing the same character of rotors motion there is no need to connect rotors in both pairs kinematically: it is
Self-synchronization of four mechanical vibroexciters at various variants of kinematical connection

enough to make it only for one pair. The other pair is self-synchronized with the same phases. So, for example, if we connect rotors in the upper pair, supposing that \(\sigma_3 = -\sigma_4 = 1\); \(\alpha_3 = \alpha_4 + \pi\) then at \(\sigma_1 = -\sigma_2 = 1\) potential function \(D\) will be

\[
D = -m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M} + \frac{b^2}{2I}\right)\cos(\alpha_1 - \alpha_2) + C_1
\]

where \(C_1\) - a constant. The minimum of this function will be reached at \(\alpha_1 = \alpha_2\), i.e. phasing of the first case will be steady.

4 The case of kinematically unconnected rotors

In this the most general case the research of possible steady modes of synchronous rotation of rotors comes down to the finding the points of a function strict minimum

\[
D = \sigma_1\sigma_2m_h^2\varepsilon_h^2\omega^2\cos_2\left(\frac{1}{M} + \frac{h^2}{2I}\right) + \sigma_1\sigma_3m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M}\cos\alpha_3^* - \frac{\sigma_3}{2I}\sin\alpha_3^*\right) + \sigma_2\sigma_3m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M}\cos\alpha_3^* - \frac{\sigma_3}{2I}\sin\alpha_3^*\right) + \sigma_1\sigma_4m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M}\cos\alpha_4^* - \frac{\sigma_4}{2I}\sin\alpha_4^*\right) + \sigma_2\sigma_4m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M}\cos\alpha_4^* - \frac{\sigma_4}{2I}\sin\alpha_4^*\right) - \sigma_3\sigma_4m_h^2\varepsilon_h^2\omega^2\left(\frac{1}{M} + \frac{b^2}{2I}\right)\cos(\alpha_3^* - \alpha_4^*),
\]

where \(\alpha_2^* = \alpha_2 - \alpha_1\); \(\alpha_3^* = \alpha_3 - \alpha_1\); \(\alpha_4^* = \alpha_4 - \alpha_1\).

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References


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Influence the dispersion on disturbance in solid mechanics for great gradient

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ABSTRACT

The work is devoted to alternative formulation of equilibrium conditions as conditions of equilibrium angular moment for continuous mechanics. Then equilibrium conditions of forces are the special case of more common conditions of equilibrium of angular moment. The modified equations of conservation are conservation laws of density, linear moment, energy and new law is law for angular moment are suggested. The stress tensor is not symmetric. The nonsymmetrical stress tensor is determined from the phenomenological theory of elasticity. The law of angular momentum in an elementary volume is employed, for gas this law is received from the modified Boltzmann equation. The boundary conditions are discussed. Some examples is adduced. Keywords: angular moment, conservation laws, nonsymmetrical stress tensor, Boltzmann equations, Chapman-Enskog method, conjugate problem

1 Introduction

Gas-surface interaction plays an essential role in processes connected with atmosphere re-entry vehicles that is essential to solute the conjugate problem at any height of the flow. It is necessary to know aerodynamic characteristics of the spacecraft for the rarefied gas, transitional rarefied – flow regimes and continues regimes. The particles interact, using forces and moments. The principle difference between ours and classical equations for the description of the continuous mechanics consists in consideration of the angular moment variation in an elementary volume, as usually it is disregarded. Influence of the variation the angular moment in an elementary volume is studied for gas, liquid and solid mechanics in [1-4]. The asymmetric press tensor is obtained. Its value of asymmetric is received. The degree of asymmetric stress tensor we received from moment equation ( in projections ). Determination of
mechanical properties of nanostructures with complex crystal using moment interaction at microscale is discussed in [5]. Usually equilibrium conditions are postulated as conditions of equilibrium of forces. Then the angular moment law is fulfilled if stress tensor is symmetric. The second type of equilibrium is equilibrium of moment. We analyzed some macroscopic effects for some this cases. The problem was considered for the distribution of the stress in point K of the infinite plate under the uniform load along the segment BC lying inside the plane and having the angle with the axis y and for twisting. The Prandtl problem for two and three dimension were investigated. It was received the second solution in this tasks. Some experimental facts [6, 7] tell us about importance of gradients physical parameters. There is the connection between moment theory and the gradient theory. Besides the minimum of functional with moment for these problems has the local minimums. As at conclusion the volume value was rejected as value is more small in comparison with surface value. It should be mentioned that this values tell from another by one order. So the global minimum one have too but it is less and the destruction stress is less too.

2 Influence of the dispersion in the fluid mechanics

The angular moment does not contain the new dimension constants and nonstationary contains in density and velocity but not have the nonstationary term. Then we received the modified Navier-Stokes equations and conservation equations

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} + \frac{1}{\rho} \left( \nabla \cdot \mathbf{P} \right) = 0.
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} \left( \rho u_i + P_{ij} + x_j \frac{\partial P_{ij}}{\partial x_i} \right) - \frac{\mathbf{F}}{m} = 0.
\]

\[
\frac{\partial}{\partial x_i} \left( \rho \left( \frac{3}{2} RT + \frac{1}{2} u^2 \right) + \frac{\partial}{\partial x_i} \left[ \rho u_i \left( \frac{3}{2} RT + \frac{1}{2} u^2 \right) + u_k P_{kj} + q_j \right] + \frac{\partial}{\partial x_i} \left[ \rho u_i \left( \frac{3}{2} RT + \frac{1}{2} u^2 \right) + u_k P_{kj} + q_j \right] = 0.
\]

The law of the angular momentum in an elementary volume is employed. We obtain the equation for angular moment from the modified Boltzmann equation.

\[
\frac{\partial \mathbf{M}}{\partial t} + \nabla \times \mathbf{F} = 0,
\]

For the small gradients angular moment \( M \approx 0 \). The last equation for usual Boltzmann equation degenerates in equality \( P_{ij} = P_{ji} \). Then new equation of the gasdynamics are constructed. There are: \( t \)-time, \( x \)-coordinate, \( \rho \)-density, \( P_{ij} \)-stress tensor, \( u \)-velocity, \( T \)-temperature. For the kinetic theory the boundary conditions at infinity are as in classical case. There are another on surface and include the gradient of the distribution function in longitudinal direction. That is can follow from the modified Boltzmann equation to write at surface. It is possible to write the equation for the \( N \)-distribution function in region

\[
|x_1 - x_2| \leq \sigma
\]
\[
\frac{\partial P_N}{\partial t} + \xi_1 \cdot \frac{\partial P_N}{\partial x_1} + \xi_2 \cdot \frac{\partial P_N}{\partial x_2} + \sum_{j=3}^{N} \xi_j \cdot \frac{\partial P_N}{\partial x_j} + X_{12} \cdot \frac{\partial P_N}{\partial \xi_1} + X_{21} \cdot \frac{\partial P_N}{\partial \xi_2} = 0
\]

The equation for two-part distribution function is [8]

\[
\frac{\partial P_{N}^{(2)}}{\partial t} + \xi_1 \cdot \frac{\partial P_{N}^{(2)}}{\partial x_1} + \xi_2 \cdot \frac{\partial P_{N}^{(2)}}{\partial x_2} + X_{12} \cdot \frac{\partial P_{N}^{(2)}}{\partial \xi_1} + X_{21} \cdot \frac{\partial P_{N}^{(2)}}{\partial \xi_2} = 0
\]

It is possible to depend one particle from gas and another is from surface. At the boundary of \(|x_1 - x_2| \leq \sigma\) the distribution function is the Chapman-Enskog function. The flow of molecules through boundary is reaching surface without collisions. The model of interaction the gas with surface can be as in [9]. After integration on \(x_2\) we have the force influenced at one-particle function. From the modified Navier-Stokes equations after integration on \(y\) we have the boundary conditions for continuous medium with addition term along longitudinal coordinate. Additional term one can obtain from the Boltzmann equation.

### 3 The Prandtl problem

The degree of asymmetric the stress tensor we can received from moment equation (in projections)

\[
y \left( \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z \left( \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) + \tau_{zy} - \tau_{yz} = 0,
\]

\[
x \left( \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z \left( \frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \tau_{zx} - \tau_{xz} = 0,
\]

\[
x \left( \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) - y \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \tau_{yx} - \tau_{xy} = 0
\]

Thus we have (fig.1)

\[
\frac{\partial}{\partial y} \left[ x \left( \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) - y \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) \right] = \Delta_{yx}
\]

\[
\frac{\partial}{\partial z} \left[ x \left( \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z \left( \frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) \right] = \Delta_{xz}
\]

For the same index (ii, kk, jj) it is necessary to calculate the gradient of physical values but it give the classical stress tensor. To define connection the stress tensor with the velocity (rheology) should be found the point into elementary volume with forces are equal zero. Then we have to consider the Taylor series to coordinate. Another variant is to employment the classical processes to keep uniformity of designation for gas and for solid body we shall be \(S \approx \sigma\)

\[
\hat{S} \left( \begin{array}{c}
\dot{S}_{xx} \\
\dot{S}_{xy} \\
\dot{S}_{xz} \\
\dot{S}_{yx} \\
\dot{S}_{yy} \\
\dot{S}_{yz} \\
\dot{S}_{zx} \\
\dot{S}_{zy} \\
\dot{S}_{zz}
\end{array} \right) = \left( \begin{array}{ccc}
\frac{\partial u}{\partial x} & \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{1}{2} \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \\
\frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \\
\frac{1}{2} \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) & \frac{1}{2} \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & \frac{\partial w}{\partial z}
\end{array} \right)
\]
We consider the Prandtl problem of compression layer by two rough plates in [2]. We make use the equations of equilibrium. This formulation of problem of moment theory is not well. The theory contradicts the Navie equations as in equilibrium the movement is absent. We suggest that

\[
\frac{\partial}{\partial y} \left[ x \left( \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) \right] - \frac{\partial}{\partial x} \left[ y \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) \right] = \Delta_{yx},
\]

\[\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0,\]

from here is

\[
\frac{\partial^2 \sigma_{yy}}{\partial y^2} - \frac{\partial^2 \sigma_{xx}}{\partial x^2} = 0, \quad \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} = k,
\]

\[\sigma_{yx} = k_1 y, \quad \frac{\partial \sigma_{yy}}{\partial x} = k - k_1 = k_2, \quad \sigma_{xx} = k_2 x + \varphi(y), \quad \frac{\partial \sigma_{yy}}{\partial x} = 0,
\]

\[\frac{\partial}{\partial x} \left\{ (x \frac{\partial \sigma_{yy}}{\partial y}) - y k \right\} + \frac{\partial \sigma_{yy}}{\partial y} = 0, \quad \frac{\partial \sigma_{yy}}{\partial y} + x \frac{\partial^2 \sigma_{yy}}{\partial x \partial y} + \frac{\partial \sigma_{yy}}{\partial y} = 0,
\]

\[\partial \sigma_{yy} = f(x), \quad k_2 + k_1 - k = 0.
\]

One of the solution is

\[u = -ax \pm ah \sqrt{1 - \left( \frac{y}{h} \right)^2} + c_1, \quad v = ay, \quad c_1 = \text{const}
\]

Conclusions

Present paper is continuation of the previous works. We discuss the problems that can be appearing to considerate the angular moment variation in an elementary volume near the surface.

REFERENCES
The efficiency of using the stress recovery procedure for the finite element method on the example of the problem with small deformations

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Abstract

The proposed stress recovery procedure allows us to construct the stress field for the problem without numerical differentiation of the displacement field obtained by the finite element method. In this paper, the idea of the procedure is demonstrated in the framework of the small deformation theory. In accordance with this procedure the distributed forces are defined on the internal surfaces of the body. The problem is reduced to solving the systems of linear algebraic equations. Using the Cauchy relation, the components of the stress tensor are computed for the nodes of the finite element grid. This method has been used to solve the problem and proved to be effective enough.

1 Introduction

In solid mechanics numerical realization of the virtual displacement principle by the finite element method (FEM) usually leads to a fairly good approximation of the displacement field and to a considerably worse approximation of the stress field. This is connected with the need to differentiate the displacement field for constructing the stress field. A number of algorithms have been proposed to solve this problem in the framework of the Lagrange statement. The first algorithm is based on changing the positions of the finite element nodes without increasing the degrees of the finite element freedom. The other algorithms involve increasing the degrees of the finite element freedom by means of adaptive remeshing of the finite element grid, or by increasing the approximation degree of the required variables in the finite elements.

Numerical realization of the virtual displacement principle by the finite element method (FEM) can also be accomplished by the well-known stress recovery methods. These methods include the mean stress technique for elements adjacent to a given node with subsequent extrapolation of the obtained nodal values to the body.
boundary; the conjugate approximation method; the technique of the spline functions for smoothing the displacement field; the fundamental solution method. The methods are not equivalent neither in accuracy nor in complexity of numerical realization. Here we use the stress recovery procedure, in which the nodal forces are defined with the help of the FEM stiffness matrix. It was first proposed by Navaratna [1] and Striklin [2] and was developed further by Rogovoy [3, 4, 5] and Kalinin [4]. The stress recovery procedure is rather effective both in accuracy and required computer resources.

2 The idea of the stress recovery procedure

Let us consider the variational statement of the boundary-value problem of small deformations in the framework of solid mechanics

\[
\int_S \vec{q} \cdot \delta \vec{u} \, dS + \int_V \rho \vec{K} \cdot \delta \vec{u} \, dV - \int_V \vec{\bar{T}} \cdot \delta \vec{\varepsilon} \, dV = 0, \tag{1}
\]

where \(\vec{q}\) is the vector of external surface forces, \(\vec{K}\) is the vector of mass forces, \(\vec{u}\) is the displacement vector, \(\vec{\bar{T}}\) is the stress tensor and \(\vec{\varepsilon}\) is the tensor of small strains. According to the FEM for numerical realization of this equation we approximate the displacement vector \(\vec{u}\) using its nodal values \(\vec{u}_k\) and the shape functions \(\psi_k^{(j)}\):

\[
\vec{u} = \sum_{k=1}^{n} \vec{u}_k \sum_{j \in M^V_k} \psi_k^{(j)}, \quad j = 1, 2, \ldots, m, \tag{2}
\]

where \(M^V_k\) is a set of numbers for elements adjacent to the \(k\)-th node in the volume \(V\), \(n\) and \(m\) are the numbers of nodes and finite elements. The solution of problem (1), taking into account the approximation (2), gives the values of the displacement vector at the nodes.

Let us choose within the body a sufficiently smooth surface \(l\), formed by the sides of the finite elements and dividing the body into two parts. Neglect one of the parts. The distributed force \(\vec{p}\), acting on the surface \(l\) of the remaining part of the body on the side of the neglected one, is the unknown quantity. The vectors \(\vec{Q}_k\) of the forces reduced to the nodes are found from the forces distributed over the element surface and the shape functions. On the other hand, the force reduced to the nodes can be defined as the product of the stiffness matrix for this node and the obtained nodal displacement vector. Thus we obtain the system of the Fredholm integral equations of the first kind:

\[
\sum_{j \in M^S_k} \int_{S_1} \vec{q}_* \psi_k^{(j)} \, dS_1 = \vec{Q}_k, \quad k \in N_*, \tag{3}
\]

where \(N_*\) is the set of numbers for nodes belonging to the surface \(l\), \(M^S_k\) is the set of numbers for elements adjacent to the node \(k\) and forming the surface \(S_k = S_1 \cup l\) by their sides, \(\vec{q}_*\) is the prescribed vector on the surface \(S_1\) \((\vec{q}_* = \vec{q})\) or the unknown vector on the surface \(l\) \((\vec{q}_* = \vec{p})\).
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Let the distributed force $\vec{p}$ be approximated on the surface $l$ with the help of its nodal values $\vec{p}_k$ and the shape functions $\psi_{(i)}^k$:

$$\vec{p} = \sum_{k=1}^{K} \vec{p}_k \sum_{j \in M_k} \psi_{(i)}^k,$$  \hspace{1cm} (4)

where $K$ are the numbers of nodes belonging to the surface $l$, $M_k$ is the set consisting of the numbers of elements adjacent to the $k$-th node and forming the surface $l$ by their sides. Note that vectors $\vec{u}$ (2) and $\vec{p}$ (4) have the same approximation order.

To define the unknown quantities $\vec{p}_k$ in expression (4) we apply the method of the least squares and minimize the functional with respect to $\vec{p}_k$

$$\min_{\vec{p}_k} \int_l \left( \vec{p} - \sum_{k=1}^{K} \vec{p}_k \sum_{j \in M_k} \psi_{(i)}^k \right) \cdot \left( \vec{p} - \sum_{k=1}^{K} \vec{p}_k \sum_{j \in M_k} \psi_{(i)}^k \right) \, dl + \alpha R(\vec{p}_k),$$ \hspace{1cm} (5)

where $R(\vec{p}_k)$ is the regularizer with parameter $\alpha$. The relation for $R(\vec{p}_k)$ can be written as

$$R(\vec{p}_k) = \sum_{k=1}^{K} \sum_{i > k} (\vec{p}_k - \vec{p}_i) \cdot (\vec{p}_k - \vec{p}_i).$$

Thus, we obtain the system of linear algebraic equations determining $\vec{p}_k$.

Knowing the values of the distributed force at the nodes of the surface $l$ we can write the Cauchy relation for each node on this surface:

$$\vec{n}_l \cdot \tilde{T}_k = \vec{p}_l,$$ \hspace{1cm} (6)

where $\vec{n}_l$ is the unit normal at the node $k$, $\tilde{T}_k$ is $\tilde{T}$ at the node $k$. For a two-dimensional problem the tensor $\tilde{T}_k$ is represented by three independent coordinate components. So we obtain an underdetermined system where the number of equations is less than that of the unknown quantities. Choose within the body another surface $t$ going through the node $k$. Let us define the nodal values $\vec{n}_t$ of the distributed force on this surface and write down an additional equation to relation (6)

$$\vec{n}_t \cdot \tilde{T}_k = \vec{p}_t,$$ \hspace{1cm} (7)

Now we obtain an overdetermined system where the number of the equations is more than the number of the unknown quantities. Solving this system (two vector equations (6) and (7)) by means of the least square method we get the components of the stress tensor $\tilde{T}$ at the node $k$.

3 The axial symmetry problem under small deformations

We use the proposed stress recovery procedure to solve the problem with small deformations. Let the elastic cylindrical specimen be stretched by external distributed
forces applied to its end. Owing to the symmetry of the problem we shall consider only one quarter of the specimen axial section (Fig. 1(a)) with the following boundary conditions:

\[
  \begin{align*}
  r = 0 & : \quad u_r = 0, \; T_{rz} = 0; \\
  z = 0 & : \quad u_z = 0, \; T_{rz} = 0; \\
  r = a & : \quad T_{rr} = 0, \; T_{rz} = 0; \\
  z = b & : \quad T_{zz} = p_z(r), \; T_{rz} = 0.
  \end{align*}
\]

The finite element discretization of the domain is made using the grid \( m \times n \)

\[(\text{Fig. 1(b))}. \] The problem has been solved on the grids \( m \times n = 5 \times 10, \; 10 \times 20 \) and \( 20 \times 40 \) with linear and square approximation of the displacement field and triangular finite elements. The nodal stresses have been calculated using the standard mean stress technique for elements adjacent to the given node and the stress recovery procedure with \( \alpha = 10^{-6} \) and \( \alpha = 1 \) (in (5)). Geometry of the specimen has been defined by the quantities \( a = 1 \) and \( b = 2 \). The distributed forces applied to the end have been given as a function \( p_z(r) = 0.1(1+5r^4) \). The material constants have been assumed as \( \lambda = 1.5 \) and \( G = 1 \).

Figure 2 demonstrates the distribution of the tangent stresses \( T_{rz} \) over the horizontal cross-section of the specimen at \( z = b/2 = 1 \). Curves 1 and 2 (Figure 2(a)) have been calculated using the standard mean stress technique with the linear and square approximation of the displacement field. Curve 3 has been calculated by the recovery procedure developed for the vertical surfaces with \( \alpha = 10^{-6} \).

Curve 1 (Fig. 2(b)) has been calculated using the recovery procedure for the vertical surfaces with \( \alpha = 10^{-6} \). Curves 2 and 3 have been calculated by the recovery procedure for horizontal surfaces with \( \alpha = 10^{-6} \) and \( \alpha = 1 \). We note that curve 2 has oscillations at vertical surfaces which is characteristic of the Gibbs effect. Its smoothing (curve 3) reduces the oscillation, but does not lead to the prescribed zero boundary values at the vertical surfaces.

Figure 3 demonstrates the distribution of the tangent stresses \( T_{rz} \) over the vertical cross-section of the specimen at \( r = a/2 = 0.5 \). Curves 1 and 2 (Figure 3(a)) have been calculated using the standard mean stress technique with the linear and
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Figure 2: The stress $T_{rz}$ at the horizontal cross-section ($z = b/2 = 1$) square approximation of the displacement field. Curve 3 calculated by the developed recovery procedure for vertical surfaces with $\alpha = 10^{-6}$.

Figure 3: The stress $T_{rz}$ at the vertical cross-section ($r = a/2 = 0.5$)

Curve 1 (Fig. 3(b)) has been calculated using the recovery procedure for horizontal surfaces with $\alpha = 10^{-6}$. Curves 2 and 3 calculated by the recovery procedure for vertical surfaces with $\alpha = 10^{-6}$ and $\alpha = 1$. It should be noted that curve 1, calculated for horizontal surfaces, has zero values at the boundary points, while curves 2 and 3, calculated for vertical surfaces, show oscillations at these points.

It should be emphasized, that with the stress recovery procedure we can obtain the same approximation order of the stresses more quickly than with the standard mean stress technique.

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Analysis of Grinding Media Motion in Planetary Ball Mills

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Abstract

In planetary ball milling, the feed material is exposed to different stress conditions, resulting in varying product fineness. The stress conditions depend on the grinding media motion. Knowledge of the relationship of process parameters and stress conditions can help in the development of a stress model for this mill type. A stress model provides the means to estimate process parameter values needed to obtain a certain distribution of stress energies and therefore product quality.

The influence of important process parameters on the grinding media motion is assessed by experimental as well as numerical methods. High speed video shots of moving media were obtained in a laboratory scale mill. In a first qualitative analysis of the experimental results, the influence of mill speed ratio and friction is illustrated. Furthermore, a discrete element model was devised to simulate the ball motion in a planetary ball mill. The simulation results are compared to the video shots with respect to motion trajectories and velocities.

1 Motivation

Planetary ball mills consist of one or more rotating grinding chambers which are situated on a revolving sun wheel (Figure 1). The grinding chamber contains grinding media and the product material. A rotation of the grinding chamber is superimposed to a revolution of the sun wheel. Consequently, the grinding media are exposed to superimposed centrifugal forces and therefore posses high kinetic energies. They collide among one another or with the chamber wall, which results in the stressing of the product material.

Due to their high energy density planetary ball mills are especially suited for the fine grinding of hard and brittle material, mechanical alloying and mechanochemical reactions. In comparison to other mill types like tumbling mills, higher stress intensities can be generated due to the centrifugal field. The stress intensity describes to
what extent the product particles are stressed in a process. Planetary ball mills are
built almost exclusively for batch operation, peripherals like pumps or complex pro-
cess control equipment are barely needed. This makes planetary ball mills relatively
cost-effective while being straightforward in handling. Another benefit is the simple
sterilisability of the grinding chamber, being especially favourable for applications
which imply high purity requirements like the pharmaceutical industry.

On the other hand, planetary ball mills also possess some drawbacks due to their
working principle: above certain installation sizes, major technical difficulties in the
mills’ drive systems emerge. Beyond that cooling of the grinding chamber in dry
grinding is a major issue. So far, these effects are controllable only in small scale
planetary ball mills, which limits this mill type to laboratory application. Another
issue is the design of feeding and product removal for continuous operation. Al-
though there have been some solutions presented, they remain technically extremely
demanding. This is why planetary mills are usually operated in batch mode.

As a result of the benefits mentioned, planetary ball mills are very interesting
for application in process development i.e. new processes can be developed in a
laboratory scale planetary ball mill. For the production scale, the process is then
transferred to another mill type such as ball mills, vibrating mills or stirred media
mills. This requires knowledge about the stress conditions in the planetary mill,
in order to ensure similar conditions during the transfer. Knowledge about the
stress conditions is necessary not only for these transfer tasks but also for research
regarding mechanical alloying and mechanochemical reactions.

In order to characterise the stress in planetary ball mills information about the
motion patterns of the grinding media present in this mill type is needed. The
grinding media movement varies depending on the mill operating parameters, so
these have to be considered carefully. In the following the major parameters are
introduced:

The angular velocities of the grinding chamber $\omega_G$ and the sun wheel $\omega_S$ are
related by the speed ratio $k$:

$$k = \frac{\omega_G}{\omega_S}$$

The speed ratio $k$ is defined as positive for both angular velocities having the
same direction of rotation. For instance, a speed ratio of $k = -2$ describes the
case where the grinding chamber rotates with the double absolute value of the sun wheel’s angular velocity and in opposite direction.

Important geometric parameters are the diameter ratios of the sun wheel related to the grinding chamber inner diameter

\[
\frac{d_S}{d_G} = \frac{\text{sun wheel diameter}}{\text{grinding chamber diameter}} \tag{2}
\]

as well as grinding chamber inner diameter related to grinding media diameter

\[
\frac{d_G}{d_{GB}} = \frac{\text{grinding chamber diameter}}{\text{grinding media diameter}} \tag{3}
\]

Another process parameter of influence is the grinding media filing ratio, which is defined as the grinding media bulk volume over the grinding chamber volume:

\[
\varphi_{GM} = \frac{\text{grinding media bulk volume}}{\text{grinding chamber volume}}. \tag{4}
\]

Furthermore, different parameters are used to describe the amount of product material, depending on whether grinding is carried out in dry or wet: In dry grinding, the product filling ratio \(\varphi_C\) is applied as follows

\[
\varphi_P = \frac{\text{product bulk volume}}{\text{grinding media void volume}}. \tag{5}
\]

In contrast, the suspension filling ratio

\[
\varphi_S = \frac{\text{product suspension volume}}{\text{grinding media void volume}} \tag{6}
\]

and solids content \(c_m\)

\[
c_m = \frac{\text{mass of product particles}}{\text{suspension mass}} \tag{7}
\]

are used for the characterisation of wet grinding processes. Other parameters of influence in planetary ball milling are milling time and material parameters like density, particle size and friction.

Figure 2 shows the occurrence of different motion patterns of grinding media in a planetary ball mill according to Höfl [1]. From theoretical considerations Höfl deduced this diagram where the four different patterns are displayed in dependence of the speed ratio and diameter ratio of sun wheel and grinding chamber. The lines limit the zones of different motion patterns. In the so called sliding regime the bulk of grinding media slips on the grinding chamber wall. A motion where the grinding
media experience a lift by the chamber wall and in the following carry out a rolling motion upon each other is designated the cascading regime. The cataracting regime occurs, when grinding media detach from the wall due to centrifugal forces and cross the grinding chamber in flight. In the case of high centrifugal forces occurring, the grinding media will be supported by the grinding chamber wall and follows its rotating motion being centrifuged. This motion pattern is undesirable in most applications, since the product particles are only slightly stressed.

As mentioned before, the relationships described are based upon theoretical considerations. Other publications contain theoretical deductions of grinding media motion as well [2, 3]. A systematic analysis of the grinding media motion in planetary ball mills by means of experiments is lacking so far.

The Discrete-Element-Method (DEM), developed by Cundall and Strack [4], has been increasingly used in research on ball milling processes since the 1990s. Utilizing DEM simulation, Mishra [5] showed a quantitative analysis of the grinding media movements in planetary mills with respect to their dependence on several operating conditions like grinding media filling ratio, relative speed ratio and friction coefficient. He underlined the strong impact of varied friction coefficients on the motion pattern of the grinding media. Amongst others, Mishra’s results show an increased amount of high-energy impacts and a loosening of the grinding chamber load for increased friction coefficients. Consequently, the analysis of friction is an essential element in the investigation of stress conditions in planetary ball mills. Yet, friction is neglected in the analytical studies existing at present. In other works by Kano et al. [6] a method was developed and validated enabling the estimation of a rate in a planetary ball mill by simulating the specific impact energy of grinding media. The same group further published results on the influence of the rotational direction and the speed ratio on impact energy, based on DEM-simulation and grinding experiments [7]. The results principally correspond with those summarized by Höffl [1] in Figure 2. At the moment, impact energies can be controlled by a skillful choice of
operating conditions. Furthermore the results concerning grinding media motion indicate the possibility to affect the amount of grinding media contacts. A systematic study, as for instance in the case of stirred media mills, has not yet been conducted.

2 Experimental

A laboratory scale planetary ball mill (*Retsch PM400*) was equipped with a test rig which enables the observation and recording of the grinding media motion inside the grinding chamber (Figure 3). For this, a high speed camera (*Prosilica GC640*) was placed on top of the grinding chamber lid. Lighting is supplied by several LEDs incorporated in the lid as well. The camera is fixed on the grinding chamber and therefore carries out the same rotating motion. As a result the relative motion of grinding media and grinding chamber is observed. The camera is connected to a computer, enabling recording and analysis of the images at a rate of 250 frames per second.

The planetary ball mill possesses an effective sun wheel diameter $d_S$ of 300 mm. The stainless steel grinding chambers are interchangeable so that different chamber volumes can be employed. A change in volume implies also a change in grinding chamber diameter $d_G$, so the diameter ratios are affected by this change. Stainless steel grinding media of different diameters (see Table 1) were used as grinding media. The filling ratio was $\varphi_{GB} = 0.3$. Other parameters were varied as listed in Table 1.

With this setup, image sequences of the grinding media motion are captured. In this early stage of study, no product material was added in order to keep analysis simple. Utilising the recorded image sequences, the motion of certain marked
Table 1: Variable operating parameters of the laboratory planetary ball mill

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value(s) / range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>speed ratio $k$</td>
<td>-3; -2.5; -2; -1</td>
<td>-</td>
</tr>
<tr>
<td>sun angular velocity $\omega_S$</td>
<td>3 - 42</td>
<td>s$^{-1}$</td>
</tr>
<tr>
<td>diameter $d_G$</td>
<td>65; 70; 100</td>
<td>mm</td>
</tr>
<tr>
<td>diameter $d_{GM}$</td>
<td>3; 10; 20</td>
<td>mm</td>
</tr>
</tbody>
</table>

grinding media was analysed by particle tracking software.

## 3 Simulation

In addition to experimental investigations, the grinding media motion is examined by simulation. A three-dimensional model of the laboratory mill was created using the commercial software *Itasca PFC3D*. The dimensions and operating conditions of the mill used here are the same as described above for the experiments. Figure 4 displays the model in the program view with grinding media being represented by spheres, wireframe representations of the grinding chamber (right) and a wireframe arm to simulate the mill’s sun wheel (left).

The simulation incorporates a linear contact model as described for example by Mishra [5]. The parameters needed are either taken from the literature or determined experimentally. Since the grinding chamber and grinding media are made of stainless steel, density is set to 7800 kg/m$^3$. A reduced stiffness of $10^5$ N/m is employed in order to keep simulation time reasonably short. The damping coefficient is calculated from a measured restitution coefficient. This is in turn derived from drop tests as described by Mishra or Heinrich [5, 8]. A grinding media is dropped from the height, $h_1$, onto a fixed plate. By means of a digital camera the rebound height, $h_2$, is measured. The coefficient of restitution $e$ can then be calculated from the ratio of rebound height to falling height and the ratio of velocities after, $v_2$, and before the collision, $v_1$: 
Table 2: Speed ratios analyzed with respect to grinding media motion and the corresponding motion pattern as predicted by Höfl (Figure 2)

<table>
<thead>
<tr>
<th>speed ratio k</th>
<th>motion pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3</td>
<td>centrifuging</td>
</tr>
<tr>
<td>-2.5</td>
<td>cascading</td>
</tr>
<tr>
<td>-2</td>
<td>cascading</td>
</tr>
<tr>
<td>-1</td>
<td>sliding</td>
</tr>
</tbody>
</table>

\[ e = \frac{v_2}{v_1} = \sqrt{\frac{h_2}{h_1}}. \]  \hspace{1cm} (8)

Values of the friction coefficient given in the literature vary in a range of 0.7 - 0.9. According to Cleary [9] \( e = 0.75 \) for steel media is selected as a first approximation. Later on, friction coefficients shall be measured experimentally.

4 Results

The impact of mill speed ratio \( k \) on grinding media motion was investigated using the described mill test rig. Speed ratios were set as given in Table 2. The revolution speed of the sun wheel \( n_S \) was held constant at 180 min\(^{-1}\) (corresponding to \( \omega_S = 18.8 \text{ s}^{-1} \)). The grinding chamber diameter \( d_G \) was 100 mm and as media diameter \( d_{GB} \) of 10 mm was chosen for this series of measurements. The resulting grinding media motion is depicted in Figure 5. The comparison of the shots show that no differences in grinding media motion occur when the speed ratio is varied. In all four cases cascading of the media is observed. This is emphasized even better by analysis of the recorded image sequences when played in total. First results of the DEM-model for different speed ratios are in agreement with the experimental observation. According to these findings in contrast to Höfl [1] and other theoretical calculations by Raasch [2], the mill speed ratio does not influence the grinding media motion at all for the investigated mill parameter configurations. The reason for this observed difference is subject of further investigations currently conducted.

In order to show the influence of a product material being present, a comparison of the grinding media motion with the absence and presence of limestone product particles was conducted. The feed limestone fraction possessed a size distribution between 1000 and 4000 \( \mu \text{m} \) with a median size \( x_{50} \) of 1925 \( \mu \text{m} \). The filling ratio was set to \( \varphi_P = 0.5 \). The revolution speed of the sun wheel \( n_S \) was held constant at 180 min\(^{-1}\) (corresponding to \( \omega_S = 18.8 \text{ s}^{-1} \)) while speed ratio was \( k = -3 \) for this case. The charge was milled for 1 min before the recording of the image sequence in order to allow for mixing and adhesion of product on the grinding media.

The resulting motion patterns are shown in Figure 6. Arrows indicate the rotational directions of the grinding chamber (grey) and the grinding media relative to the grinding chamber (white). Considerable differences in motion can be observed. While the grinding media carry out a steady clockwise motion as a bulk in case of no charge added, several rotational directions and velocities can be monitored.
Figure 5: Video shots of grinding media motion for different speed ratios $k$

Figure 6: Video shots of grinding media motion without charge (left, $\varphi = 0$) and with limestone charge (right, $\varphi = 0.5$). $k = -3$, $\omega_s = 18.8 \text{ s}^{-1}$ for both cases.
in the presence of limestone. In the chamber’s centre some media carry out small circular and clockwise movements with a superimposed counterclockwise rotation. A similar counterclockwise motion at low velocities is observed for a ring-shaped group of grinding media moving along the chamber wall. Last, one or few grinding media move on top of the others at high velocities in clockwise direction.

Figure 6 clearly shows that grinding media motion strongly depends on the combination of material employed and therefore the present friction conditions. DEM-simulation with varied coefficient of friction in the range of 0.1 to 0.8 also show a strong influence on the grinding media motion. These results are in good agreement with prior findings by Mishra [5].

5 Conclusions

Planetary ball mills exhibit desirable properties which make them very interesting for an application in the lab scale stage of process development. Possible applications are fine grinding, mechanochemical reactions as well as mechanical alloying. In order to allow the scale-up to production, knowledge about the stress conditions in the planetary mill is necessary. These depend on the grinding media motion inside the grinding chamber.

A test rig was built with a high speed camera attached to the grinding chamber lid, enabling the observation of relative motion of grinding media and grinding chamber. On the basis of video camera shots, considerable differences between the theoretically derived predictions from the literature and experimental observations of grinding media motion are demonstrated. The mill speed ratio \( k \) was designated a key influencing parameter of grinding media motion in the literature. In the experiments conducted, no influence of speed ratio could be observed in a range \(-3 < k < -1\). More detailed investigations are conducted to clarify the impact of the speed ratio. Other operating parameters have to be looked at, too. Furthermore, a strong impact of friction on the grinding media motion could be identified from the experiments. Thus, friction necessarily has to be considered in future studies on stress conditions in the planetary ball mill. Experimental as well as simulation techniques are currently being employed to gain further insight to the correlation of grinding media motion and stress conditions in the planetary mill.

References


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The approach to estimating local stress in block boundaries in interfacially-structured materials and media on basis of interface response to dynamic loading

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Abstract

The effect of local shear stress on strain response of block boundaries (interfaces) to dynamic loading in interfacially- and block-structured media has been studied through computer-aided simulation using movable cellular automaton method. The study provided grounds for an extended approach to estimating proximity of local shear stress in the interfacial zone to critical (ultimate) value as well as to diagnosing belonging of local stress state to quasi-elastic or quasi-plastic stage of material or medium deformation.

1 Introduction

An important direction in deformable solid physics and mechanics is investigation of features of mechanical response of so-called interfacially structured (or controlled) materials. This term combines materials, which mechanical behavior is defined significantly by processes of strain localization in boundaries between structural elements (i.e. in interface regions). Class of interfacially controlled materials/media with relatively highly deformable interface regions is wide enough. In particular, it includes nanostructured materials, various composites as well as hierarchically organized block-structured geological media [1, 2, 3]. At this takes place, typical scale of structural elements (grains, blocks and so on) of interfacially structured materials of different nature can be from parts of micron (in case of nanostructured materials) up to tens - thousands kilometers (in case of lithospheric plates).

Main peculiarity of structure of interfacially controlled geological media is hierarchical organization of block structure [3, 4]. Fragments of rock massifs are separated by planar discontinuities, which sizes vary in very wide scale range. Because of this feature one of main deformation mechanisms of stressed block-structured geological
medium is relative displacement of structural elements (rock slabs) along the boundaries (interfaces), which are usually filled by highly damaged and lower strength material in comparison with material of blocks themselves [5, 6]. The regime and velocity of block motion along active boundaries are controlled by local geometry, structure and stress, as well as by natural and man-caused external forcing. The characteristic velocities can vary from a few millimeters per year (creep) to a few meters per second during coseismic (unstable) slip in large earthquakes as interfaces reach the critical shear stress. Therefore, estimating local stress in zones of active faults has been among priority objectives in rock mechanics and geomechanics. It appears reasonable to represent local stress by relative shear stress which is the key parameter that measures the proximity of an interface to the critical state where it becomes prone to unstable slip.

As shown in [7], local stress state of block interface can be characterized by the value of relative block displacement induced by testing impulse-like dynamic action. At the same time use of more complex loading conditions gives the possibility to analyze larger number of parameters of deformation response of interfacial region. The present paper is devoted to theoretical study of influence of shear stress level on features of deformation response of model interblock boundary in interfacially controlled (block structured) medium to complex dynamic (vibration) loads. Theoretical study based on computer-aided simulation by means of movable cellular automaton (MCA) method [8].

2 Problem statement and simulation results

The MCA simulation was performed with a qualitative 2D model of a boundary between structural elements of block-structured medium (Fig. 1a). The model sample consisted of two monolithic high-strength blocks separated by a discontinuity with the mechanic response of the latter imitating mechanical properties of cataclastic rock and characterizing by long segment recording irreversible deformation. The response functions of the movable cellular automata that simulated the blocks and interface region are shown in Fig. 1b (note that response function is a some analog of unified hardening curve in deformable solid mechanics). The interface was presumed to be strongly deformed and to involve damage of different scales. The damages much smaller than the CA size were included implicitly through the response function (see curve 1 in Fig. 1b), whereas those of the CA scale were simulated by disconnected (broken) CA pairs.

The model samples were loaded according to the following scheme. The lower elements in the lower block were locked and the load was applied to the upper elements in the upper block (Fig. 1a). In the model being considered dissipative and inertial influence of the environment was taken into account indirectly by an additional viscous force applied to the automata of the block side faces along the X (horizontal) axis ($F_{\text{visc}} = -\alpha V_x$, where $V_x$ is the velocity component of the corresponding automaton, see Fig. 1a). The system was driven to its initial stress and strain by applying an external force with a normal ($F_y$) and a shear ($F_x$) components to the upper CA of the sample and the following relaxation (Fig. 1a). In all experiments we used the same $F_y$ with its specific value about 20% of the yield stress of
The approach to estimating local stress in block boundaries in interfacially-structured materials and media on basis of interface response to dynamic loading

Figure 1: A 2D model of interface between elements of a structured medium: (a) structure and loading of sample; (b) response function of automata that simulate interface (curve 1) between blocks (curve 2). Dashed line corresponds to unloading.

The interface material (curve 1 in Fig. 1b). The automaton $S$ of the upper block was used as a local vibratory energy source situated near the boundary (Fig. 1a). Vibration loading was realized in the following way. Periodically changing normal repulsion force acted in all interacting pairs of automaton $S$ with its neighbors in addition to "conventional" potential and viscous interacting forces (Fig. 2):

$$F_{ij}^{rep} = \begin{cases} S_{ij} P_{\text{max}} \sin(2\pi \nu (t - t_{\text{start}})), & (n - 1)/\nu < t - t_{\text{start}} < (n - 1/2)/\nu \\ 0, & (n - 1)/\nu < t - t_{\text{start}} < (n - 1/2)/\nu. \end{cases}$$

where $S_{ij}$ is square of contact of interacting automata, $\nu$ is frequency, $t_{\text{start}}$ is time of vibration start, $t$ is current time, $P_{\text{max}}$ is amplitude of vibration pressure, $n$ is vibration cycle number.

Figure 2: Scheme of action of local vibratory energy source imitated by movable cellular automaton $S$.

It is known that the sample eigenfrequencies connected with propagation of longitudinal ($V_{\parallel}$) and transverse ($V_{\perp}$) elastic waves play an important role under vibration loading. For the present system (Fig. 1a) the eigenfrequency region is restricted within the values $\nu_{L} = V_{\perp}/2L$ and $\nu_{H} = V_{\parallel}/2H$, where $L$ is sample length and $H$ is sample height. In the described calculations frequency of vibration varied over a wide range including interval of eigenfrequencies of the simulated sample.

In Fig. 3, resistance of the model sample to steady shear ($F_{\text{res}}$) is plotted against shear displacement ($l_{sh}$), at user-specified value of $F_{y}$. The variables $F_{\text{res}}$ and $l_{sh}$

In Fig. 3, resistance of the model sample to steady shear ($F_{\text{res}}$) is plotted against shear displacement ($l_{sh}$), at user-specified value of $F_{y}$. The variables $F_{\text{res}}$ and $l_{sh}$
are normalized to the maximum strength $F_{\text{max}}$ and the interface thickness $h_{\text{intf}}$, respectively. The shear strength curve includes three intervals corresponding to the quasi-elastic (stage I in Fig.3), quasi-plastic flow (stage II), and supercritical (softening and residual strength, stage III) stages. In described calculations various shear stresses (characterized by the value of $F_x$) were considered. Some of them are marked in the loading curve (Fig.3) by points.

![Figure 3: Normalized shear resistance of model active fault wall ($F_{\text{res}}/F_{\text{max}}$) vs. relative shear displacement ($l_{sh}/h_{\text{intf}}$). Shear deformation was carried out with constant velocity $V_x=0.1$ m/s. Points on the load diagram mark some selected stress levels: 1 - $F_{\text{res}}=0.56F_{\text{max}}$; 2 - $F_{\text{res}}=0.66F_{\text{max}}$; 3 - $F_{\text{res}}=0.76F_{\text{max}}$; 4 - $F_{\text{res}}=0.82F_{\text{max}}$.](image)

Simulation results have shown that under conditions of applied constant force $F_x$ local vibration leads to gradual accumulation of irreversible strains in different areas of interface region and subsequent formation of damages. This results in initiation of dynamic but low-amplitude irreversible displacements, which can be considered as small "stable" slips (Fig. 4a) As may be seen from the Fig. 4b, these slips are accompanied by "bursts" of velocity of upper block displacement. Initiated slips contribute to acceleration of irreversible damage accumulation process in different areas of interface region. At this takes place, increase of number of damages leads to "amplitude" and typical velocity of upper block dynamic slips. So, these two processes becomes mutually accelerating. On the certain stage effective shear strength of the interface region becomes lower than specific value of applied force $F_x$, and next dynamic displacement of the upper block becomes non-stop, that is to say, unstable relative slip of blocks takes place (Fig.4).

Analysis of simulation results have shown that character and peculiarities of relative block displacement in the stage of "stable" deformation (preceding initiation of unstable dynamic slip) are in many respects defined by parameters of vibration loading. In particular, Fig.5a illustrates dependences of total "stable" displacement $l_{sh}$ of the upper block on vibration frequency. It can be seen that in domain of "low" frequencies (which are lower than eigenfrequencies of the simulated system) the value of $l_{sh}$ rapidly falls as the frequency is increased. When passing to the region of eigenfrequencies the value of $l_{sh}$ reaches some level and remains nearly constant with further increase of frequency. As illustrated in Fig.5a, when the value of applied shear stress (characterized by the value of $F_x$) approaches stress level corresponding to the beginning of stage of quasi-plastic response of the interface (stage II in Fig.3), total "stable" shear displacement $l_{sh}$ step-wise falls (see curves 2 and 3). This effect
The approach to estimating local stress in block boundaries in interfacially-structured materials and media on basis of interface response to dynamic loading

![Graph](image1)

Figure 4: Dependence of relative relative shear displacement $l_{sh}/h_{intf}$ (a) and tangential component of upper block motion velocity $V_x$ (b) on number of cycles $N_{vibr}$ of local vibration ($F_{res}/F_{max}=0.66$, $\nu = 2\nu_{hi}$, $P_{max}=122.5$MPa).

...is connected with change of character of deformation of the interface. Distribution of local stresses in the interface region is very inhomogeneous. In this case vibration loading leads to appearance and accumulation of local irreversible strains in the most stressed areas. Strengthening of these areas results in involving other areas in processes of strain accumulation. It is evident that in case of less stressed sample such processes take place in larger number of areas (i.e. in larger volume). This provides relatively high deformation ability of the interface. Increase of the value of applied shear stress results in increase of volume concentration of highly stressed areas with initial stress state close to ultimate one. In this case even a weak vibration action lead to "coordinated" deformation of considerable part of interface region and hence to quick reaching of ultimate state of the interblock boundary. So, character of change of total "stable" displacement length (namely, its step-wise fall) indicates the "true" value of the shear stress corresponding to beginning of quasi-plastic flow stage for interblock boundary.

![Graph](image2)

Figure 5: Dependences of total value of "stable" relative block displacement $l_{sh}$ and number of "stable" low-amplitude slips $N_{dd}$ (b) on vibration frequency (vibration pressure amplitude $P_{max}=490$ MPa): 1 - $F_x=0.56F_{max}$; 2 - $F_x=0.66F_{max}$; 3 - $F_x=0.76F_{max}$; 4 - $F_x=0.82F_{max}$.

As noted above, relative motion of blocks in the stage of "stable" shear deformation is achieved mainly owing to low-amplitude dynamic slips (Fig.4). The number of such "stable" slips ($N_{dd}$) is nearly independent on vibration frequency, however it...
is defined to a great extent by stress state (Fig. 5b). As shown in Fig.5b, decrease of number of stable slips begins at shear stresses, which are much lower than "formal" point of transition from quasi-elastic to quasi-plastic deformation stage of interface (Fig.3), and has quite smooth character. Simulation results have shown that further decrease of applied shear stress (the value of $F_x$) doesn’t lead to noticeable increase of $N_{dd}$. Hence the interval of $F_x$ corresponding to curves 1 and 3 in Fig.5 indicates the length of "true" transition region between intervals of quasi-elastic and quasi-plastic response of considered interface.

An important part of research of behavior of block-structured media under dynamic actions is analysis of frequency spectrum of velocities of structural element. Because of this, frequency spectrum of mass velocity $V_x$ of the upper block in the stage of "stable" sample deformation was analyzed. Particular attention has been given to frequency interval below the maximum sample eigenfrequency $\nu_{eig}$. This interval includes periodic components of complex cooperative motion of the system (including dynamic slips). Fig. 6 shows typical frequency distribution of upper block velocities obtained by means of Fourier transform of dependence $V_x(t)$. It can be seen that this distribution is characterized by pronounced peaks corresponding to loading frequency ($\nu_{vibr}$), its derivative, maximum sample eigenfrequency ($\nu_{eig}$) (in Fig.6 $\nu_{eig}$ shifted to the left in consequence of plastic deformation of the interface region) and dynamic slips. Analysis of simulation results have shown that some integral characteristics of frequency distribution of upper block velocities strongly depend on the level of sample stress state.

Figure 6: Fourier transform of time dependence of mass velocity of the upper block in the stage of "stable" deformation of the sample (here $\nu_{vibr}/\nu_{H} =0.54$).

Fig.7a gives dependences of relative amplitude ($A_{rel}$) of the peak corresponding to vibration frequency on the value of (in this case, $A_{rel}$ was defined as a ratio of absolute amplitude of this peak to total amplitude of other peaks, which exceed background level by order of magnitude). One can see that while in the region of quasi-elastic system response the value of $A_{rel}$ decreases several times with increasing load frequency (curves 1 and 2), $A_{rel}$ becomes nearly constant (curve 3) as the "true" beginning of quasi-plastic deformation regime is approached (curve 3). On further increasing of initial stress level (curve 4), step-wise increase of $A_{rel}$ takes place. This effect is concerned with quasi-homogeneous character of plastic deformation of the interface region and therefore with sharp decrease of the number, amplitude and velocity of "stable" dynamic slips. An important result was obtained in analysis of energy of frequency spectrum of upper block mass velocities ($W$). As may be seen
The approach to estimating local stress in block boundaries in interfacially-structured materials and media on basis of interface response to dynamic loading from Fig. 7b, on reaching the ”true” transition region between intervals of quasi-elastic and quasi-plastic response of the interface, the value of $W$ decreases by an order of magnitude in all considered vibration frequency range. Further increase of initial stress doesn’t lead to noticeable change of this characteristic.

Figure 7: Dependence of relative amplitude ($A_{rel}$) of the peak corresponding to vibration frequency $\nu$ (a) and dependence of energy ($W$) of frequency spectrum of upper block mass velocities (b) on the value of $\nu$ ($F_{max}=490$ MPa): 1 - $F_x=0.56F_{max}$; 2 - $F_x=0.66F_{max}$; 3 - $F_x=0.76F_{max}$; 4 - $F_x=0.82F_{max}$.

3 Discussion of results and conclusion

Some years ago authors proposed an approach to estimating relative value of local shear stress (as compared with ultimate stress) in fragments of active block boundaries in faulted crust [7]. This approach is based on initiation of displacements in fault zone fragments by means of local testing impulse actions, registration and analysis of initiated displacements. Relevance of proposed approach is concerned in particular with possibility of its application for estimating local stress state of fragments of active tectonic faults in the earth’s crust. At the same time above described simulation results demonstrate that capabilities of this approach can be extended by use of serial (including vibration) actions. In particular, analysis of stress state of interface region can be done with several parameters of interface deformation response. These parameters are total value of initiated relative tangential (shear) block displacement, number of low-amplitude irreversible dynamic slips as well as characteristics of frequency spectrum of velocities of relative block displacement along the boundary (relative amplitude of the peak corresponding to vibration frequency, energy of frequency spectrum and possibly some other characteristics). Study of deformation response of investigated fragment of interblock boundary to local testing vibrations with various frequencies makes possible construction of dependences similar to shown in Fig. 5-7 and use them for more rigorous estimation of characteristic level of shear stress in the interface region.

It is important to note that use of vibration actions doesn’t replace previously proposed testing impulse-based approach, but supplements it. This allows us to propose an extended approach to diagnosing stress state in fragments of active block boundaries in block-structured media. The approach could be based on long-time
monitoring of dynamics of natural and man-caused displacements in studied part of active interface. Periodical carrying out of tests with use of impulse and vibration loading allows researcher to estimate proximity of stress state of the interface region to ultimate state as well as to diagnose belonging of stress state to quasi-elastic or quasi-plastic deformation stage and reveal the moment of passing into transition region between them. Importance of information about proximity of stress state to quasi-plastic stage is concerned with the fact that on passing into this stage even small stress variations can lead to quick reaching the ultimate state (Fig. 3).

In conclusion it may also be noted that in view of reasonable generality of considered model presented simulation results are qualitatively valid for various interfacially-controlled materials/media (in particular for nanostructured materials) and may be used to develop new methods to estimating their stress-strain state.

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The approach to estimating local stress in block boundaries in interfacially-structured materials and media on basis of interface response to dynamic loading

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Effect of surface topography on material flow in milli-scale deep drawing

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Abstract

One of the most important process factors in metal forming related to the tool/material design is the interfacial behavior between material and tool. Especially in micro scale region, it would be prefer not to use lubricant from the standpoint of not only environmental load but also the releasability from tools, clogging of lubricant, and also that of influence of meniscus force and viscous force on formability. In dry friction condition, dominant factor over the frictional behavior between tool and material is the contact behavior of surface topography. This study aims to clarify the effect of surface topography of tool and materials on deep drawing characteristics in dry friction condition. To investigate the effect of surface asperity of tool and material on forming behavior, an experimental study of cylindrical deep drawing process was conducted using mirror-polished and air-blasted tool sets and materials in milli-scale region, which is classified as the intermediate region between micro- and macro-scales. Tribological behavior results from the different surface topography were evaluated from comparison of drawing punch force and surface quality of drawn cup. Corresponding to this tribological behavior, by considering from the results of drawn cup thickness strain distribution, the effect on material flow in deep drawing process was discussed. As a result, it was demonstrated that the formability of deep drawing process in dry friction condition could be controlled by surface topography on tools and material.

1 Introduction

Metal forming has been widely prevalent as a manufacturing process in mass production. In recent years, against the trend toward more and more products having higher and higher electronic content, microforming technology, which has applied from conventional macro scale region to micro scale region, has been paid great attention as one of the most economical mass production methods for sub-millimeter-scale microparts [1].
One of the most important process factors in the metal forming related to the tool/material design is the interfacial behavior between material and tool. In particular in sheet metal forming, accuracy of products and forming failure such as fracture or wrinkling is strongly influenced by frictional behavior between material and tool. Since the frictional behavior depends upon local contact condition such as local surface roughness, pressure and relative speed between contact surfaces, many researches focused on local frictional behavior [2]. These frictional behaviors have been taken for granted to explain with condition using lubricant to enhance the formability and quality of products.

In micro scale region, however, it would be prefer not to use lubricant from the stand point of not only environmental load but also the releasability from tools, clogging of lubricant, and also that of influence of meniscus force and viscous force on formability. In dry friction condition, since the friction force depends on the real contact area and the shear strength of the asperity contact during sliding [3], it can say that a dominant factor over the frictional behavior between tool and material is the contact behavior of surface asperities. Meanwhile, the effect of local surface topography on the global forming behavior has not been revealed previously under the dry friction condition.

To consider the local and global factor simultaneously, this study focused on milli-scaled order, which is classified as intermediate region between micro- and macro-scale [4]. At milli-scaled order, there are some advantages as follows:

* It is easy to conduct the experimental investigation compared with micro-scale
* The results would be applicable to both the macro and micro scales.
* The surface roughness as a local geometrical factor can be considered in finite element (FE) model, which is difficult in macro-scale.

Within the above background, this study aims to investigate the effect of surface topography of tool and materials on deep drawing characteristics in dry friction condition. In this report, to investigate the effect of surface asperity of tool and material on global forming behavior under un-lubricated condition, an experiment of cylindrical deep drawing process for producing cups of 10.5mm in diameter and 0.3mm in thickness was conducted using mirror-polished and air-blasted tool sets and materials in milli-scale region. To evaluate the effect of surface properties on formability and forming accuracy, punch force during the process, surface accuracy, and thickness strain distribution of drawn cups were investigated experimentally.

## 2 Experiment

### 2.1 Material

A circular blank material was cut to 16.5mm in diameter from rolled stainless steel thin sheet (JIS; SUS304-H) of 0.3mm in average thickness. Table 1 shows the mechanical properties of the blank. It was obtained from tensile test whose specimen was referred to JIS No.13B test piece. Aside from the as-received material with rolling marks, air-blasting treatment was conducted to make the different surface asperities of the blank specimens. As the condition of air blasting treatment, glass powder of 53-63 µm size was irradiated for 1min on both sides of the sheet. Figure 1
shows the surface images of as-received blank and air-blasted blank of SUS304-1/2H sheet, which have obtained by confocal laser scanning microscope. As shown in Figure 1, rolling marks was removed by air blasting and the rough surface asperities were made by glass powder irradiation. Maximum surface roughness of air-blasted sheet is about 3 times rougher than that of as-received material. To eliminate the influence of work-hardening on the surface because of air-blasting treatment, both sheets of different surface asperities were annealed (Ar gas, 800, 1h).

![Surface images of the blank used in milli-scale drawing experiment](image)

**Figure 1: Surface images of the blank used in milli-scale drawing experiment**

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<table>
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<tr>
<td><strong>Young’s modulus E</strong>/GPa</td>
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<tr>
<td><strong>Yield strength</strong>(\sigma_y)/MPa</td>
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<tr>
<td><strong>Tensile strength</strong>(\sigma_b)/MPa</td>
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<tr>
<td>(r \text{ value} )</td>
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<tr>
<td><strong>Elongation</strong>(\lambda)/%</td>
<td>37</td>
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**Table 1: Mechanical properties of the blank used \((*\sigma = F\epsilon + \sigma_y)\)**

### 2.2 Tool set

milli-scale tool set was designed to producing cups of 10.5 mm in diameter and 1.6 of drawing ratio. Figure 2 shows the appearance of designed drawing die and drawing punch and the schematic illustration of geometries of the milli-scale tool set used. All tools were made of sintered WC-Co hard alloy (JIS: V20 tungsten-carbide-cobalt alloy). To make the different surface asperities of the tools, in addition to the un-treated lap finished tool, air-blasting treatment was conducted in same as the material mentioned above. For the air-blasting treatment, glass powder of 53-63 \(\mu m\) size was irradiated for about 30min on the tool surface and rough surface was made.

Figure 3 shows 3D surface images of un-treated and air-blasted drawing punch obtained by confocal laser scanning microscope. For the untreated tools, the surface
of the drawing punch has quite smooth surface quality of 0.022 mm maximum surface roughness. On the other hand, for the air-blasted tools, the maximum height of surface roughness was significantly rough as shown in Figure 3. The machine traces of untreated tool were removed and directional property was disappeared. Additionally the surface became extremely rough surface with the asperity of dimple as shown in the figure.

2.3 Experimental procedure

By using above blank material, tool set, milli-scale deep-drawing experiments were conducted using the erichsen-cupping tester. To consider only the influence of tool surface roughness, the experiment was carried out under a un-lubricated condition. Drawing speed was 0.5mm/s and blank holder force was not applied to examine only the influence of contact behavior of sliding on the die corner radius,
so that the constant gap between the drawing die and blank holder was set up to be 0.45mm.

To evaluate the formability of each surface condition, punch force was measured. Additionally, the drawn cup surface roughness and thickness strain distribution were measured. For cutting the milli-scale cup in half to measure the cup geometry and inner surface roughness, the high-precision fine cutter was used. After cutting the micro cup in half, the cut plane was polished to eliminate the burr and the drawn cup geometry and thickness distribution were measured from the digital images obtained by a digital microscope observation. Surface roughness of the cup was measured by a digital image analysis of confocal laser scanning microscope images.

3 Results and discussion

3.1 Influence of surface topography on formability

To investigate the drawability in each surface conditions, punch force was measured during the process. Figure 4 (a) shows the comparing data of punch load-stroke curves between 4 different surface conditions of tools and blanks. Figure 4 (b) shows the appearance of the drawn cup of fractured sample and succeeded sample. As shown in Figure 4(a) and (b), it could not form successfully in the conditions with lapping tool, though in the condition of blasted tool could complete the process. The fracture was occurred at the point of cup-corner in every fractured specimen, which drawn by lapping tool. Additionally, as the shape of the load-stroke curve shows, it has two peaks of maximum value. The first peak of the curve indicates the drawing force and the second peak is caused by the ironing process. For the drawing force, in the condition of air-blasted tool demonstrated slightly higher load than lapping tool. Also for the ironing process, in the condition of air-blasted tool indicated higher load and the difference of each load curve became larger. That is to say, in the condition with lapping tool the process could not complete, although the forming load is lower than that with air-blasted tool.

In order to study the contact behavior, which brings about the different tribological condition, surface property of drawn cups was observed. Figure 5 shows the surface images of upper side of the drawn cup wall of outer surface. As shown in Figure 5, strong adhesion traces with die or scratch marks and sliding traces in the axial direction could also observe. Especially in the condition with lapping tool and blasted blank, the maximum surface roughness have not so big difference with initial surface roughness(Rz=2.94 mm). It means that the effect of smoothing with lapping die could not work on the surface of the blank. Therefore it can be consider that in the condition with lapping tool indicated low forming force, caused by less contact area between die and material. Meanwhile, for the condition with air-blasted tool, the contact traces with die can be observe on the surface of the drawn cup. In other words, it can be consider that because that the resistance force with adhesion or plowing would be easy to occur in the condition with rough tool surface, the high drawing force was indicated especially under the ironing process, which the normal load is relatively high.

To consider how these tribological conditions caused by difference of surface
Figure 4: Compared data of drawability between lapping tool and air-blasted tool

Figure 5: Surface images of drawn cup outer wall surface and surface profile in different tool surface conditions
topography effect on the global deformation, thickness strain distribution were measured. Figure 6 shows the thickness strain distribution, which compared the data of lapping tool and blasted tool with untreated material. As shown in Figure 6, tendency of the thickness distribution is quite different between each condition. For the condition with lapping tool, the thickness strain decreases gently from the cup bottom until the end of cup corner radius. In other hands, local thickness reduction was occur at only the region of end of the cup corner for the condition with air-blasted conditions.

![Figure 6: Comparison of thickness strain distribution data between lapping tool and air-blasted tool](image)

Corresponding to the consideration of tribological conditions, the reason of the fracture in the condition with lapping tool can be considered by means of material flow depend on the frictional behavior caused by different surface conditions. As mentioned above, the fracture occurred at cup coner radius, where the large thickness reduction was observed in the condition of lapping tool. That is to say that the friction force in the contact between punch corner and blank is law and the material is easy to flow because of the tensile force at the cup wall and cup bottom, so that the reduction of the thickness and the fractured was easy to occur. Contrarily, for the rough tool, the high friction force of the contact between punch corner and blank resisted the material flow at the cup corner and the thickness was maintained.

### 3.2 Effect for enhancement of drawability

For a validation of the consideration mentioned above, an experiment was conducted with a combination of air-blasted punch (rough surface) and lapping die. As a results of that, by changing the surface asperity of punch surface to rougher, it could be success to complete the drawing process with lapping die. It is thought to be similar phenomenon as a differential lubrication. By reducing the friction resistance at the die flange and die corner radius, the drawing force became lower.
Additionally, by increasing the friction resistance at punch corner radius, the loaded part for drawing force moved from bottom side of cup corner radius to wall side of cup corner radius, so that the fracture force would be higher and be resistant to fracture. These low drawing force and high fracture force bring the enhancement of drawability. Figure 7 shows the data of punch load-stroke curves compared between the conditions of lapping tool, air-blasted tool, and lapping die-blasted punch. As shown in the figure, for the drawing force, the condition of lapping die-blasted punch indicated the lowest load, and for the ironing force, the condition indicated the highest force. Nevertheless the drawing force could complete. From the results, it can say that the frictional property was changed by surface property and it works on the enhancement of drawability. In other words, in the dry friction condition, there are some possibility to control the frictional behavior with a surface topography to enhance the drawability.

![Figure 7: Load-stroke curves comparing with different combination of tool set](image)

### 4 Conclusions

In this study, aimed to clarify the effect of surface topography of tool and materials on deep drawing characteristics in "dry" friction condition, cylindrical deep drawing process using mirror-polished and air-blasted tool sets and materials in milli-scale region was conducted. Tribological behavior results from the different surface topography were evaluated from comparison of drawing punch force, surface quality and thickness distribution of drawn cup. The following results were obtained.

1. Although the condition of air-blasted rough tool could succeed the drawing process, the condition of lapping smooth tool could not complete the process.
2. The above results are strongly related to the tribological condition of contact behavior of surface topography between tool and material. Particularly in a milli-scale region, it was found that smooth tool surface tends to indicate the low friction force because of less contact area, and rough tool surface tends to indicate the high friction force caused by adhesion and plowing effect. Especially under the high normal load like ironing process, the curve indicated higher with a condition of rough material surface.

3. It was shown that the contact behavior of different surface topography indicates the different material flow in the process, so that the loaded part moved and it would affect the formability.

4. By changing the surface asperity of punch surface to rougher, it could be success to complete the drawing process even with lapping die. It means that drawability could enhance in dry friction by controlling the surface topography of tool surface topography.

References


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Convection and heat transfer in a horizontal cylindrical layer of the saturated porous medium

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Abstract

The present study deals with the convective motions in a horizontal cylindrical layer of the saturated porous medium. A numerical experiment has been performed with the help of a finite-difference method for various models of porous medium (Darcy, Brinkman, Forchheimer) in Buussinesq’s approximation in a wide interval of dimensionless parameters Grashov, Prandtl and Darcy. Temperatures of restricting surfaces relied with stationary values, and the temperature of the interior cylinder is more, than exterior. New unsymmetrical solutions of the equations of a convective filtration are found out. Their occurrence, areas of existence and stability is explored. One of them represents the multivortex structure with the asymmetrical vortexes in subpolar area. Other asymmetrical motion is implemented as a convective plume, refracted from a vertical. Both solutions can arise either strong or soft fashion and exist in a restricted interval of values of Grashov number. Preferred rotation of a fluid in the asymmetrical vortex is possible as clockwise and counter-clockwise and arises in a casual fashion (breakdown of symmetry).

1 Introduction

The investigations of a natural convection in saturated porous mediums are of interest for a solution of scientific and engineering problems. There is a large number of the experimental and theoretical studies devoted to this problem; most complete review is submitted in [1]. The theoretical study was carried out more often within the framework of Darcy model of a porous medium and for cavities of various geometries. One of frequently explored configurations is the horizontal cylindrical layer. As a rule, authors were restricted to observation of the symmetric crescent motion which has the shape of two symmetric vortexes, formed by streams, rising near to a heated interior surface and lowered near cold exterior boundary, and to establishment of associations of heat transfer from defining parameters of a problem.
In thin layers and in layers of the moderate thickness (the ratio of radiuses of cylinders $R > 0.2$) symmetric motions with several additional vortexes in the top part of an annulus were observed. Research of transitions between symmetric movements with various number of vortexes in subpolar area of a thin cylindrical layer of a usual liquid by pseudo-spectral method was dealt in [2].

Alongside with known symmetric solutions in the form of two or other even number of vortexes, earlier authors for Darcy’s and Brinkman’s porous medium had been found new asymmetric solution of the equations of convective filtration [3-5]. One of them represents structure with asymmetrical vortexes in subpolar area. Other solutions is realized at greater Grashof number in the form of convective a plume rejected from a vertical. Occurrence of an asymmetric plume is accompanied by strong pulsations of temperature in the top part of a layer which amplitude decreases with distance from a vertical axis.

A variety of natural and artificial porous materials causes use of various models of the porous medium. If velocity of a filtration is not small (Reynolds’s number defined on the size of pore is more than unit), for high-porous medium often use Brinkman’s and Forchheimer’s models. The comparison of conditions of occurrence of asymmetric convective motions for various models of the porous medium is of interest. Some results for Darcy’s and Brinkman’s models have been received earlier in works [4, 5].

The purpose of the present study is research of conditions of occurrence, stability, character of heat transfer both symmetric, and asymmetric convective motions in a horizontal cylindrical layer of the saturated porous medium for Darcy’s, Forchheimer’s, and Brinkman’s models.

2 Problem Formulation

Let’s analyse a horizontal layer of saturated porous medium, restricted by rigid cylindrical surfaces with radiuses $R_1$ and $R_2$. The viscous incompressible fluid with a density $\rho_f$, viscosity $\nu$ and a thermal capacity $(c_p)_f$ fill up the layer. Internal and external boundaries of a cylindrical cavity are kept at the constant temperatures $T_1$ and $T_2$ with $T_2 < T_1$. The porous medium is characterized by porosity $\varphi$ and permeability $K$. Both these properties for various mediums vary in rather wide limits: $K \approx (10^{-8} \div 10^{-15}) m^2, \varphi \approx 0.02 \div 0.90$. Therof, the equation of a convective filtration of a fluid in Bussinesk’s approximation has a various form [1]:

$$Da\varphi^{-1}\frac{\partial \vec{v}}{\partial t} = -\nabla p - \vec{v} + Gr \vec{\gamma} \quad \text{(Darcy’s model)}$$

$$Da\varphi^{-1}\frac{\partial \vec{v}}{\partial t} = -\nabla p - c_F Da^{1/2} |\vec{v}| \vec{v} - \vec{v} + Gr \vec{\gamma} \quad \text{(Forchheimer’s model)}$$

$$Da\varphi^{-1}\frac{\partial \vec{v}}{\partial t} = -\nabla p - \vec{v} + Da \Delta \vec{v} + Gr \vec{\gamma} \quad \text{(Brinkman’s model)}$$

In the equations (1) - (3) $c_F$ - Forchheimer’s coefficient, which magnitude depends on nature of porous material (in calculations of many authors it was fixed $c_F = 0.55$); value $c_F = 0$ correspond to Darcy’s model.
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It is necessary to add to the momentum equations (1) - (3) the heat conduction equation and continuity equation:

\[
\frac{b}{\partial t} = \frac{1}{Pr} \Delta T - \vec{v} \nabla T \tag{4}
\]

\[
\text{div} \vec{v} = 0 \tag{5}
\]

In the system (1) - (5) standard symbols of velocity \( \vec{v} \), pressure \( p \) and temperature \( T \) are used. We have chosen as units of measurements of distance, time and \( \vec{v}, T, p \) accordingly \( R^2, \nu^2, \nu/R_2^2, T_1 - T_2, \rho c \nu^2/K \).

Boundary conditions in the non-dimensional form will become:

\[
r = R: \; v_n = 0; \; T = 1; \quad r = 1: \; v_n = 0; \; T = 0 \tag{6}
\]

Boundary value problem (1) - (6) contains some the dimensionless parameters - Grashof number \( Gr \), Prandtl number \( Pr \), Darcy number \( Da \), the ratio of radiuses \( R \) and parameter \( b \), representing the ratio of thermal capacities of a medium and a fluid:

\[
Gr = \frac{g \beta (T_1 - T_2) R_2 K}{\nu^2}; \; Pr = \frac{\nu}{\chi_m}; \; Da = \frac{K}{R_2^2}; \; R = \frac{R_1}{R_2}; \; b = \frac{(\rho c_p)_m}{(\rho c_p)_f} \tag{7}
\]

In these parameters \( \chi_m, (c_p)_m \) are thermal conductivity and specific heat capacity of saturated porous medium; \( \beta \) is the coefficient of thermal expansion of fluid, \( g \) is the gravity acceleration.

The most of calculations was realised in a 2D dimensions in polar coordinates \( r, \theta \) for variables \( T \), a stream function \( \psi \) and a vorticity of a filtrational flow \( \xi \):

\[
\nu_r = \frac{1}{r \partial \psi}, \; \nu_\theta = -\frac{\partial \psi}{\partial r}, \; \xi = -\Delta \psi \tag{8}
\]

The solution of the time-dependent problem (1)-(6) was obtained by a finite deference method with use of explicit and implicit schemes. The most calculations were carried out on the uniform grids with a mesh size of 0.005 on radial coordinate and of 1.8° on a polar angle.

The value of porosity was fixed \( \varphi = 0.3 \) and parameter \( b = 1 \) in all calculations.

3 Results and Discussion

Let us consider stationary regimes of a convective filtration. In this case structures of arising convective motions practically do not depend on model of a saturated porous medium. The structures of symmetric flow submitted on Fig. 1. The symmetric flow (Fig. 1), consisting of two crescent vortexes (further S1), arises at as much as small values of Grashof number and exists in a wide range of values of parameters of a problem. As the Grashof number increases a convective plume is formed above internal cylinder, and near to borders of a cavity a boundary layers are shaped.
Figure 1: Isolines (a, b, c) and isotherms (d, e, f) of convective motions in cylindrical layer for Darsy’s model at $Gr = 400$, $Pr = 1$, $Da = 10^{-6}$, $R = 0.3$ (a, b, d, e), $R = 0.8$ (c, f)

From the figure follows, that at the given values of parameters both are possible: the symmetric motions, concerning a plane $\theta = 0$, and the asymmetrical motions.

Other symmetric solution (S2) contains additional convective vortexes in subpolar area of a cylindrical layer. Such a motion is presented in Fig. 1b. A reason of formation of these additional vortexes is instability of Rayleigh’s type: in rather thin cylindrical layer of fluid thermal conditions in an upper part become similar to those in the plane layer, which is heated from below. In layers of moderate thickness, for example with $R=0.3$, there is only one symmetric solution with two additional vortexes. As a layer is thin, there are some solutions with different number of vortexes: with two, with four etc. Motions with four additional vortexes is realized in a layer with $R = 0.7$ (Fig. 1c). Such a motion with six vortexes exists for $R = 0.8$. Symmetric flow S2 arises in a jump fashion at finite Grashof number and exists in a restricted range of its values. In thick layers ($R < 0.16$) multivortex solutions do not exist and crescent flow is observed only.

Stationary symmetrical solutions lose stability with growth of Grashof number and become non-stationary. The structures of these flows are shown on Fig. 2. The loss of a stability of a regime with two crescent vortices (S1) represents special interest. In layers with $R < 0.7$ (thick enough layers) in a neighborhood of a plume thermal waves arise, which are spread along exterior boundary. Eventually the waves running in any side from a plume amplify, therefore the plume is deflected in an op-
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Figure 2: Isolines (a, b, c) and isotherms (d, e, f) of convective motions in cylindrical layer for Darcy’s model at $R = 0.3$, $Da = 10^{-6}$, $Gr = 3000$, $Pr = 1$ (a, d), $Gr = 250$, $Pr = 15$ (b, e), $Gr = 400$, $Pr = 1$ (c, f)

posite side. The streamlines and isotherms of this asymmetrical motion (further A1) are submitted on Fig 2 a, b, d, e. The deflection of a plume from a geometrical plane of symmetry of a layer in this or that side occurs randomly and may be interpreted as spontaneous breakdown of symmetry of convective current. Magnitude of a plume deviation angle from a vertical axis for all models makes approximately $20° – 40°$. As the Grashof number increases the position of a plume and its structure vary in an oscillatory fashion. The amplitude of an angle of deflection makes about $6°$. With a decrease of Grashof number transition from an asymmetrical plume to the symmetric solution (S1) happens to a hysteresis.

The structures of other asymmetrical flow are shown on Fig 2 c, f. This motion differs from S2 loss of a symmetry concerning a plane $\theta = 0$: intensity of vortex motions in the left-hand and right half of layer become different, and a more intensive flow is implemented in any half of cavity by a casual fashion. This solution arises in layers of moderate thickness and exists, as well as symmetric solution S2, in a restricted interval of values of Grashof number.

Transitions of structure of convective movements from symmetric (S1) to an asymmetric plume (solution A1) for considered models of the saturated porous medium depending on value of Darcy number and can occur both “strong”, and “soft” fashion.

Quantitatively the degree of asymmetry of current can be defined by means of
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Figure 3: The dependence of asymmetry parameter from Grashof number at $R = 0.3, Pr = 1, c_F = 0.55, Da = 10^{-3}(1), Da = 10^{-6}(2)$.

Markers 3 correspond to symmetrical mode.

Figure 4: The dependence of critical Grashof number from Prandtl number at $R = 0.3, Da = 10^{-5}$ for Darcy’s (1), Forchheimer’s (2) and Brinkman’s (3) models.

Parameter

$$As = \int_0^1 \int_0^{2\pi} \psi_r dr d\theta$$

This quantity is proportional to $z$-projection of the moment of a liquid. For vortexes with clockwise rotation of a liquid $As > 0$. Examples of "soft" and "strong" change of character convective motions are presented on Fig. 3 (curves 1 and 2). The deviation of a plume from a geometrical plane of symmetry of a layer in this or that party occurs in the casual image, therefore the curve 1 on Fig. 3 represents the top part of symmetrical bifurcation curve or so-called fork-wise bifurcation.

Occurrence of an asymmetric plume is accompanied by intense pulsations of temperature in the top part of a layer which amplitude decreases with distance from a vertical axis. Amplitude of fluctuations in a point near to an external surface (a point A on fig. 2) makes 0.3 difference of temperatures between internal and external cylinders. The amplitude of fluctuations of temperature in a point B (Fig. 2a), essentially less and account about 0.1 differences of temperatures of cylindrical surfaces.

The spectral analysis of pulsations of temperature in a point A has shown, that the first dimensionless frequency $\omega_0$ and multiple harmonics from 2 up to $7\omega_0$ are present. Amplitudes of higher harmonics decrease on exponential law. The temperature oscillations are kept low-frequency harmonics with removal from an axis of symmetry of a cavity.

The numerical experiments have shown, that formation of asymmetric motion is preceded with occurrence of thermal waves near to a surface of the external cylinder.
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Figure 5: The dependence of critical Grashof number from ratio of radiiuses at $Pr = 1, Da = 10^{-5}$ for Darcy’s (1), Fochheimer’s (2) and Brinkman’s (3) models

Figure 6: The variation of Nusselt number with Grashof number at $R = 0.3, Pr = 1, Da = 10^{-5}$ for Darcy’s (1), Forchheimer’s (2) and Brinkman’s (3) models

Research of dependence of a threshold of stability from Prandtl number therefore is of interest. Corresponding curves are presented on Fig.4 for all concerned models of porous medium. For values $Pr > 1$ dependencies $Gr^*(Pr)$ for all models of the porous medium in case of $R = 0.3$ and $Da = 10^{-5}$ are well approximated by formula $Gr^* = 4.3 \cdot 10^3 Pr^{-1.2}$. Loss of stability of a symmetric plume in the porous medium occurs at much smaller Prandtl number, than similar instability in a horizontal annulus of the usual liquid, investigated experimentally in [6].

As it has noted been above, threshold value of Grashof number of formation of an asymmetric plume depends not only on Prandtl number, but also from thickness of a cylindrical layer. On Fig.5 dependencies $Gr^*$ from parameter $R$ defining thickness of a cylindrical layer are represented for concerned models. From schedules follows, that for value $Da = 10^{-5}$ occurrence of an asymmetric plume for Darcy’s model take place at a greater size of Grashof number, than in Forchheimer’s model. For all models the inclined plume exists only in layers of large thickness $R \leq 0.6$. Calculations for values $R < 0.05$ demand fine grid and, hence, substantial growth of time of computations.

For a quantitative analysis of heat transfer, it is convenient to use Nusselt number:

$$Nu = \frac{1}{2\pi R \ln R} \int_0^{2\pi} \left( \frac{\partial T}{\partial r} \right)_{r=R} d\theta$$ (10)

Diagrams of dependence of a Nusselt number on Grashof number for three models of porous medium at $R = 0.3, Pr = 1, Da = 10^{-5}$ are shown in Fig. 6. According to the figure, considerable deviations of $Nu$ values for these models begin for Grashof numbers $Gr > 1500$. From diagrams follows, that transition from the symmetric
convective motions to asymmetrical is not accompanied by an abrupt change of a Nusselt number. Points $A$ on curves 1-3 corresponds to occurrence of an asymmetric plume (mode A1) by strong fashion. A letter $B$ marks points of transition to a symmetric mode S1.

Figure 8: Isolines of $z$-projection of stream function for three-dimensional convective flow in cylindrical annulus for $z=2.5$ at $Pr=1, Da=10^{-6}, Gr=500, l=5$: a - $R=0.2$, b - $R=0.5$, c - $R=0.7$

Change of a local heat transfer $q$ on a surface of the internal cylinder for three models is shown on Fig.7. We shall note substantial growth of convective heat transfer in comparison with molecular, its small change for different models and significant increase of maximum value $q$ for transition from mode S1 (Fig.7a) to A1 (Fig.7b). Breaks on the schedules, corresponding an asymmetric mode, correspond to area of an arrangement of a plume. The maximal value of density of a heat transfer for all models is carried out at $\theta = \pi$ in the bottom part of a surface of the internal cylinder. On a surface of the external cylinder the value $q$ is maximal at $\theta = 0$ and it has minimal value close $\theta = \pi$. 
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The calculations in three-dimensional statement for a cylindrical cavity with the longitudinal size \( l = 5R_2 \) have shown, that except for small neighborhoods near to end faces the convective motion inside a cavity has flat character. For layers with size \( R > 0.2 \) the symmetric solutions similar S1 and S2 were observed. Examples of these structures for Darcy’s model are presented on Fig.8. Asymmetric plume for three-dimensional area is realized for values of parameters \( R = 0.5, \Pr = 1; 7, D\alpha = 10^{-6} \) for Darcy’s and Forchheimer’s models.

**Conclusion**

For three models of porous medium (Darcy’s, Forchheimer’s and Brinkman’s) asymmetric solutions of the equations of convective filtration in a horizontal annulus are found out. Their occurrence, areas of existence and stability is explored in a wide interval of values of Grashof, Prandtl and Darcy numbers and rations of radiuses of interior and exterior cylinders. One of them represents multivortical structure with asymmetrical vortexes in subpolar area. Other asymmetrical motion is implemented as a convective plume, refracted from a vertical. Primary circulation of a liquid in asymmetrical vortexes is possible as on clockwise or counter-clockwise and arises in the casual image (spontaneous breakdown of symmetry).

**References**


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Theoretical investigation of fluids and gases filtration in heterogeneous porous medium

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Abstract

The present study deals with hydraulic flows of incompressible fluid or ideal gas in channels, filled with heterogeneous porous medium; exactly supposed, that the porosity changes along the channel. Plane-parallel motions were examined analytically. The method of finite elements was applied for investigation of steady and transient modes of flow at high Reynolds numbers. Numerical calculation is executed in three-dimensional statement for the channel of square section, with a length in 5 times exceeding the cross-section sizes. The study has shown that motion is unsymmetrical due to gradient of porosity. Comparison of the results received with two models of the porous media – Darcy’s and Forchheimer’s – has shown essential difference between them.

1 Introduction

Studying of a filtration in non-uniform porous mediums is of interest for the decision both engineering, and scientific problems. The full review of experimental and theoretical works is presented in [1]. A plenty of works is devoted to studying of a pressure filtration in multilayered and non-uniform grounds. As a rule, it was supposed, that heterogeneity of medium is caused only by space gradients of permeability, and porosity was considered as a constant. Rather recently there were works in which it is shown, that the account of heterogeneity of porosity leads to interesting effects [2].

Theoretical studying, as a rule, was spent on the basis of Darcy’s model, that is robust for enough small speed of a filtration. But if Reynolds’s number defined on the size of pore is more than unit, Darcy’s model become inaccurate, and another models of the porous medium are actual. If speed of a filtration is not small often use Forchheimer’s model, using linear and quadratic resistance terms of an impulse equation. The linear on speed term represents viscous losses and the quadratic term
represents inertial losses. For high-porous mediums often use Brinkman’s model in which an impulse equation contain not only Darcy’s force of resistance but also viscous friction. In a sense it is intermediate between Darcy’s model of saturated porous medium and a usual liquid.

The purpose of the present work is theoretical study of a pressure filtration of liquids and gases in porous mediums with the heterogeneity caused by a gradient of porosity. Objects of research are also the area of existence and stability of modes of a filtration, and symmetry of existing solutions to a direction of flow. The attention is paid to comparison of the results received by means of various models of the porous medium.

2 Problem description and basic equations

Let’s consider movement of a viscous fluid in the channel filled by a porous material which physical properties (namely coefficient of porosity) are assumed non-uniform on space. Movement of a fluid in the channel arises under pressure difference on an input (in) and an output (out) of the channel. The porous material of a channel is characterized by factor of porosity \( \varepsilon \) and permeability \( K \). These characteristics for various materials change in rather wide limits: \( K \approx (10^{-8} \div 10^{-15})m^2 \), \( \varepsilon \approx 0.02 \div 0.90 \). As a result the equations describing a filtration of fluids have a various form (see [3]):

\[
\begin{align*}
\varepsilon^{-1} \frac{\partial \vec{v}}{\partial t} + \left( \frac{\vec{v}}{\varepsilon} \right) \nabla \vec{v} &= -\nabla p + \rho_f \vec{v} \\
\varepsilon^{-1} \frac{\partial \vec{v}}{\partial t} + \left( \frac{\vec{v}}{\varepsilon} \right) \nabla \vec{v} &= -\nabla p + c_F Da^{1/2} |\vec{v}| - \vec{v} \\
\varepsilon^{-1} \frac{\partial \vec{v}}{\partial t} + \left( \frac{\vec{v}}{\varepsilon} \right) \nabla \vec{v} &= -\nabla p + \rho_f + Da \Delta \vec{v}
\end{align*}
\]

In the equations (1) - (3) \( \vec{v} \) – speed of a filtration, \( c_F \) – Forchheimer’s coefficient, which magnitude depends on nature of porous material (in calculations of many authors it was fixed \( c_F = 0.55 \)), \( \rho_f \) – density of a liquid. As speed of a filtration is usually small, often neglect nonlinear members in acceleration. However in a considered problem it is impossible, as nonlinear items define effects in the non-uniform porous medium.

It is necessary to add to the momentum equations (1) - (3) the continuity equation and the gas law for incompressible fluids:

\[
\begin{align*}
\text{div} \vec{v} &= 0; \quad \rho_f = 1, \quad (4)
\end{align*}
\]

and for gases:

\[
\begin{align*}
\frac{\partial \rho_f}{\partial t} + \text{div}(\rho_f \vec{v}) &= 0; \quad \rho_f = p/p_{\text{ref}}, \quad (5)
\end{align*}
\]

where \( p_{\text{ref}} \) is dimensionless atmospheric pressure.
In system (1)-(5) as units of measure of distance, time, speed, density and pressure are chosen accordingly \( L, L/v_0, v_0, \rho_0, \rho_0 v_0^2 \). Letter \( L \) designates the characteristic size of the channel (for example, its width), \( \rho_0 \) – density of fluid at atmospheric pressure and \( v_0 = L \nu/K \) represents characteristic speed of a problem.

Boundary conditions in the non-dimensional form look like:

\[
\begin{align*}
\nu_n |_{r=0} &= 0; \\
p_{in} &= p_1; \\
p_{out} &= p_2
\end{align*}
\]

Boundary value problem (1), (4 - 6) contains one dimensionless parameter \( \Delta p = p_1 - p_2 \) – a difference of pressure on an input and an output of the channel. Boundary value problems (2), (4 - 6) and (3), (4 - 6) contain one more dimensionless parameter – Darcy number \( Da = K/L^2 \).

We considered that the characteristic size of the channel is not too small, thus Darcy number is much less than unit. In this case Brinkman’s model provide the results close to Darcy’s model. Therefore in the analysis and calculations only two models of the porous medium were used: Darcy’s and Forchheimer’s.

Boundary value problems (1), (4 - 6) and (2), (4 - 6) were investigated analytically for a case of the steady plane-parallel flow. Solutions of the full non-stationary equations of a filtration was spent numerically with finite-element method. Calculations were carried out for the three-dimensional channel of square section, with a length in 5 times exceeding the cross-section sizes. The channel filled by a porous material with constant permeability, but porosity was considered non-uniform and varied under the linear law from value \( \varepsilon_1 \) on the left border up to value \( \varepsilon_2 \) on the right border. At processing results of calculation all variables be translated in a dimensionless kind.

3 Filtration of incompressible fluids

Let’s consider primarily the one-dimensional established movement of a liquid — a plane-parallel flow along an axis \( x \) the cartesian system of coordinates. In Darcy’s model it is described by the equations:

\[
\frac{1}{2} v_x^2 e^{-3 \varepsilon'} = -p' - v_x, \quad v'_x = 0
\]

In these equations the stroke means a derivative on coordinate \( x \). On an input \( x = x_1 \) and on an output \( x = x_2 \) of the channel boundary conditions (6) are satisfied. The solution of the given problem can be received analytically and looks like:

\[
v_x = \left( - (x_2 - x_1) \pm \sqrt{(x_2^2 - x_1^2) + 2\left( \frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1} \right)(p_1 - p_2)} \right) \left( \frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1} \right)
\]

The dependence of filtration speed \( v_x \) from a difference of pressure \( \Delta p = p_1 - p_2 \) is presented on Fig.1a. These charts received under the formula (8) for a case \( \varepsilon_1 = 0.3, \varepsilon_2 = 0.9 \). The main feature is presence of two solutions at values \( \Delta p < p_A \). A continuous line designates the steady solution. A shaped line designates the unstable solution. Both solutions converge in a point of extremum \( A \) at value
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\[ \Delta p = \Delta p_A. \] At pressure exceeding \( \Delta p_A \), solutions of a boundary value problem \((7), (6)\) are absent.

The analysis of Fig.1a find the asymmetry relative to direction of a gradient of porosity: more intensive flow is realized at \( p_1 > p_2 \), i.e. when flow is directed aside increases in porosity of medium.

Let’s consider results of the numerical solution of the full three-dimensional equations. They are presented on Fig.1a by triangular markers. Flow has stationary character and with the big degree of accuracy coincides with a steady branch of the analytical solution \((8)\). The numerical solution too has an extreme point. Thus at \( \Delta p > \Delta p_A \) are absent not only stationary solution of system \((7)\), but also any solutions of a full problem \((1), (4), (6)\).

Let’s estimate value of an extreme pressure \( \Delta p_A \). We shall allow the channel in length of \( 0.1 \text{ m} \) is filled by a porous material with constant permeability \( 4 \cdot 10^{-8} \text{ m}^2 \) and the non-uniform porosity varying under the linear law from value 0.3 on left border up to value 0.9 on right border. The porous material of the channel is saturated by water at temperature \( 25^\circ \text{C} \). In this case in an extreme point the pressure makes \( \Delta p_A = 277 \text{ Pa} \), also speed of \( 0.23 \text{ m/s} \). If length of the channel to increase up to \( 1 \text{ m} \), having kept values of other dimensional parameters, for pressure and speed of current we shall receive much great values of \( \Delta p_A = 27700 \text{ Pa} \) and \( 2.3 \text{ m/s} \) accordingly.

Let’s address now to the results received on the basis of Forchheimer’s model. The plane-parallel stream along an axis \( x \) the cartesian system of coordinates is described by the equations:

\[
-\frac{1}{2}v_x^2\varepsilon^{-3}\varepsilon' = -p' - v_x - c_F D a^{-1/2} |v_x| v_x, \quad v_x' = 0
\] (9)
The solution of a problem (9), (6) looks like:

\[ p_1 > p_2 : v_x = \frac{-(x_2 - x_1) \pm \sqrt{(x_2^2 - x_1^2) + 4\left(\frac{1}{2}\left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1^2}\right) + c_f \text{Da}^{-1/2}\right)(p_1 - p_2)}}{\frac{1}{2}\left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1^2}\right) + c_f \text{Da}^{-1/2}} \]  

(10)

\[ p_1 < p_2 : v_x = \frac{-(x_2 - x_1) \pm \sqrt{(x_2^2 - x_1^2) + 4\left(\frac{1}{2}\left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1^2}\right) - c_f \text{Da}^{-1/2}\right)(p_1 - p_2)}}{\frac{1}{2}\left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1^2}\right) - c_f \text{Da}^{-1/2}} \]  

(11)

The dependence of speed of a filtration on a pressure \( \Delta p \) for a case \( \varepsilon_1 = 0.3 \), \( \varepsilon_2 = 0.9 \) is presented on Fig.1b. There are two solutions in all range of values. One of them is steady and is described with a plus sign before a root at expressions (10-11). This branch of the chart is designated by a continuous line. The second solution is unstable and it is corresponds a minus sign before a root in expressions (10-11). It is designated by a shaped line. As follows from Fig.1 Forchheimer’s model does not lead to occurrence of extreme points as it was in Darcy’s model.

Small asymmetry of the solution for positive and negative values \( \Delta p \) may be note. Let’s enter the parameter defining asymmetry of flow: \( \text{As} = (v_+ - v_-)/v_+ \), where \( v_+ \) and \( v_- \) are values of speed at positive and negative directions of flow. In examined area of \( \Delta p \) this parameter is small and has values 0.025–0.03.

The filtration flow, described by Forchheimer’s model of the porous medium, was investigated numerically for the three-dimensional channel. Results of the numerical simulation are presented on Fig.1b by triangular markers. Good concurrence to the steady analytical solution is observed.

Comparison of the results, received for incompressible liquids with use of two models of the porous medium, shows significant enough difference. The values of speed calculated in Darcy’s model, appear in 2-3 times overestimated. It, apparently, explained that the given model considers only viscous resistance, but ignores inertial resistance which becomes significant at greater speeds. Besides this, the solution, received on Darcy’s model, has points of an extremum and area of absence of solution that does not prove to be true by practice. At the same time Forchheimer’s model provides results which are comprehensible and do not conflict with data of experiments and observation (see [1]).

**Filtration of gases**

The equations, describing filtration of elastic liquids and gases, should include compressibility and thermal effects. In a number of works (see [1]) it has been shown, that the pressure filtration of gases can be considered as isothermal as the changes of temperature, arising at variations of pressure, are compensated by heat exchange with a porous material. So in the present work thermal effects were ignored, and the basic system of equations was (3), (5). A finite-element method was used to numerical simulation of flow of ideal gas in the channel with the non-uniform porous medium. Calculations were carried out for the three-dimensional channel of square section, with a length in 5 times exceeding the cross-section sizes.
Theoretical investigation of fluids and gases filtration in heterogeneous porous medium

Figure 2: The dependence of a mass flow density from pressure at $\varepsilon_1 = 0.3$, $\varepsilon_2 = 0.9$, $D\alpha = 10^{-5}$ for ideal gas

It is known, that characteristic speed of a filtration of gases at the certain pressure difference appears on the order above, than for liquids. Therefore at studying a pressure filtration in gases Forchheimer’s model was used as it yields good results even at rather high speeds of a filtration.

When effects of compressibility at high pressure are developed, speed of a filtration is not a constant along the channel. Then the another characteristic of a filtration is more suitable – the density of a mass flow:

$$W = \int_S \rho \vec{v} \cdot d\vec{S}$$  \hspace{1cm} (12)

where S is the area of cross-section of the channel. This quantity is a constant along an axis of the channel. The combination $\rho_0 v_0$ is possible to use as unit of measure $W$ for transition in a dimensionless kind.

Results of numerical simulation are presented on Fig.2. The chart displays dependence of density of mass flow $W$ on a pressure. The diagram is show, that Forchheimer’s model in application to compressible fluids provide results similar to that took place for incompressible liquids. A steady solution exist in all range of $\Delta p$. The extreme points, arising at use of Darcy’s model, here are absent. Small asymmetry of the solutions for positive and negative values of flow directions takes place: the parameter $A_s$ accepts values within the limits of $0.02 \div 0.04$.

The range of pressure presented on Fig.2, is wide enough. It begins from small values at which gas is incompressible, and obtain values at which the density inside of the channel strongly changes. Distributions of density and filtration speed along an axis of the channel (conterminous with an axis x the cartesian system of coordinates) are presented on Fig.3. At values of pressure $\Delta p < 70$ ideal gas behaves as incompressible fluid; at $\Delta p = 680$ density of gas changes inside of the channel in 4 times. However, both for small and for greater pressure, Forchheimer’s model gives the satisfactory description of a filtration of gas in the porous medium. We shall
Figure 3: The distribution of density (a) and filtration velocity (b) along the channel at $\Delta p = 23$ (1), $68$ (2), $226$ (3), $679$ (4) for ideal gas

note, that for considered pressures the speed of a filtration is less than the speed of a sound equal of 16.5 dimensionless units.

Conclusion

The results indicate to presence of asymmetry of a pressure filtration of liquids and gases in the non-uniform porous medium. Fluids flow in a direction of growth of porosity with greater speed, than in the opposite direction. The quantitative analysis of a pressure filtration in the non-uniform porous medium essentially depends on a choice of model of the porous environment. So in Darcy’s model presence of an extreme point is possible: at some pressure exists two solutions, and at others - neither. Forchheimer’s model gives other result: solutions exist at any a pressure. The results, received on the basis of the theoretical analysis and numerical modelling, will well be agreed. Comparison with data of experiments and field observation [1] testifies that Forchheimer’s model is more comprehensible at quantitative analysis for heterogenous porous mediums.

References


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Investigation of structure and rheological simulation of AMg6 alloy under height temperature deformation

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Abstract

Simulation of rheology of AMg6 alloy under height temperature plastic deformation has been made taking into account relaxation processes and structure formation.

Essential influence on rheological properties of strained metals renders conditions of deformation. Under a cold strain there is only a hardening of a material, at a hot deformation alongside with a hardening in metal intensively there are processes of a softening. For a softening at the hot deformation in absence of phase changes processes of dynamic recovery, polygonization and recrystallization are responsible. Interacting of processes of a hardening and softening define behavior of a material during a hot deformation, being reflected on change of a strain resistance. Therefore the strain resistance can be used for an estimation of physical-mechanical properties and a structural condition of metal after a hot deformation.

In an article [1] a mathematical model in the form of a differential equation system, presenting change of the strain resistance depending on history of change of deformation rate intensity $H = \sqrt{3}\dot{\varepsilon}$ is offered at high-temperature plastic deformation:

$$\begin{align*}
\sigma &= \sqrt{3}k + \sigma_v, \\
\dot{k} &= \rho V_n - \rho \dot{V}_r, \\
\dot{\rho} &= a_1 \exp(-a_2 \rho) H - a_3 \rho, \\
\dot{V}_r &= a_5 \Lambda_r R^2 \frac{dr}{dt}, \text{ if } V_r \leq a_6,
\end{align*}$$

(1)
\[ \dot{\mathbf{V}}_r = \dot{\mathbf{V}}^*_r \left( \frac{1 - V_r}{1 - a_6} \right)^{a_7} \]

if \( V_r > a_6 \), \( \dot{\mathbf{V}}^*_r = \dot{\mathbf{V}}_r \) at \( V_r = a_6 \),

\[ \Lambda_r = \int_{t_0}^t H dt, \quad \frac{d\sigma}{dt} = H \rho, \]

\[ \sigma_\nu = a_8 \ln(1 + a_9 H). \]

Here \( k(t) \)–a yield stress under Mises yield condition \( a_0 = k(0) \); \( t \)–a time; \( \sigma_\nu \)– a viscous component of stresses; \( \rho \)–a magnitude proportional to an increment of density of dislocations due to a plastic deformation; \( \dot{\epsilon} \)–strain rate; \( V_n, V_r \)– unrecrystallized and recrystallized parts of volume of metal, \( V_n + V_r = 1 \); \( R \)–radius of a nucleus of recrystallized grains, \( R(t_r) = 0 \); \( t_r \)–the point of time of onset of the dynamic recrystallization, defined condition \( \rho = a_4 \); \( a_i, i = 0, ..., 9 \)–the parameters of a model which are a subject identification on experimental data.

The given work is devoted to study of applicability of the model (1) for description of change of the strain resistance of AMg6 alloy with low stacking-fault energy under hot temperature deformation.

From AMg6 alloy (Si - 0.14; Fe-0.34; Cu - 0.05; Mn - 0.05; Mg - 6.44; Zn - 0.05; Ti - 0.06 %) have made cylindrical specimens in the diameter 8 ± 0.1 mm and the height 12 ± 0.1 mm. For smoothing mechanical properties of metal by volume specimens preliminary have been kept in the furnace at temperature 325°C during three hours with the subsequent cooling on air.

Experiments on compressing of specimens performed on the automated installation created in the Institute of Engineering science of the Ural Branch of the RAS. Installation provides a strain rate in range 0.01 up to 10 s\(^{-1}\). A specimen with two strikers placed into the container and heated up in the electric furnace to temperature 300°C.

The heated container with a specimen was carried from the furnace to holding devices of the installation and strained. Deformation of specimens from AMg6 alloy carried out in a high-speed range 0.1 - 4 s\(^{-1}\). Tests performed without application of lubrication, using polished strikers. During deformation measured displacement of holding devices, force of a straining and temperature of a specimen surface. Change of temperature of a specimen surface measured professional thermal imager system NEC TH-9100WL through a slotted hole in a funnel of the container, containing a specimen. In connection with radiation coefficient at aluminum alloys at the given temperature low for decrease part of effect of erroneous measurements as a result of thermal reflection from walls of the container, a surface of the specimen from AMg6 coated a thin layer of a high-temperature paint of the black color, standing heated up to 530°C.

Deformation of an aluminum alloy occurred on the bottom limit of recrystallization temperature, therefore effect on a softening, besides the contribution of dynamic recrystallization, could render and dynamic polygonization. Although the model does not consider softening of an alloy due to dynamic polygonization, the received results show that it well enough describe processes of a hardening and a softening on the bottom limit of temperature of a flowing dynamic recrystallization.
References


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Simulation of mode of deformation under scratch test using the Berkovich indenter

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Abstract

The numerical simulation has been made for a scratch test by the Berkovich indenter under different orientation of indenter. The next assumptions have been applied under simulation — surface of material is flat and material is elastoplastik.

Scratch test is mainly used to study mechanical properties of materials near their surface. Understanding of this test is of great interest to both academic and industrial communities. The value of scratch hardness and surface deformation mechanisms of materials depend on the indenter geometry, the orientation of indenter, on the rheology of the material, the friction at the interface. The analysis of the residual groove, the pile-in, the sink-in and stressedly-deformed state is important to understand what it occurs during a scratch test. The purpose of this study is to determine the influence of orientation of indenter on the stressedly-deformed state.

Figure 1: Geometry of a indenter Berkovich showing the edge and face scratching directions

Elastic-plastic scratch test was performed using the the ANSYS version 9.0 software package using the large strain feature with uniaxial stress-strain input data.
The Berkovich indenter was used and its edge and face was directing towards the scratch direction as illustrated on fig.1.

The specimen is rectangle specimen witch constrained both in horizontal and vertical directions. Due to the symmetry of the problem, the indenter are treated as one-half part of three-dimensional body and specimen as one-fourth part of three-dimensional body. SOLID185 is used for meshing of the specimen and the Berkovich indenter. It is defined by eight nodes having three degrees of freedom at each node: translations in the nodal x, y, and z directions. The meshes along the scratch groove needed to be very fine to be able to describe the deformation and stress gradient below indenter with sufficient accuracy. The indenter and the specimen are shown in Fig. 2 with the appropriate boundary conditions for the problem. The nodes on the side 1 can not move along the x-axis, the nodes on the side 2 can not move along the z-axis and all the nodes on the bottom of the mesh are fixed. The friction coefficient $\mu$ between the indenter and the specimen was assumed to be 0.1.

![Figure 2: The finite element mesh of the scratch test and boundary condition](image)

The indenter was modeled as a linear elastic -plastic isotropic material with Young’s modulus $E = 1140$ GPa, Poisson’s ratio $\nu = 0.07$. The indenter tip was perfect.

![Figure 3: Stress-strain hardening curve](image)
The specimen was modeled as a multilinear elastic-plastic material with isotropic hardening behavior and assumed to be initially stress free. Purely elastic deformation takes place only during the beginning of the indentation process and follows Hook’s law. The plasticity follows von Mises yield criterion and power law hardening – $\sigma_s = a \cdot e^b$. The Von Mises yield criterion is applied for determining the occurrence of the plastic deformation. The multilinear elastic-plastic behavior is shown in Fig. 3 [1].

![Figure 4: The contours of the equivalent plastic strain were carried out in: a — the edge direction; b — the face direction](image)

Fig. 4 shows the contours of the equivalent plastic strain after a scratch simulation on a copper specimen with the Berkovich indenter in both the face and edge directions.

It can be seen from these figures that a smooth groove was created on the top surface of the specimen and the plastic strain concentrates mainly within the groove.

![Figure 5: The contours of Y displacement were carried out in: a - the edge direction; b - the face direction](image)

The formation of scratch results from plastic forming of the material without separation its. The mechanism of the formation of scratch consists in: the elastic deformation inside the groove, the elastic deflection of the surface responsible for the vertical displacement of the edge of the contact, the plastic deformation which is result in the remaining groove and the pile-up.

In case the scratch was made in the edge direction, the pile-in forms all along the length of scratch and on both sides of the groove. In case the scratch was made
in the face direction, the pile-up forms mainly front face. The pile-up is the higher than the pile-up, formed in the edge direction (fig. 5).

The simulation results were analyzed and there was defined that: the kinetics of accumulation of shear deformation under the scratch test, mechanism of the equivalent plastic strain distribution, the distribution of the stressed state index.

**References**


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Identification of elastic waves generated in friction zone. Computer simulation

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Abstract

Computer simulation is performed by combined discrete-continual approach. The movable cellular automaton method is used to describe discrete part of the friction couple (contact area). Analysis of Fourier spectra for time series of such parameters as velocity components, pressure and stress intensity allows to reveal the frequencies specific for the numerical model, the geometry and the processes occurring in contact area.

Introduction

Sliding friction, which takes place during the relative motion of conjugated solid surfaces, is accompanied by elastic oscillations of various frequencies. It is believed that the main factors responsible for these oscillations are a decrease in the friction coefficient with increasing relative velocity [1] and the friction force fluctuations in real contacts, related to differences in the local friction coefficient [2]. Rubtsov and Kolubaev [3] demonstrated that elastic waves could be generated as a result of the plastic flow in a real contact of materials with temperature-dependent mechanical properties. Gardos and Gabelich [4] believe that the friction coefficient is insufficient to describe a friction couple and consider the friction noise as a necessary additional characteristic of this system. From the general considerations, it is clear that this noise represents a superposition of elastic oscillations generated in the real contact (due to adhesive interactions, separation of worn particles, etc.) and their resonance at the eigenfrequencies of a tribological system. Therefore, the detected sound (longitudinal elastic waves in air) offer an integral characteristic of the entire system. The initial elastic waves generated at the sites of real contact bear more information about their sources. The extraction of this information in dynamic regime is still a difficult task in the experimental tribology.

This paper describes an attempt to use the results of computer simulation in order to identify elastic waves responsible for the processes taking place in the contact region of a model friction couple.
1 Formulation of the problem

We have considered numerical models of the contact interaction between solids, which is accompanied by the generation and propagation of elastic waves. Numerical calculations were performed within the framework of a combined discrete-continuum approach [5]. This approach was successfully checked in solving problems for the propagation of elastic wave of various types in a discrete medium (modeled by the method of movable cellular automata) and in a continuum (described by a system of equations of motion solved by the finite difference method) and their passage via the conjugation boundary of the two-component medium [5]. Previously, we have theoretically studied the nature of the stationary regime of deformation in solids, which was also related to the wave processes [6]. In both cases, the elastic waves were described in terms of the vector fields of velocities at the points of the medium, while the numerical parameters of these waves were not considered.

In the initial stage of this investigation, we performed calculations devoted to the “detection” of single propagating waves (both forward and reflected) generated in semi-infinite medium by a point impact on the free surface. In the bulk of the medium we placed “gages” and analyzed time series of such parameters as velocity components, pressure and stress intensity. It was found that the stress intensity (in contrast to the pressure) revealed the propagation of both longitudinal and transverse waves. Since the stress intensity is determined by the squares of the principal stress components [7], this quantity is positive and the frequency of its oscillations during the passage of a compression wave is twice as large as the frequency of pressure oscillations [8].

In the second stage, we considered a source of continuous signal, whereby the velocity component perpendicular to the surface at the point of loading was described by a harmonic function of time during the entire period of calculation. In this case, waves continuously propagate from the source, reflect from the boundaries, and superimpose on the following waves. Accordingly, the field of velocity vectors resembles “chaos” and cannot be analyzed without recourse to special mathematical methods. An analysis of the Fourier spectra of the time series of the pressure and stress intensity, determined at the same point as in the case of a single wave, showed that the peaks of main frequencies became narrower. For the stress intensity, a peak corresponding to the propagation of longitudinal waves is more intense than that for the transverse waves.

These results indicated that, in the case of friction, where many wave sources are continuously operating, an analysis of the Fourier spectra will probably also reveal the main frequency corresponding to the generation of elastic waves in the regions of real contact interactions. Accordingly, in the third stage we considered the friction of two steel bodies and analyzed the spectra of the main parameters for this system.

2 Results of numerical simulation

We have numerically simulated the friction between two steel bodies, with the material properties (\( \rho = 7800 \text{ kg/cm}^3 \), \( v_p = 5.95 \text{ km/s} \), \( v_s = 3.19 \text{ km/s} \)) and the geometry (0.25×0.5156 µm in size, shown in Fig. 1) analogous to those used previ-
ously [9, 11]. The method of movable cellular automata was used to simulate only a narrow region near the contact surface [10]. In Fig. 1, regions $a$ were described within the framework of continuum mechanics, regions $b$ were simulated using the method of movable cellular automata, and region $c$ corresponds to a quasi-liquid layer in the contact zone. The top and bottom surfaces of the bodies were loaded by applying compressive pressures $P = 250$ MPa and horizontal velocities $V = 10$ m/s. Periodic boundary conditions were applied at the left and right sides. The movable automata were 5 nm in size and the data were recorded at a time step of $10^{12}$ s. The “gages” were placed in the discrete region, closer to the boundary of conjugation with the grid.

![Figure 1: A sample for the simulation of friction using a combined discrete-continual approach.](image)

Figure 2 shows the typical Fourier spectra determined for of the time series of the main characteristics. The frequency is expressed in terms of the unit inverse to the interval of recording ($10^{12}$ Hz). As can be seen, all spectra display narrow peaks at a frequency of 0.004, which characterizes the discrete model (artificial roughness) rather than a physical process, and is determined by the ratio $V/d$, where $V = 20$ m/s is the relative velocity in the friction couple and $d$ is the automaton size. All spectra also exhibit the second harmonic (0.008) related to this feature of the model.

The most clearly pronounced physical peak is observed at a frequency of $\approx 0.003$ in the spectrum of the horizontal velocity component. In order to understand the meaning of this peak, let us determine the eigenfrequencies of the system under consideration. For a plane sample, we have two stripes with one end moving at a preset velocity and the other end free. Their frequencies can be determined by
identification of elastic waves generated in friction zone. Computer simulation

Figure 2: Fourier spectra of the time series of (a) the x-component of velocity and (b) the stress intensity in a friction couple.

analogy with a cantilever fixed at one end [9]: \[ p_k = v(k - 0.5)/2l, \] where \( v \) is the elastic wave velocity and \( l \) is the stripe height (half of the whole assembly height). The transverse sound velocity is \( v_S = 3.19 \text{ km/s} \) and the sample height is \( 5.156 \times 10^{-7} \text{ m} \). Therefore, the first harmonic is 3 GHz, which corresponds to 0.003 in the adopted frequency units, accordingly, the second harmonic corresponds to 0.009. These very frequencies are observed in the spectrum of the horizontal velocity component. A change in the sample height leads to the corresponding frequency variation (Fig. 3a). The spectra of the vertical component of velocity exhibits no such peaks and is independent of the sample width, which is explained by the use of periodic boundary conditions.

A change in the automaton size leads to the variation of only peaks corresponding to the artificial roughness. The only (smeared) peak that remains unchanged when the dimensions of the sample and automata are varied corresponds to a frequency of 0.002 in the spectra of pressure, stress intensity, and vertical velocity component. This frequency characterizes the average lifetime of coupled automata in the quasi-liquid layer near the contact surface and it can be interpreted as a characteristic frequency of motion at a microscopic level in the stick-slip regime. This value varies depending on the criterion of bond restoration between unbound automata (Fig. 3b), which can be related, for example, to an increase in the contact zone temperature.

We also varied the structure of the interacting bodies (Fig. 4). First, we varied...
initial roughness in the contacting zone, namely length and number of asperities. When friction layer was forming in these bodies Fourier spectra could differ but when steady-state process was established the spectra where practically the same. Second, we used materials of heterogeneous structure consisting of hard inclusions and soft layer. In this case the Fourier spectra had the peaks corresponding to shifting the interacting bodies at the character size of inhomogeneity.

3 Conclusions

We have numerically modeled dynamic contacts between solid bodies, which are accompanied by the generation and propagation of elastic waves, and analyzed the Fourier spectra determined for the time series of velocity components, pressure, and stress intensity at given points. Preliminarily, changes in these spectra were considered for the reflection and superposition of single waves and waves from a continuous source. This experience was used in the analysis of elastic waves propagating in a model friction couple, which allowed frequencies characteristic of the model, problem geometry, and process in the contact zone to be revealed.

Therefore, we have demonstrated the possibility to identify processes taking place
Identification of elastic waves generated in friction zone. Computer simulation

Figure 4: Contacting zone of samples (area modeled by the method of movable cellular automata) with various structure at (a) initial time and (b) steady-state regime of friction.

in the real contact regions by an analysis of elastic waves observed in the friction couple.

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Motion of a deformable particle in an oscillating medium:
continuous model

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Abstract

Analysis of free sinking of a solid particle in a fluid and of rising up of a deformable particle (an individual gas bubble or a gas bubble with an attached particle) are generic model problems in the theory of the enrichment processes [1,3]. Therefore, the analysis of an influence of fluid’s oscillations upon the average velocity of particle’s steady motion is of considerable practical relevance. This study is also interesting for the theory of flotation process, which occurs under conditions of turbulent pressure pulsations in a fluid, and also in connection with possibilities to control particle’s motion by means of fluid’s oscillations.

In this paper, the motion of solid and deformable particles in a viscous incompressible fluid performing time-harmonic oscillations with a given frequency and the amplitude is examined. A particle is modeled as a spherical shell with an elastic rod inside. Under the assumption, that the fluid’s resistance to motion of particle is of a nonlinear nature, analytical formulas for an average velocity of the particle are obtained. Formulas suggest that the magnitude of this velocity is reduced due to effect of oscillations of the volume of a fluid. The presence of resonance frequencies is revealed. The decrease may be particularly large in the case of a deformable particle (for example, an air bubble) due to the resonant effects, i.e., when the frequency of fluid’s oscillations is close to the natural frequency of the particle.

The concept of vibrational rheology is used for the solution of problem [4]. In accordance with its content the discussed effects are explained as being introduced by modification of rheological characteristics of particles with respect to their ‘slow’ motions due to the effect of ‘fast’ motions (oscillations).

Several aspects of the influence of vibrations on motion of particles in a fluid have been considered in [6-8]. Results reported in these references and experimental data are in a good agreement with conclusions of the present paper. The simplest model of a deformable particle has been studied in reference [9].
1 A model and equation of motion of a particle

A model of a deformable particle in an oscillating fluid-filled vessel is shown schematically in Figure 1.

This model includes an 'external' mass and an elastic rod. We assume that a rod and an external mass may move along the axis $u$, which is built in a vessel and directed downwards. Equations of motion of a particle have the following form:

\[
M \ddot{u} |_{\xi=0} = -F(\dot{u} |_{\xi=0}) + m(1 - \Delta)(A\omega^2 \sin \omega t + g) + ES \frac{\partial u}{\partial \xi} |_{\xi=0} \]

\[
-\frac{\partial^2 u}{\partial \xi^2} + \frac{\rho}{E} \ddot{u} = \frac{\rho}{E} A\omega^2 \sin \omega t + \frac{\rho}{E} g \]

Here $u$ - the displacement of a rod, the axis $\xi$ is rigidly attached to the external particle, directed downwards, its beginning coincides with the base of rod (see Fig. 1); $M = m + m_0$, where $m_0$ - the added mass of a fluid, $\Delta$ - the ratio of the density of the fluid $\rho_0$ to the density of the particle $\rho$; $A$ - the amplitude, and $\omega$ - the frequency of the oscillations of the vessel.
Time differentiation is designated by dot. We assume that displacement of the external mass equals \( u|_{\xi=0} = 0 \).

Boundary condition for the displacement \( u \) is: \( \frac{\partial u}{\partial \xi} \bigg|_{\xi=l} = 0 \).

In equation (1), \( F(\dot{u}|_{\xi=0}) \) designates a fluid resistance force, which as in previous publications [1-3] is approximated by the formula:

\[
F(\dot{u}|_{\xi=0}) = \rho_0 D^2 \Psi(Re) \dot{u}^2\big|_{\xi=0} \text{sign} \dot{u}|_{\xi=0}
\]

Where \( \rho_0 \) - a density of the fluid, \( D \) - a diameter of the particle, and \( \Psi(Re) \) is a resistance coefficient, which depends on Reynolds number \( Re = \frac{DV}{2\nu} \) as predicted by classic Rayleigh diagram (\( V \) - characteristic velocity, and \( \nu \) - kinematic viscosity of a fluid). Inasmuch we are concerned with a case of non-linear (quadratic) resistance, we assume:

\[
Re > 500, \Psi(Re) \approx 0,2
\]

2 Solution of a problem; vibro-rheological characteristic of resistance force and equations of slow motion of a particle

To solve the problem, we use the methodology of vibrational mechanics and use the method of direct partition of motions[4]. We seek a solution of the system of equations (1), (2) in the form:

\[
u = U(t) + \nu(t, \omega t)
\]

where \( U \) is a ”slow” time, and \( \nu \) is a ”fast”, \( 2\pi \) - periodic in non-dimensional time variable \( \tau = \omega t \), with vanishing magnitudes averaged over period in \( \tau \):

\[
\langle \nu(t, \omega t) \rangle = 0
\]

(angular brackets designate averaging in \( \tau \)). Following standard procedure of the method of direct partition of motion, we obtain the following equations of fast and slow motions, respectively:

\[
M \ddot{U}|_{\xi=0} = -\left\langle F((\dot{U} + \dot{\nu})|_{\xi=0}) \right\rangle + m(1 - \Delta)g + ES \frac{\partial U}{\partial \xi}\bigg|_{\xi=0} + \frac{\partial^2 U}{\partial \xi^2} + \frac{\rho}{E} \ddot{U} = \frac{\rho}{E} g
\]

(8)

\[
M \ddot{\nu}|_{\xi=0} = -\left\langle F((\dot{U} + \dot{\nu})|_{\xi=0}) \right\rangle + \left\langle F((\ddot{U} + \ddot{\nu})|_{\xi=0}) \right\rangle + m(1 - \Delta)A\omega^2 \sin \omega t + ES \frac{\partial \nu}{\partial \xi}\bigg|_{\xi=0} - \frac{\partial^2 \nu}{\partial \xi^2} + \frac{\rho}{E} \ddot{\nu} = \frac{\rho}{E} A\omega^2 \sin \omega t
\]

(10)
The boundary conditions are: \( \frac{\partial U}{\partial \xi} \bigg|_{\xi=l} = 0, \quad \frac{\partial \upsilon}{\partial \xi} \bigg|_{\xi=l} = 0 \).

Firstly, equations of fast motions (9), (10) should be solved. The essential advantage of the direct partition of motions method is a possibility to solve equations of fast motions in an approximate manner, if, as is typical, the equation of slow motion is of the fundamental interest. In this case, in the course of solving equations (9), (10) we assume that resistance forces \( F(\dot{U} + \dot{\upsilon}) \bigg|_{\xi=0} \) are negligible in comparison with other forces.

Solution of equations (9-10) is sought as \( \upsilon = \upsilon_1(\xi) \sin \omega t \). Apparently, the solution of equation (10) is:

\[
\upsilon_1(\xi) = C_1 \sin \sqrt{\frac{\rho}{E}} \omega \xi + C_2 \cos \sqrt{\frac{\rho}{E}} \omega \xi - A
\]

Thus, the constants \( C_1 \) and \( C_2 \) should be determined. We apply boundary conditions: \( \upsilon'(l) = 0 \) and equation (9). It yields:

\[
C_1 = C_2 \frac{\sin \sqrt{\frac{\rho}{E}} \omega l}{\cos \sqrt{\frac{\rho}{E}} \omega l}, \quad C_2 = A \frac{M - m(1 - \Delta)}{M} \frac{1}{1 + \frac{\sqrt{\rho E}}{M \omega l} \tan \sqrt{\frac{\rho}{E}} \omega l}
\]

To solve equation of slow motion, we have to determine \( \upsilon|_{\xi=0} \) from equations (9) and (10). As follows from (11):

\[
\upsilon|_{\xi=0} = (C_2 - A) \sin \omega t
\]

We use equation (12) to get:

\[
\upsilon|_{\xi=0} = B \sin \omega t,
\]

where:

\[
B = -A \frac{\delta \omega \cos \omega d + \eta \sin \omega d}{\omega \cos \omega d + \eta \sin \omega d},
\]

\[
\delta = \frac{m(1 - \Delta)}{M}, \quad \eta = \sqrt{\rho E S} M, \quad d = \sqrt{\frac{\rho}{E}}.
\]

To derive equations of slow motion (7), (8), it is sufficient to find \( R(\hat{\upsilon}|_{\xi=0}) = \langle F((\hat{U} + \hat{\upsilon})|_{\xi=0}) \rangle \). As follows from (3) - (5) and (14) with identities \( \langle \cos \omega t \rangle = 0 \), \( \langle \cos^2 \omega t \rangle = \frac{1}{2} \) taken into account, we obtain:

\[
R(\hat{\upsilon}|_{\xi=0}) = \langle F((\hat{U} + \hat{\upsilon})|_{\xi=0}) \rangle = 0.2 \rho_0 D^2 (\hat{U}_0^2|_{\xi=0} + \frac{1}{2} B^2 \omega^2 \text{sign} \hat{U}|_{\xi=0}).
\]

In this formula, we use the assumption that a velocity of the particle \( \hat{\upsilon}|_{\xi=0} = (\hat{U} + \hat{\upsilon})|_{\xi=0} \) in the motion we consider preserves the same sign, i.e., \( \hat{\upsilon}|_{\xi=0} > 0 \). With this assumption being ignored,
formulas acquire more complicated form, but it does not alter the reported results qualitatively.

Formula (15) defines the effective resistance force to the steady motion of a particle in an oscillating fluid (its vibro-rheological characteristic). With this formula taken into account, equations of slow motion of a particle (7), (8) acquire in the following form:

\[
M \ddot{U} \bigg|_{\xi=0} = -0,2 \rho_0 D^2 (\dot{U}^2) \bigg|_{\xi=0} + \frac{1}{2} B^2 \omega^2 \text{sign} \dot{U} \bigg|_{\xi=0} +
\]
\[
+ m(1-\Delta)g + ES \frac{\partial U}{\partial \xi} \bigg|_{\xi=0} + \frac{\partial^2 U}{\partial \xi^2} + \frac{\rho}{E} \dddot{U} = \frac{\rho}{E} g
\]

Integration of equation (17) from 0 to 1 yields:

\[
\frac{\partial U}{\partial \xi} \bigg|_{\xi=0} + \frac{\rho}{E} \int_0^1 \ddot{U} d\xi = \frac{\rho}{E} l g
\]

Equation (16) gives:

\[
M \ddot{U} \bigg|_{\xi=0} = -0,2 \rho_0 D^2 (\dot{U}^2) \bigg|_{\xi=0} + \frac{1}{2} B^2 \omega^2 \text{sign} \dot{U} \bigg|_{\xi=0} + m(1-\Delta)g +
\]
\[
+ \rho l S g - \rho S \int_0^1 \ddot{U} d\xi,
\]

### 3 Velocity of stationary sinking (rising up) of a particle

Stationary (steady state) motion of a particle is characterized by the magnitudes of \( \dot{U} \big|_{\xi=0} = \dot{X}_s = \text{const} \) and \( \dot{U} = \text{const} \). Then the velocity \( \dot{X}_s \) is determined from equation:

\[
[m(1-\Delta) + \rho S l]g = 0,2 \rho_0 D^2 (\dot{X}_s^2 + \frac{1}{2} B^2 \omega^2) \text{sign}\dot{X}_s
\]

Therefore:

\[
\dot{X}_s = \pm V_0 \sqrt{1 - \frac{1}{2} \left( \frac{B \omega}{V_0} \right)^2},
\]

where

\[
V_0 = \sqrt{\frac{|m(1-\Delta) + \rho S l| g}{0,2 \rho_0 D^2}}
\]

- magnitude of a mean velocity of motion of a particle in the absence of vibrations, with sign ”+” in equation (21) presenting a sinking particle when \( m(1-\Delta) + \rho S l > 0 \) and \( \dot{X}_s > 0 \). Sign ”−” corresponds to a rising particle when \( m(1-\Delta) + \rho S l < 0 \) and \( \dot{X}_s < 0 \).
If the particle has a spherical shape and it is non-deformable, i.e. $\eta = 0$, then formula (14) for the amplitude $B$ is considerably simplified:

$$B = -\frac{m(1 - \Delta)A}{M}$$

As follows from (21-22), mean velocity of sinking and rising up is significantly reduced due to vibrations, and this reduction is particularly pronounced in the resonant cases, when the amplitude of fast vibrations of a particle $B$, defined by formula (14), grows in comparison with its non-resonant magnitude. A function $|B/A|$ for $\delta = \frac{1}{2}$, $\eta = 3$, $d = 1$ is plotted in Figure 2.

<table>
<thead>
<tr>
<th>$B/A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

Figure 2: Dependence of the amplitude of fast oscillations on the excitation frequency.

It should be noted that infinitely large amplitudes at resonant frequencies are developed due to neglecting of the energy dissipation in analysis of fast motions. Therefore, strictly speaking formulas (14) and (21), as well as the graph in Figure 2 are valid for frequencies, slightly detuned from resonances. It does not present serious difficulties to take into account effects of damping in analysis of fast motions. However, it makes algebra more cumbersome.
4 Eigenfrequencies of a gas bubble and of the model of a particle

It is helpful to compare eigenfrequencies of the considered model and of a gas bubble. Cornfeld has derived the following formula for eigenfrequencies of a bubble [10]: 
\[ \omega_n^2 = \frac{\sigma}{\rho R^3} n(n + 2)(n + 3), \]
where \( R \) is the radius of a bubble, \( \sigma \) - is a surface tension, \( \rho \) the density of a fluid. Our problem formulation does not involve surface tension. So that we compare magnitudes of eigenfrequencies scaled by the magnitude of the lowest one 
\[ \omega_n = \omega_1 \sqrt{\frac{n(n+2)(n+3)}{12}}. \]

Let us explore the influence of variations in parameters \( \delta, \eta \) and \( d \) on distribution of eigenfrequencies. As a criterion, we adopt the ratio of gaps between neighboring frequencies, for example \( (\omega_2 - \omega_1)/(\omega_4 - \omega_3) \). Apparently, parameter \( \delta \) has no influence on this ratio. Variation in \( d \) affects this ratio very weakly (because the gaps between frequencies vary equally with variation in parameter \( d \)). Parameter \( \eta \) influences on the distribution of frequencies, as it grows, gaps \( (\omega_{n+1} - \omega_n)/(\omega_{n+3} - \omega_{n+2}) \) decrease. Maximum value of \( (\omega_{n+1} - \omega_n)/(\omega_{n+3} - \omega_{n+2}) \) equals 1 and it is attained when \( \eta \to 0 \). Hence, variation in parameters \( \delta, \eta \) and \( d \) weakly affects distribution of eigenfrequencies.

Eigenfrequencies predicted in the present paper and in [10] are compared in the table for \( \delta = \frac{1}{2}, \eta = 3, d = 1 \).

<table>
<thead>
<tr>
<th>Frequency number</th>
<th>Scaled magnitude</th>
<th>The present model</th>
<th>Cornfeld</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.4556</td>
<td>2.4556</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>5.23294</td>
<td>4.48337</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>8.20453</td>
<td>6.72506</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>11.256</td>
<td>9.18818</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>14.3434</td>
<td>11.8618</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>17.449</td>
<td>14.7333</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>20.5652</td>
<td>17.7928</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>23.6879</td>
<td>21.0283</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>26.815</td>
<td>24.4333</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>29.945</td>
<td>27.9986</td>
<td></td>
</tr>
</tbody>
</table>

5 Conclusion

Relatively simple formulas for the averaged speed of a solid and a deformable particle in an oscillating fluid are obtained. These formulas suggest that the magnitude of the speed decreases as a result of the pulsations. This decrease can be particularly significant in the case of the deformable particle, for example, the air bubble. The results reported in the paper can be used for analysis and optimization of the processes of gravity concentration and flotation, and also for an active control of these processes.

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References


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Adaptive algorithms for suppressing beam vibration of dual cantilever mass absorber

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Abstract

Generally, the vibration absorber is one of the most common methods used to control vibration via the stiffness of the vibration absorber which is adjusted to have the natural frequency equal to the frequency of harmonic force that acts on the system. However, the nature of exciting forces is usually in a dynamic form which has a broad range of frequencies. The passive vibration and active dynamic absorbers are limited in usage while the adaptive vibration control achieves attenuation of harmonic excitation through tuning a reactive device. Therefore, the adjustment of absorber stiffness to the optimized natural frequency has a limit to suppress the vibration of system. The objective of this study is to investigate the use of adaptive dynamic vibration absorber for suppressing beam vibration of dual cantilever mass absorber with gradient method and Lyapunov's direct method.

1 Introduction

The absorber typically consists of an inertial device which changes the dynamic response of the original vibrating system over a certain range of frequencies. The absorbing device may be a linear mass-spring oscillator, rotary oscillator, a fluid or a distributed elastic structure. Generally, vibration absorber is designed to have the natural frequency or absorption frequency (\(\omega_a\)) equal to the frequency of exciting force in order to protect the resonance which occurs when the exciting frequency (\(\omega_f\)) is equal to the natural frequency of the primary system (\(\omega_n\)). After installing the vibration absorber, the vibration of the main system approaches to zero at the resonance frequency. That means the efficiency of the vibration absorber is highest at this frequency and the efficiency is reduced when the frequency of the exciting force is changed. Therefore, the vibration absorber is invented and can be tuned to the absorption frequency by adjusting damp, mass or stiffness for the coincide of the variable frequency. However, the harmonic vibration occurs in the
mechanical system whose amplitude and frequency of the force are always varied. Thus, adjusting the absorption frequency is not efficient enough for suppressing the harmonic vibration that occurs in the system.

The concept of the vibration absorber was first developed in 1902 by Frahm, who designed a fluid tank system for the reduction of rolling motion in the German ships. The dynamic vibration absorber was firstly discovered in 1909, which is a passive system that consists of mass spring and damper. Den Hartog [1] presented the principle of reducing the maximum amplitude of the main system by using the damped vibration absorber and in 1993 Korenev and Reznikov [2] applied the vibration absorber to the tower structures, and ventilation pipes. Hunt [3] presented the active dynamic vibration absorber (ADVA) to apply in the helicopter by developing the hydraulic rotor system. In addition, two sensors and feedback devices were attached to the rotor and body of helicopter. Both signal was amplified and controlled servo valve for controlling hydraulic between rotor and body of helicopter. Lamancusa [4] did the experiment by using the adaptive-passive absorber for sound radiation in the engine. The result showed vibration occurred in a narrow band of response. It was summarized that the adaptive-passive vibration absorbers worked well to reduce the vibration. Franchek, Ryan and Bernhard [5] studied about controlling the vibration of four-floor building model with a tunable vibration absorber mounted on the top floor. The base of the building was excited by the frequencies of 6.1-7.4 Hz. by using the criteria adjusting absorption frequency equal to the exciting the frequency. From the test, the tunable vibration absorber could minimize the vibration up to 24 dB. In 1997, Buhr, Franchek and Bernhard [6] developed the adaptive-passive vibration control from previous studies in a non-collocated situation by using the previous building model. The second and third floors were controlled by the vibration control which used the phase difference obtained from demodulation in processing. The result revealed that when the structure was excited at a frequency of 6 Hz, the tuned vibration absorber achieved a 19.4 dB and 23 dB reduction in the amplitude of the second and third floors, respectively. Charneal, Charette and Fuller [7] studied the use of the adaptive tune vibration absorber (ATVA) to minimize sound radiated from a simply supported plate by using the stiffness adaptation which is controlled by two different tuning algorithms. The results demonstrated that in the 156 Hz case the ATVA can increase the average sound pressure levels radiated at 12 dB and reduce the sound pressure levels by and average of 16.5 dB compared to the base line case.

Christopher [8] studied the comparison of two different vibration absorbers (a) enclosed-air and (b) dual cantilever masses. Both absorbers will adapt the absorption frequency to implement equal to the exciting frequency by the stiffness adjustment of the vibration absorber. From the experiment, the enclosed-air absorber was able to reduce the vibration to 10 dB which worked in 47-60 Hz and had the resonance frequency at 53 Hz. The efficiency depended on types of diaphragm that were used in the enclosed absorber. Dual cantilever mass absorber has the higher flexibility and efficiency in use. The system was used the dual mass absorber with an extended frequency range of 47-95 Hz. Simon [9], [10] followed Christopher by using the same vibration absorber which was dual cantilever mass to control the vibration of a rectangular plate and the large electric transformer.
Adaptive algorithms for suppressing beam vibration of dual cantilever mass absorber

The system response with passive absorber has low performance and the system with the tuning absorption frequency method has enough performance to suppress the beam vibration but it is difficult to adjust the stiffness of absorber when the frequency of the exciting force has more than one. Although the dual cantilever mass absorber has many advantages. The studies of Chritopher and Simon presented that the important conditions affecting the efficiency of the absorber in the exciting force with a single frequency. In fact, the vibration system has the complex amplitude and frequency, and also it has multi-amplitude and frequency. Finally, this paper studies and analyzes the gradient method and Lyapunov’s direct method for adjusting the optimized stiffness of the vibration absorber. Moreover, the most efficiency to minimize the vibration and automatic work was obtained by using LabVIEW version 7.1 and MATLAB version 7.0 programs in the measurement of the vibration and the stiffness adjustment of the vibration absorber.

2 Mathematical description

The active dynamic vibration absorber (ADVA) uses the dual cantilever mass vibration absorber in this study because it is easy to make at low cost and can adjust the stiffness of the vibration absorber. From the characteristics of this vibration absorber, there are absorber masses at both ends of the rod as shown in Figure 1. Adjusting the displacement (L) of absorber masses at both sides will change the stiffness of the absorber. Therefore, the natural frequency of the absorber or the absorption frequency will be changed.

The important criteria in designing the vibration absorber is the absorption frequency of the absorber \( \omega_a \) must be equal to the frequency of the exciting force \( \omega_f \), which is the absorption frequency of the vibration absorber related with the stiffness. Therefore,

\[
\omega_a^2 \propto \frac{k_a}{m}
\]

where \( k_a \) is the stiffness of the absorber and \( m \) is the absorber mass.

The absorption frequency of the absorber is calculated by the Dunkerley approximation that is,

\[
\omega_a = \sqrt{\frac{k_a}{m}} = \sqrt{\frac{76.2EI}{(3m_b + 25.4m_a)L^3}}
\]

Therefore,

\[
k_a = \frac{76.2EI}{L^3}
\]

where

- \( E \) = Modulus of elasticity
- \( I \) = Moment of inertia
- \( L \) = Rod length (displacement between absorber mass and body)
- \( m_a \) = Absorber mass
- \( m_b \) = Rod mass.
The main system in this study is a straight beam. It has a rectangular cross section which is 25 mm. width, 13 mm. thick and 840 mm. long. The vibration source is circular disc which was perforated with a hole, connecting with the motor shaft. It has been set up at the middle of beam. Then, it makes the harmonic force due to the rotating unbalance mass, which varies with a square of circular velocity of the motor and let the working speed of the motor is in a range of 600-2400 rpm (62.83-251.32 rad/sec) and the attached vibration absorber is under the beam as middle as the motor as shown in Figure 2.

The experiment is performed following Figure 3. The relationship between the stiffness of the vibration absorber and rod length has the nonlinear characteristic. We can approximate the range of rod lengths of 0.085-0.15 m. or the stiffness of the vibration absorber of 3327-11320 N/m and the equation is

\[ k_a = -6.43 \times 10^7 L^3 + 2.36 \times 10^7 L^2 - 2.95 \times 10^6 L + 1.32 \times 10^5 \]  

(4)

The mathematical model of the beam is attached absorber which has the harmonic force acting on the system as shown in Figure 4. When the mass, stiffness, damping and displacement of the primary system are defined as \( M, k, c \) and \( X \) respectively and \( m, k_a, X_a \) are respectively mass, stiffness and displacement of the absorber. The system is excited by the harmonic force \( F(t) \). Thus, the equation of
Adaptive algorithms for suppressing beam vibration of dual cantilever mass absorber

Figure 3: The relation between the stiffness of the vibration absorber and rod length.

Figure 4: The mathematical model of the beam with undamped absorber.

motion in the state space form is

$$
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\dot{x}_3 \\
\dot{x}_4
\end{bmatrix} =
\begin{bmatrix}
0 & 1 & 0 & 0 \\
-\frac{k-k_a}{M} & -\frac{c}{M} & \frac{k_a}{M} & 0 \\
0 & 0 & 0 & 1 \\
\frac{k_a}{m} & 0 & -\frac{k_a}{m} & 0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix} +
\begin{bmatrix}
0 \\
\frac{1}{M} \\
0 \\
0
\end{bmatrix}
F(t)
$$

(5)

and the state output is

$$
y =
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix}
$$

(6)

where $x_1 = X$; $x_2 = \dot{X}$; $x_3 = X_a$ and $x_4 = \dot{X}_a$. 
3 Adaptive algorithms for stiffness adjustment

The first control algorithm of the vibration absorber is the gradient method which adjusts the stiffness of the dual cantilever mass vibration absorber. The second control algorithm vibration absorber is Lyapunov’s direct method. The objective of algorithms is to adjust the stiffness of the dual cantilever mass vibration absorber until the displacement is close to zero.

Gradient method: One possibility is to adjust the parameters in such a way that the loss function is minimized

$$ J(\hat{k}_a) = \frac{1}{2}X^2 $$  \hspace{1cm} (7)

and assign the parameters in the negative gradient of $J$

$$ \frac{\partial \hat{k}_a}{\partial t} = -\gamma \frac{\partial J}{\partial \hat{k}_a} = -\gamma X \frac{\partial X}{\partial \hat{k}_a} = -\gamma XD $$ \hspace{1cm} (8)

then give the following adaptation law, so that $\left( \frac{\partial X}{\partial \hat{k}_a} \right)$ is

$$ M \frac{\partial^2 D}{\partial t^2} + c \frac{\partial D}{\partial t} + (k + \hat{k}_a)D = X_a - X $$ \hspace{1cm} (9)

where $D = \frac{\partial X}{\partial \hat{k}_a}$ is the sensitivity function and $\gamma$ is the adaptation gain.

Lyapunov’s direct method: Lyapunov function is selected as

$$ V(X, \hat{k}_a) = \frac{1}{2} \left( \frac{k + \hat{k}_a}{M} \right) X^2 + \frac{1}{2} \dot{X}^2 + \frac{M}{2\gamma} \left( \frac{k_a + \hat{k}_a}{M} \right)^2 $$ \hspace{1cm} (10)

Then, we get the time derivative of $V$ as

$$ \dot{V}(X, \hat{k}_a) = -\frac{c}{M} \dot{X}^2 + \frac{1}{\gamma} \left( \frac{k_a + \hat{k}_a}{M} \right) \left( \frac{\partial \hat{k}_a}{\partial t} + \gamma X_a \dot{X} \right) $$ \hspace{1cm} (11)

The rate of change of $\hat{k}_a$ is

$$ \frac{\partial \hat{k}_a}{\partial t} = -\gamma X_a \dot{X} $$ \hspace{1cm} (12)

4 Experiment and Simulation Results

Experiment and Simulations are performed the system with vibration absorber. The first experiment and simulation are concerned system with gradient method algorithm. The second simulation is concerned system with Lyapunov’s direct method algorithm. The parameters of the system are $M = 3.72$ kg, $m = 0.512$ kg, $k = 77485$
N/m, \( k_{a_{\text{initial}}} = 5500 \) N/m and \( c = 5.9 \) N-s/m.

Part I: The sinusoidal function is used for the exciting force with \( A \sin (\omega t) \), where \( A = 0.0002581 \omega^2 \) and use the starting frequency (\( \omega \)) at 94.24 rad/sec, switch up to 144.51 and 125.66 rad/sec in 100 sec and 200 sec. The results of the response with the gradient method are compared with experiment and simulation as shown in Figures 5 and 6. The result of the simulation with Lyapunov’s direct method is shown in Figure 7.

![Figure 5](image1)

Figure 5: Experimental result of the system response of \( X(t) \) with gradient method.

![Figure 6](image2)

Figure 6: Simulation result of the system response of \( X(t) \) with gradient method.
Part II: The excitation force with \(2.29 \sin(94.24t) + 5.38 \sin(144.51t)\) switch up to \(4.07 \sin(125.66t) + 2.50 \sin(82.50t)\) in 500 sec. The result of the simulation with the gradient method is shown in Figure 8 and Figure 9 presents the adjusting parameter of the stiffness absorber. In the first period, the absorber’s stiffness is 10770 N/m and in the second period is 8056 N/m. The result of the simulation with Lyapunov’s direct method is shown in Figure 10 and Figure 11 presents the adjusting parameter of the stiffness absorber. In the first period, the absorber’s stiffness is 10660 N/m and in the second period is 8070 N/m.

Figure 7: Simulation result of the system response of \(X(t)\) with Lyapunov’s direct method.

Figure 8: Simulation result of the system response of \(X(t)\) with gradient method.
Figure 9: Absorber’s stiffness adjusted with gradient method.

Figure 10: Simulation result of the system response of $X(t)$ with Lyapunov’s direct method.

The result of the simulation with Lyapunov’s direct method is shown in Figure 10 and Figure 11 presents the adjusting parameter of the stiffness absorber. In the first period, the absorber’s stiffness is 10660 N/m and in the second period is 7905 N/m.
5 Conclusions

This study is aimed to demonstrate a method for optimizing the stiffness of the dual cantilever mass absorber. The control algorithms of Lyapunov’s direct method and gradient method for the vibration absorber have the same highest efficiency to reduce the vibration of a beam. Although the system with the gradient method shows high performance to adjust the stiffness of absorber, the stability of the system must be defined first. The adaptive algorithms could adjust the optimum stiffness of the absorber to well reduce the vibration in both cases of the single and multi exciting forces. Therefore, the adaptive algorithms are the high efficiency method for the adjusted stiffness of the dual cantilever mass absorber.

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Adaptive algorithms for suppressing beam vibration of dual cantilever mass absorber


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Stability analysis of tension-torsion process of one mechanical system

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Abstract

The stability process of tension-torsion process is described in this article. The stability failure conditions are found for rigid and soft loading.

Mechanical system consisting of two elastic circular cylinders 1 and 2, transmitting the loading to a hollow cylindrical sample 3 (fig. 1) is considered. The rigidity of rod 1 working only under tension (torsion is blocked) is equal to $\lambda_1$. The tensile forces with resulting force $P$ are given on the transversal cross-section $A–A$ (soft loading) or the section points have the displacement $u$ (hard loading). The rigidity of rod 2 working only under torsion (tension is longitudinal displacement of section $C–C$ is blocked) is equal to $\lambda_2$. The rotation moment $M$ is given on the transversal cross-section $D–D$ (soft loading) or the rotation angle $\psi$ is given (hard loading). Deformation is realized isothermally with small velocity (quasi-static deformation).

Tensile stress $\sigma$ and deformation $\varepsilon$ with tangent stresses and shear deformations appear in the sample under given loading. The sample is considered to have unit height and unit average cross-section radius, and the wall thickness is equal to $\frac{1}{2\pi}$. In this case the value of tensile force applied to the sample is equal to the stress $\sigma$. 
and the displacement sample edge adjoining to the rod \( \varepsilon \) is equal to the deformation \( \varepsilon \). The tangent stresses and shear deformations can be substituted by the values of tangent stress \( \tau \) and shear deformation \( \gamma \) on the mean line of transversal section. Then the rotation moment in sample section \( C-C \) is equal to \( \tau \), and rotation angle is equal to \( \gamma \).

Before system stability analysis we determine the sample properties. The sample is loaded with rigid control of \( \varepsilon \) and \( \gamma \) deformation. Two real numbered ordered systems \((\varepsilon, \gamma)\) can be considered as the elements of two-dimensional Euclidean deformation space \( R^2_{\varepsilon} \). The points \((\varepsilon, \gamma)\) will move along continuous curve \( \chi \), (the deformation path) in Cartesian rectangular coordinates.

By means of some mapping \( \chi \), defined by continuously - differentiated functions \( \sigma = \sigma(\varepsilon, \gamma), \tau = \tau(\varepsilon, \gamma) \), the points of the curve \( \chi \) correspond the points \((\sigma, \tau)\) in the stress space \( R^2_{\sigma} \), which form the loading curve. If the Jacobian \( I \) of this mapping is not degenerated then the mapping \( \chi \) is homeomorphism (biunique and mutually continuous mapping). If the Jacobian \( I \) is degenerated \((\det I = 0)\), in some point of curve \( \chi \) then no unequivocal mapping \( R^2_{\varepsilon} \rightarrow R^2_{\sigma} \), exists in the vicinity of this point though the mapping \( \chi : R^2_{\varepsilon} \rightarrow R^2_{\sigma} \) remains unequivocal. Such points are critical points of mapping \( \chi \). After their imagination to the \( R^2_{\sigma} \) space the return point is formed on a curve. The detailed analysis shows, that in the transition of material from hardening to softening occurs in the first critical point when the reduction of at least one stress is observed under active deformation.

The points \((\sigma, \tau) \in R^2_{\sigma} \) space are the coordinates of some vector \( \mathbf{p}(\sigma, \tau) \). Applying the Hamilton operator \( \nabla_2 \), determined in the space \( R^2_{\varepsilon} \), we find, that \( \nabla_2 \mathbf{p} = I \). Further, the vector field \( \mathbf{p} \), formed by the mapping \( \chi \), can be to spread out as a sum of potential and solenoid fields. The vector field is supposed to be potential, that is \( \mathbf{p} = \nabla_2 \Pi \) (\( \Pi(\varepsilon, \gamma) \) is the field potential). Hence, the stress work does not depend on the view of deformation path and is equal to the value of function \( \Pi \) in the achieved point of path and the vector \( \mathbf{p} \) is orthogonal to the lines of potential level \( \Pi \) in the space \( R^2_{\varepsilon} \). Now \( I = \nabla_2 \nabla_2 \Pi \) and the Jacobian of mapping \( \chi \) is the Gesse matrix of the function \( \Pi \). Thus, the set of critical points is defined by the equation solutions

\[
\det H_2 = c_{11}c_{22} - c^2 = 0, 
\]

where \( H_2 = \nabla_2 \nabla_2 \Pi, c_{11} = \Pi_{\varepsilon\varepsilon}, c_{22} = \Pi_{\gamma\gamma}, c = \Pi_{,\varepsilon\gamma} \). The points \((\varepsilon, \gamma)\), satisfy the equation \((1)\) and form the line on the plane \( R^2_{\varepsilon} \) dividing the stable (hardening) and unstable (softening) states of material.

Since \( \nabla_2 \mathbf{p} = \frac{d\mathbf{p}}{d\mathbf{e}} \), where \( \mathbf{e} \) is the vector with components \((\varepsilon, \gamma)\), the following incremental correlations

\[
d\sigma = c_{11}d\varepsilon + c_{12}d\gamma, \quad d\tau = c_{21}d\varepsilon + c_{22}d\gamma, 
\]

are fulfilled where parameters \( c_{11}, c_{22}, c \) determine the instantaneous material properties (instantaneous modules), that vary during deformation. In elasticity \( c_{11} = E \) (the Young module), \( c_{22} = G \) (the shear module), \( c = 0 \). The typical feature of correlations \((2)\) consists in the fact that additional loading due to deformation increment in one direction (for example, \( d\varepsilon \neq 0, d\gamma = 0 \)) from some point of deformation path
where $\det H_2 \neq 0$, results in stress change in both directions. Such effect is obtained in experiments. And if the Gessian has a diagonal view (elasticity) this effect is impossible.

In the case of rigid loading (fig. 1) the mechanical system is described by potential function

$$V = \frac{\lambda_1 (u - \epsilon)^2}{2} + \frac{\lambda_2 (\psi - \gamma)^2}{2} + \Pi.$$ 

If the mechanical system is located in the equilibrium state (stable or unstable) then $\nabla^2 V = 0$. The equilibrium type is determined by eigenvalues of the Gessian $H = \nabla^2 \nabla^2 V$ [1]. All the eigenvalues of the Gessian $H$ are positive under loading from elastic state. In this case the 0 saddle of Morse of function $V$ takes place. The 0 saddles of Morse have local minimum in the equilibrium point in this case and so only such saddles are locally steady. The change of sign at least of one eigenvalue and hence the equilibrium type occurs after the degeneration of the Gessian $H$. Thus, the condition of stability loss of tension with torsion process is the fulfillment of equality.

$$\det \nabla^2 \nabla^2 V = (\lambda_1 + c_{11})(\lambda_2 + c_{22}) - c^2 = 0.$$ \hspace{1cm} (3)

In the three-dimensional space with coordinates $c_{11}, c_{22}, c$ the equation (3) forms a conic surface or a discriminant cone (fig. 2).

With gradual increase of the loading parameters $\psi$ and $u$ the representing process point $M(c_{11}, c_{22}, c)$ firstly moves inside the cone. With the material characteristics $c_{11}, c_{22}, c$, change the point comes nearer to the cone surface and after crossing it the stability loss of deformation process happens. The sample suddenly (discontinuously) collapses.

With increase of rigidities $\lambda_1$ and $\lambda_2$ the discriminantal cone extends. So the equilibrium deformation depending on these values is possible also after path crossing
of line formed of critical points in the $\mathbb{R}^2_+$ space (transition of sample material to the softening stage). Besides equilibrium fragmentation of the sample is also possible.

At last the soft loading is considered. In this case the system is described by a potential function.

$$U = V - \int_{0}^{u} P \, du - \int_{0}^{\psi} M \, d\psi.$$ 

Since the system state is determined by four parameters, the relationship $\nabla_4 U = 0$ fulfils in equilibrium state. Here $\nabla_4$ is the Hamilton operator in the space of states $(u, \epsilon, \psi, \gamma)$. The equilibrium type change occurs when the Gessian $\nabla_4 \nabla_4 U$, degenerates, i.e.

$$\det \nabla_4 \nabla_4 U = \lambda_1 \lambda_2 (c_{11} c_{22} - c^2) = 0.$$  

(4)

The discriminantal cone determined by the equation (4) obviously does not depend on parameters $\lambda_1, \lambda_2$. Comparing the expressions (1) and (4) we find that the illustrating point $M$ crosses the cone surface the path in $\mathbb{R}^2_+$ intersects the curve of critical points. Hence, the discontinuous destruction of the sample will always occur at once after the transition to the stage of softening.

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Thermo-magneto-convective instabilities in a vertical layer of ferro-magnetic fluid

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Abstract

We study convection in a vertical layer of ferro-magnetic fluid heated from the side and subject to a transverse magnetic field. It is found that the subsequent fluid motion is caused by interacting thermo-gravitational and thermo-magnetic mechanisms. Our experiments and computations show that the excitation of magneto-convection leads to the formation of vertically aligned stationary rolls, while gravitational convection results in horizontal rolls corresponding to a pair of counter-propagating thermal waves. The interaction of these instability modes leads to a wide spectrum of experimentally observed flow patterns including stationary rolls and standing waves of various spatial orientations. A comprehensive stability map is computed and compared with experimental flow visualisations. Disturbance energy is analysed to achieve a deeper insight into the physical mechanisms driving the fluid motion.

1 Introduction

Common non-conducting artificial magnetic fluids consist of magnetite colloids which contain ferro-magnetic nano-particles suspended in a carrier fluid, usually synthetic oil, water or kerosene. To prevent formation of magnetite aggregates and their subsequent sedimentation a surfactant such as oleic acid is frequently used [1]. One of the applications of non-conducting ferrofluids is as a heat carrier in efficient cooling systems where the heat transfer by natural gravitational convection can be significantly enhanced by applying an external magnetic field [2]. Nonuniform heating results in a nonuniform magnetisation of a ferrofluid: cooler regions contain stronger magnetised fluid. Subsequently, a ponderomotive force arises which drives stronger magnetised cooler fluid particles to the regions with a stronger magnetic field. This phenomenon is known as magneto-convection and is not associated with gravitational buoyancy forces. However in normal gravity conditions it always acts alongside with the buoyancy forces. Therefore the purpose of the current work is
to use a perturbation energy analysis to determine the parametric regions where each of these physical mechanisms is dominant as well as to determine the internal structure of the corresponding instability patterns. To achieve these goals we choose the simple geometry of a vertical wide and tall fluid layer heated from one side and placed in a perpendicular magnetic field. Such a configuration is easy to re-create experimentally and is convenient to model due to the simplicity of the boundary conditions.

2 Problem definition and stability equations

Consider a vertical layer of ferro-magnetic fluid which fills the gap between two infinitely long and wide parallel plates. The plates are separated by distance 2d and are maintained at constant different temperatures $T_\pm \mp \Theta$. An external horizontal uniform magnetic field $\vec{H}^e = (H_e, 0, 0)$ is applied perpendicular to the layer. This field causes an internal magnetic field $\vec{H}$ within the layer. Since the fluid is ferromagnetic the external field leads to its magnetisation $\vec{M}$ which is assumed to be co-directed with the internal magnetic field: $\vec{M} = \chi_\ast \vec{H}$, where $\chi_\ast$ is the magnetic susceptibility of the ferromagnetic fluid. We adopt Boussinesq approximation for the governing continuity, Navier-Stokes and thermal energy equations which are complemented by Maxwell’s equations for magnetic field as discussed in [1, 2, 3]. The equations are non-dimensionalised using

\[
(x', y', z') = d(x, y, z), \quad \vec{v} = \frac{\eta_s d}{\rho_s} \vec{v}, \quad t' = \frac{\rho_s d^2}{\eta_s} t, \quad P' = \frac{\eta_s}{\rho_s} \rho_s d, \quad T' - T_\ast = \Theta \theta, \quad \tilde{H}' = \frac{K \Theta}{1 + \chi} \tilde{H}, \quad H' = \frac{K \Theta}{1 + \chi} H, \quad \tilde{M}' = \frac{K \Theta}{1 + \chi} \tilde{M}, \quad M' = \frac{K \Theta}{1 + \chi} M, \quad \vec{g} = g \vec{e}_g,
\]

where primes denote dimensional quantities. Then we obtain

\[
\begin{align*}
\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} &= -\nabla P + \nabla^2 \tilde{v} - Gr \theta \vec{e}_g - Gr_m \theta \nabla H, \quad (1) \\
\frac{\partial \theta}{\partial t} + \vec{v} \cdot \nabla \theta &= \frac{1}{Pr} \nabla^2 \theta, \quad \nabla \cdot \vec{v} = 0, \quad \nabla \times \tilde{H} = \vec{0}, \quad (2) \\
(1 + \chi_\ast) \nabla \cdot \tilde{H} + (\chi - \chi_\ast) \nabla H \cdot \vec{e}_* - (1 + \chi) \nabla \theta \cdot \vec{e}_* &= 0, \quad (3) \\
\tilde{M} &= [(\chi - \chi_\ast) (H - N) - (1 + \chi) \theta] \vec{e}_* + \chi_\ast \tilde{H} \quad (4)
\end{align*}
\]

with boundary conditions

\[
\begin{align*}
\left[ \tilde{H}^e - [(\chi - \chi_\ast) (H - N) \mp (1 + \chi)] \vec{e}_* - (1 + \chi_\ast) \tilde{H} \right] \cdot \vec{n} &= 0, \quad (5) \\
\vec{v} &= \vec{0}, \quad \theta = \pm 1, \quad \text{at} \quad x = \mp 1, \quad (6)
\end{align*}
\]

where $\vec{e}_y = (0, -1, 0), \vec{n} = \vec{e}_* = (1, 0, 0)$. The dimensionless parameters appearing in the problem,

\[
Gr = \frac{\rho_s \beta_s \Theta g d^3}{\eta_s^2}, \quad Gr_m = \frac{\rho_s \mu_0 K^2 \Theta^2 d^2}{\eta_s^2 (1 + \chi)}, \quad Pr = \frac{\eta_s}{\rho_s \kappa_s}, \quad N = \frac{H_s (1 + \chi)}{K \Theta}, \quad (7)
\]

are thermal and magnetic Grashof numbers characterising the importance of buoyancy and magnetic forces, Prandtl number characterising the ratio of viscous and
thermal diffusion and parameter $N$ characterising thermo-magnetic properties of a working fluid, respectively. In the above $\rho_*, \eta_*$ and $\kappa_*$ are the fluids characteristic density, dynamic viscosity and thermal diffusivity, $\mu_0 = 4\pi \times 10^{-7}$ H/m is the magnetic constant, $T_*, M_*$ and $H_*$ are the temperature, the magnetisation and the magnitude of the magnetic field in the mid-plane of the layer, $\chi = \frac{\partial M}{\partial H} \big|_{H_*}$, 

$K = -\frac{2M}{\rho T_*}$. 

Equations (1)–(6) admit steady parallel basic flow solution

$$\theta_0 = -x, \quad v_0 = \frac{Gr}{6}(x^3 - x), \quad P_0 = -Gr_m \frac{x^2}{2} + C,$$

$$H_0 = N - x, \quad M_0 = \chi_* N + x,$$

where $C$ is an arbitrary constant. The buoyancy force caused by the linear variation of the temperature (and the density) across the layer are responsible for the existence of a symmetric cubic velocity profile such that the fluid rises along the hot wall and sinks along the cold one. The fluid magnetisation increases towards the cold wall while the magnetic field decreases in this direction so that the sum $H_0 + M_0 = \text{const.}$ as dictated by Maxwell’s equations in the absence of electrical currents.

As shown in [4] linearising equations (1)–(6) about (8)–(9), and then using a standard normal mode decomposition of the disturbance fields and Squire’s transformation we obtain an equivalent two-dimensional stability problem of the form

$$\sigma u + (\alpha^2 + i\alpha v_0 - D^2) u + DP + Gr_m DH_0 \theta + Gr_m \Theta_0 D^2 \phi = 0,$$

$$\sigma v + Dv_0 u + (\alpha^2 + i\alpha v_0 - D^2) v + i\alpha P - Gr \theta + i\alpha Gr_m \Theta_0 D\phi = 0,$$

$$\sigma \theta + D\Theta_0 u + \left(\frac{\alpha^2 - D^2}{Pr} + i\alpha v_0\right) \theta = 0,$$

$$Du + i\alpha v = 0, \quad \left(D^2 - \frac{1 + \chi_*}{1 + \chi} \alpha^2\right) \phi - D\theta = 0,$$

with boundary conditions

$$u_1 = v_1 = w_1 = \theta_1 = 0, \quad (1 + \chi) D\phi_1 \pm \sqrt{\alpha^2 + \beta^2} \phi_1 = 0 \quad \text{at} \quad x = \pm 1,$$

where $D \equiv d/dx$ and $\phi$ is the magnetic potential such that the disturbance magnetic field is given by $\vec{H} = (D\phi, i\alpha \phi)$. All disturbance quantities in equations (10)–(13) are functions of $x$ only, see [3, 4] for details. Equations (10)–(14) comprise an eigenvalue problem for the disturbance complex amplification rate $\sigma = \sigma^R + i\sigma^I$ for each fixed set of governing physical parameters and wavenumber $\alpha$. Marginal stability is observed when the value of $\sigma^R$ maximised over the range of $\alpha$ becomes zero.

We emphasise that two-dimensional perturbation equations (10)–(14) represent a full three-dimensional problem which is recovered using the inverse Squire’s transformation. However the goal of this short paper is to determine the physical mechanisms driving the instabilities which is possible to do by using a two-dimensional equivalent problem alone. The reader is referred to [4] for the detailed analysis of the three-dimensional unfoldings of the current results.
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Figure 1: Typical experimentally observed magneto-convective instability pattern (left), parametric stability boundary (a) and critical wavenumber (b) for combined thermo-gravitational and magnetic convection in a vertical layer of ferro-fluid at $Pr = 130$ and $\chi = \chi^* = 5$. Basic flow is stable below and to the left of the solid line and above the dashed and dash-dotted lines in plot (a).

3 Instability mechanisms and disturbance energy

Experimental observations [5] show that various types of instability patterns superposed onto the basic flow exist depending on the values of the governing parameters. The most prominent pattern has the form of vertical rolls such as the ones seen in the left photo in Figure 1. Computations show that it appears for $Gr_m > 1.39$, relatively small values of $Gr$ and wavenumber $\alpha_c \approx 1.9$ (dashed lines in Figure 1(a,b)). These values are in good agreement with the experimentally measured ones at the onset of instability. However computations also predict the existence of other instabilities for the larger values of $Gr_m$ (dash-dotted line in Figure 1(a)) and $Gr$ (solid line).

In order to determine the physical mechanisms driving instabilities we consider the disturbance energy balance. We multiply the momentum equations (10) and (11) by complex conjugate velocity components $\bar{u}$ and $\bar{v}$, respectively, add them together, integrate by parts across the layer using boundary conditions (14) and the continuity equation, and take the real part (denoted by $\Re$ below) of the result to obtain

$$\sigma^R \Sigma_k = \Sigma_{uv} + \Sigma_{m1} + \Sigma_{m2} + \Sigma_{Gr} + \Sigma_{vis}, \quad (15)$$

where

$$\Sigma_k = \int_{-1}^{1} (|u|^2 + |v|^2) \, dx > 0, \quad \Sigma_{uv} = -\int_{-1}^{1} Dv_0 \Re (u\bar{v}) \, dx,$$

$$\Sigma_{m1} = \int_{-1}^{1} -Gr_m DH_0 \Re (\theta \bar{u}) \, dx, \quad \Sigma_{m2} = \int_{-1}^{1} Gr_m DH_0 \Re (D\phi \bar{u}) \, dx, \quad (16)$$

$$\Sigma_{Gr} = \int_{-1}^{1} Gr \Re (\theta \bar{u}) \, dx, \quad \Sigma_{vis} = -\int_{-1}^{1} (|Du|^2 + |Dv|^2) \, dx < 0.$$

Since $\Sigma_k$, the kinetic energy of perturbations, is positively defined the flow is stable (unstable) if the sum of terms in the right-hand side of (15) is negative (positive).
Table 1: Disturbance energy integrals for selected marginal stability points shown by circles in Figure 1.

<table>
<thead>
<tr>
<th>$Gr_m$</th>
<th>$Gr$</th>
<th>$\alpha$</th>
<th>$\Sigma_{uv}$</th>
<th>$\Sigma_{m1}$</th>
<th>$\Sigma_{m2}$</th>
<th>$\Sigma_{Gr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>40.974</td>
<td>1.238</td>
<td>-0.006</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.398</td>
<td>39.976</td>
<td>1.256</td>
<td>-0.007</td>
<td>0.004</td>
<td>-0.002</td>
</tr>
<tr>
<td>3</td>
<td>15.775</td>
<td>16.690</td>
<td>1.696</td>
<td>-0.011</td>
<td>0.302</td>
<td>-0.086</td>
</tr>
<tr>
<td>4</td>
<td>14.468</td>
<td>6.6</td>
<td>1.853</td>
<td>-0.003</td>
<td>1.141</td>
<td>-0.318</td>
</tr>
<tr>
<td>5</td>
<td>16.353</td>
<td>4.4</td>
<td>1.463</td>
<td>0.001</td>
<td>1.795</td>
<td>-0.759</td>
</tr>
<tr>
<td>6</td>
<td>16.239</td>
<td>4.4</td>
<td>2.147</td>
<td>0.002</td>
<td>1.812</td>
<td>-0.595</td>
</tr>
<tr>
<td>7</td>
<td>16.189</td>
<td>4.4</td>
<td>3.278</td>
<td>-0.003</td>
<td>1.516</td>
<td>-0.350</td>
</tr>
<tr>
<td>8</td>
<td>1.398</td>
<td>0</td>
<td>1.936</td>
<td>0</td>
<td>1.584</td>
<td>-0.584</td>
</tr>
</tbody>
</table>

Equivalently, we can say that positive terms in the right-hand side of (15) are responsible for instability. The values of various energy balance terms are given in Table 1 for the marginal stability ($\sigma_R = 0$) points shown by circles in Figure 1(a,b). Since within the framework of a linearised stability analysis the amplitude of disturbance fields is undefined we normalise them in such a way that the viscous dissipation integral $\Sigma_{vis} = -1$ for all points. The remaining four entries in the energy balance are listed in Table 1. From this table we make the following conclusions.

- The contribution of the basic flow velocity into the disturbance energy balance ($\Sigma_{uv}$) can be either slightly positive or negative, but it remains small for all regimes. Therefore the interaction of the disturbance velocity field with the basic flow is weak. The energy exchange between basic and disturbance velocity fields is insignificant and does not play any noticeable role in flow pattern formation.

- The first of the two magnetic contributions to the energy balance, $\Sigma_{m1}$, is positive for all non-zero values of $Gr_m$. This term represents a ponderomotive force which drives stronger magnetised cooler fluid particles into the regions of a stronger basic magnetic field (i.e. from the cold wall towards the hot wall as suggested by the basic flow field distributions (8)–(9)). Therefore in the considered configuration the dependence of fluid magnetisation on the temperature always plays a destabilising role leading to the onset of a thermo-magnetic convection.

- In contrast, the second magnetic term, $\Sigma_{m2}$, always remains negative. It represents the induction of a disturbance magnetic field by displaced ferro-magnetic fluid particles. Therefore the modification of the basic magnetic field always absorbs energy and thus plays a stabilising role. It hinders the change in the primary magnetisation field. However this magnetic stabilisation effect is always weaker than the thermo-magnetic de-stabilisation. Therefore the overall magnetic influence on the basic flow in the considered geometry is always destabilising.

- The thermo-gravitational contribution, $\Sigma_{Gr}$, depends strongly on the values of both $Gr$ and $Gr_m$ and can be either positive or negative. This term represents
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Figure 2: Selected disturbance energy integrands for parameters specified in Table 1.

the buoyancy force which drives warmer and less dense fluid upwards and cooler denser fluid downwards. It is strongly destabilising in the absence of a magnetic field i.e. for $Gr_m \sim 0$, but becomes stabilising for the larger values of $Gr_m$ when the motions caused by the actions of the vertical buoyancy force and the horizontal magnetic ponderomotive force start competing with each other. The peculiar S-shape of the stability boundary shown by the solid line in Figure 1(a) is the consequence of this competition: for larger values of $Gr$ both magnetic and thermo-gravitational terms are destabilising and their combination leads to a reduction in the area of the region of stability (the solid line goes down and then turns back). However for small values of $Gr$ and larger values of $Gr_m$ the buoyancy starts playing a much stronger stabilising role so that the solid line turns to the right increasing the stability region underneath it.

In summary, the de-stabilisation of the primary parallel flow is achieved due to the action of two physical mechanisms: the action of ponderomotive magnetic and buoyancy forces. However at small values of $Gr$ the buoyancy plays a stabilising role. The integral values presented in Table 1 also identify the nature of the instabilities whose boundaries are shown by the solid and dashed lines in Figure 1: gravitational buoyancy and magnetic ponderomotive force, respectively. Yet neither the details of these two instabilities nor the nature of the third instability whose boundary is shown by the dash-dotted line are clear so far. In order to eliminate this shortcoming
we consider the spatial distribution of the three destabilising integrands, $E_{m1}$, $E_{m2}$ and $E_{Gr}$, defined in (16) and plotted in Figure 2 for points 1–8 shown by circles in Figure 1(a,b).

For small values of $Gr_m$ and large values of $Gr$ (points 1 and 2) the thermo-gravitational instability mechanism dominates, see the dash-dotted line in plots 1 and 2 in Figure 2. The energy integrand $E_{Gr}$ has two well defined symmetric maxima near the walls. This is a reflection of the well known fact that in high Prandtl number fluids such as a typical kerosene-based ferro-colloid the thermo-gravitational instability takes the form of two counter-propagating waves in the wall regions, see detailed discussion in [4] and references therein. They are almost insensitive to a magnetic field and exist even when the magnetic Grashof number is significantly increased, see plots for points 3 and 4. However as the ratio $Gr_m/Gr$ increases the thermo-magnetic effects given by $E_{m1}$ intensify significantly and eventually become dominant, see plot 4. It is noteworthy that although the dominant physical mechanism of instability changes, this happens in a continuous way, see solid lines in Figure 1. The only indication that such a change has indeed occurred is in the qualitative behaviour of the disturbance wavenumber: as $Gr_m$ increases so does the wavenumber of thermo-gravitational waves, however this trend is reversed once they are replaced with thermo-magnetic waves, see the solid line in Figure 1(b).

With decreasing $Gr$ the difference between the two counter-propagating thermo-magnetic waves becomes blurred: the wave speeds (not shown here, but see [4]) decrease, the instability pattern becomes nearly stationary and its maximum shifts from the wall regions towards the centre of the layer, see the plot for point 5. The thermo-gravitational convection mechanism continues to play a destabilising role in the centre of the layer, but its influence in the wall regions becomes stabilising. A shift of the instability production region to the centre of the layer has a profound effect on the characteristic wavenumber of perturbations: it quickly decreases, see the right end of the solid line in Figure 1(b). This has a straightforward explanation: the disturbance structures in the centre of the layer near the inflection point of the basic flow velocity profile are subject to large shear forces. They “stretch” convection rolls decreasing their wavenumber. The centrally located instability structures elongated by the shear forces then become so large that they cause a strong “flow blocking” effect. Eventually they are destroyed by the basic flow giving way to much shorter structures, see the dash-dotted lines containing point 7 in Figure 1. Plot 7 in Figure 2 shows that the physical mechanism generating them is indeed the same as that for the thermo-magnetic waves discussed above. Their size is sufficiently small (the wavenumber is large) for the basic flow blocking effect to be reduced on one hand and for the two disturbance waves propagating near the walls to re-appear on the other. We also note that although overall magneto-induction effect $\Sigma_{m2}$ is always stabilising, the energy integrand $E_{m2}$ for points 3, 4 and 7 is positive in the centre of the layer (between the counter-propagating thermo-magnetic waves) and thus it contributes to the overall de-stabilisation across the layer.

Points 6 and 8 in Figure 1 belong to the third type of stability boundary which is disjoint from the two segments discussed so far. The physical mechanism causing this instability is of purely thermo-magnetic type: $E_{m2}$ is strongly positive while $E_{Gr}$ is close to zero. Therefore the gravitational buoyancy plays essentially no role
in these regimes of convection. Major de-stabilisation occurs near the middle of the layer where basic flow velocity is zero. As a consequence, these corresponding instability patterns are stationary \[4\]. They take the form of vertical rolls similar to the ones seen in the left photograph in Figure 1.

In conclusion, our analysis of perturbation energy distribution across the layer shows that the instability in a vertical ferro-fluid layer is caused by two physical mechanisms: thermo-gravitational (buoyancy) and thermo-magnetic. These mechanisms result in three distinct types of perturbed flow patterns: counter-propagating thermal waves (large \(Gr\), small \(Gr_m\)), counter-propagating thermo-magnetic waves (large \(Gr_m\), intermediate \(Gr\)) and stationary magneto-convection rolls (intermediate to large \(Gr_m\), small \(Gr\)). The transition between thermal and thermo-magnetic waves is continuous and occurs when \(Gr\) and \(Gr_m\) are of comparable sizes while magneto-convection rolls appear independently and dominate the flow for small values of \(Gr\). We also note in passing that a spatial orientation of the detected instability patterns is strongly related to the physical mechanisms causing them: the propagating thermal or thermo-magnetic instability waves form horizontal or inclined convection rolls, while stationary magneto-convection rolls are vertical. The reader is referred to \[4\] for detailed discussion of the spatial structure of instability patterns.

Acknowledgements

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References


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Micromechanics of fine particle adhesion - contact models and energy absorption

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Abstract

The mechanical product behaviour of dry, ultrafine cohesive powders (d < 10µm) is characterized by insufficient flowability and large compressibility. These powders show a wide variety of typical flow problems that cause insufficient apparatus and system reliability of processing plants. Consequently, a comparatively large energy input is necessary to promote the non-rapid frictional shear flow in powder handling practice. Thus, it is very essential to understand the fundamentals of particle adhesion with respect to product quality assessment and process performance in particle technology.

Comprehensive models are shown that describe the elastic-plastic force-displacement and frictional moment-angle behaviour of adhesive contacts of isotropic smooth spheres. Using the model stiff particles with soft contacts, a sphere-sphere interaction of van der Waals forces without any contact deformation describes the stiff attractive term. The soft micro-contact response generates a flattened contact, i.e. plate-plate interaction, and increasing adhesion. These increasing adhesion forces between particles directly depend on this frozen irreversible deformation. Thus, the adhesion force is found to be load dependent. It essentially contributes to the tangential forces in an elastic-plastic frictional contact with partially sticking within the contact plane and microslip. The load dependent rolling resistance and torque of mobilized frictional contact rotation (spin) are also shown.

Next, the consequences of unloading and reloading paths are discussed with respect to energy absorption. The total energy absorption comprises contributions by elastic-dissipative hysteresis due to microslip within the contact plane and by fully developed friction work when the friction limits of displacements are exceeded. With increasing contact flattening by normal load, these friction limits, hysteresis and friction work increase. This knowledge is used to improve the apparatus design and the reliability of process systems in particle technology.
1 Introduction

In particle processing and product handling of fine (d < 100µm), ultrafine (d < 10µm) and nanosized particles (d < 0.1µm), the well-known flow problems of dry cohesive powders in process apparatuses or storage and transportation containers include bridging, channelling, widely spread residence time distribution associated with time consolidation or caking effects, chemical conversions and deterioration of bioparticles. Avalanching effects and oscillating mass flow rates in conveyors lead to feeding and dosing problems. Finally, insufficient apparatus and system reliability of powder processing plants are also related to these adhesion problems. The challenge is to understand the fundamentals of particle adhesion with respect to product quality assessment, process performance and control in powder technology, i.e., in particle conversion, formulation and handling.

This micromechanical philosophy in powder mechanics has been steadily continued by the author [1-11]. The fundamentals of the macroscopic cohesive powder consolidation and frictional flow have been related to the microscopic interactions between the particles that are in contact [5-10]. In this context, particle adhesion is caused by surface and field forces (van der Waals, electrostatic and magnetic forces), by material bridges between particle surfaces (liquid and solid bridges [1-3], flocculants) and by mechanical interlocking of extreme particle shapes. A comprehensive literature review may be read in previous papers [8, 11, 12].

It is worth to note here that van der Waals forces - the focus of this paper - act at the surfaces of dry ultrafine particles. They are dominant and approximately $10^4$ - $10^6$ times the gravitational force. The state of arts in constitutive modelling of elastic, elastic-adhesion, elastic-dissipative, plastic-adhesion and plastic-dissipative contact deformation response of a single isotropic contact of two smooth spheres was discussed in previous papers [6, 8, 11, 12] and is not shown here.

The dominant microscopic effect of variable adhesion forces at particle contacts has been the physical basis of universal models for particle adhesion that includes the elastic-plastic and viscoplastic particle contact behaviour with hysteresis and consequently, energy dissipation. Various contact elastic-plastic deformation paths for non-rapid loading, unloading and detachment have been discussed. As a result, the varying adhesion forces between particles directly depend on this frozen irreversible deformation. Thus, the adhesion force has been found to be load dependent [6-11].

To continue these new constitutive models, the consequences of elastic-dissipative as well as elastic-plastic, frictional unloading and reloading paths of normal and tangential forces, rolling and torsional moments are discussed with respect to the energy absorption [13]. This energy absorption comprises contributions by elastic-dissipative hysteresis due to microslip within the contact plane and by fully developed friction work when the friction limits of displacements are exceeded during contact sliding, particle rolling or rotation. Therefore one may expect that with increasing contact flattening by normal load the friction limits, hysteresis and friction work increase.
2 Constitutive models for elastic-plastic, dissipative behaviour and load dependent adhesion

This paper is intended to focus on the new model of isotropic, stiff, and linear elastic, spheres that are approaching to soft contacts by attractive adhesion forces of smooth surfaces. The soft or compliant, elastic-plastic contact displacement as response is assumed to be small $h_K/d \ll 1$ compared to the size (diameter) of the stiff particle. The particles may have the mechanical properties of limestone, which is widely used in powder mechanics as standard material. Its material stiffness is so large that the volume deformation is negligible. During surface stressing these stiff particles are not so much deformed that they undergo certain changes of the particle shapes.

2.1 Particle Contact Constitutive Model for Normal Loading

A typical normal force-displacement diagram for elastic-plastic contact behaviour is demonstrated in Fig. 1, calculated by the equations collected in Table 1. The zero-point of this diagram $h_K = 0$ is equivalent to the characteristic adhesion separation of direct contact $a_0$. This characteristic adhesion separation for the direct contact of spheres is of a molecular scale (atomic centre-to-centre distance) and amounts to about $a_0 = 0.3-0.4\text{nm}$. With respect to large specific surfaces of ultrafine particles, this separation $a_0$ depends on the properties of liquid-equivalent packed adsorbed water layers. Consequently, more or less mobile adsorption layers due to condensed humidity of ambient air influence the particle contact behaviour.

After approaching $F_N \propto a^{-2}$ (with $a = a_0 - h_K$) from an infinite distance $\infty$ to a minimum separation $a = a_0$, Fig. 1a), the smooth sphere-sphere contact without any contact deformation is formed by the short-range attractive adhesion force $F_N = -F_{H0}$ (the so-called jump in). But this direct contact is not in a state of force equilibrium and, as the response, is elastically deformed with an approximated circular contact area, Fig. 1b). A local plate-plate-contact is formed from the previous contact point. When this Hertz or DMT curve intersects the abscissa the total force equilibrium $F_N = 0$ is obtained. With increasing external normal load this soft contact starts at a pressure $p_f$ with plastic yielding at the point $Y$. This yield point $Y$ is located here below the abscissa, i.e., the contact force equilibrium $F_N = 0$ includes a certain elastic or elastic-plastic deformation as response of effective adhesion force. The maximum pressure $p_f$ within the contact plane cannot be exceeded and results in a combined elastic-plastic yield limit of the flattened plate-plate contact with an annular elastic zone and a circular centre. A confined plastic field with a micro-yield surface is formed inside of the contact circle.

The elastic-plastic yield limit for loading results in a linear function, line $Y-U$ in Fig. 1c). This elastic-plastic yield limit cannot be crossed. Between the elastic-plastic yield limit and the adhesion limit the elastic domain is located. Any load $F_N$ yields an increasing displacement $h_K$. But, if one would unload, beginning at arbitrary point $U$, the elastically deformed, annular contact zone recovers along a parabolic curve $U-A$. The reloading would run along equivalent curves from point
Figure 1: Calculated normal force - displacement diagram of contact flattening of limestone particles, modelled as smooth mono-disperse spheres, median diameter \( d_{50} = 1.2 \mu m \). For convenience, pressure and compression are defined as positive but tension and extension are negative.

A to point U forward to the displacement \( h_{K,U} \) as well. If the adhesion limit at point A is reached then the contact plates detach with the increasing distance \( a = a_0 + h_{K,A} - h_K \), Fig. 1d).

It is worth to note here that the secant unload stiffness between \( h_{K,A} \) and \( h_{K,U} \) \((450-820 \text{N/m})\) increases with increasing contact flattening \( h_{K,U} \) and with increasing load \( F_{N,U} \) [12]. Thus, with increasing external load applied at any process, e.g. in powder compaction, the particle contacts become stiffer and stiffer and approach the solid behaviour of a compressed briquette or tablet.

2.2 Load Dependent Adhesion Force

The slopes of elastic-plastic yield and adhesion limits in Fig. 1 characterise the contact softness or compliance. If one eliminates the centre approach \( h_K \) of the loading and unloading functions, a linear function for the contact pull-off force \( F_N = -F_H \) at the detachment point A is obtained [9, 10].

The dimensionless, so-called elastic-plastic contact consolidation coefficient \( \kappa \) determines the slope of adhesion force \( F_H \) influenced by predominant plastic contact failure. This displacement or flattening coefficient \( \kappa \) characterizes the irreversible particle contact stiffness or softness as well. A shallow slope implies low adhesion level \( F_H \approx F_{H0} \) because of stiff particle contacts, but a large slope means soft contacts, or in other words, cohesive powder flow behaviour in the macroscale [7]. The
total adhesion force $F_H$ consists of a stiff contribution $F_{H0}$ and a soft, displacement influenced term $\kappa \cdot (F_{H0} + F_N)$. Thus, Eq. (11) can be interpreted as a general linear constitutive contact model, i.e. linear in forces, but non-linear in material characteristics.

### 2.3 Elastic-Plastic, Frictional Tangential Force

The Coulomb friction limits of tangential forces are described by the coefficient of internal friction $\mu_i$. These limits for contact sliding, Eq. (15) in Table 2, depend on the elastic-plastic contact consolidation, i.e., elastic-plastic flattening by the normal force $F_N$ and the variable (positive) adhesion force $F_H(F_N)$ as well, Eq. (11).

The contact loses its elastic tangential stiffness at $k_{TH} = 0$ and completely mobilized contact sliding is obtained for the friction limit of displacement $\delta = \delta_{C,H}$ under load dependent adhesion force $F_H(F_N)$, Eq. (11), see grey points for yield in Fig. 2. Compared to the contact radius $r_K = 6 - 14 \text{nm}$, the elastic range is very small and limited by the tangential displacement $\delta_{C,H} < 0.06 \text{nm}$. At these Coulomb friction limits (grey points, index C) the elastic behaviour is transmitted into the frictional behaviour of contact sliding shown by constant tangential force $F_{T,C,H}$, Eq. (15). The tangential force-displacement diagram Fig. 2 is calculated by the equations of Table 2.
Figure 3: Rolling resistance force (at the centre of mass) - rolling angle diagram for limestone particles modelled as smooth mono-disperse spheres. The non-linear elastic curves by partially sticking and microslip within the flattened contact plane and the straight lines of elastic secant stiffness are shown. The hysteresis by partially sticking and microslip within the flattened contact plane is demonstrated here only for the largest normal force. One may consider the strongly increasing level of friction limits due to the adhesion within the flattened contact plane.

2.4 Elastic-Plastic, Frictional Rolling Resistance of Load Dependent Adhesive Contact

The frictional rolling resistance force of smooth soft spheres acts at the centre of mass and can be considered by a tilting moment relation of the force pair around the grey pivot at the perimeter of contact circle. As the response of contact flattening a lever arm of contact radius $r_K$ with respect to $F_N$ is generated that is equilibrated by rolling resistance $F_R$ acting perpendicular to direction of $F_N$ with the lever arm $r - h_K/2$, see in Fig. 3 the rectangular lines of the sketch right below:

The linear elastic range is very small restricted by the limit of rolling angle $\gamma_{C,H} = 8 \cdot 10^{-5} - 1.9 \cdot 10^{-4}$. At these limits the elastic behaviour is transmitted into the contact rolling shown by constant rolling resistance force $F_{R,C,H} \neq f(\gamma)$ that depends on the positive adhesion force $F_H(F_N)$, see Table 3.

2.5 Elastic-Plastic, Frictional Spinning of Load Dependent Adhesive Contact

The new constitutive torsional moment - rotation angle functions for elastic-plastic, frictional behaviour are shown in Fig. 4 and Table 4. The linear elastic range is very small and restricted by a constant friction limit of rotation angle $\phi_{C,H} = 0.0076$. At this Coulomb friction limit $\phi_{C,H}$ the elastic behaviour is transmitted into the contact spinning shown by constant torque that also depends on adhesion force.
Figure 4: Torsional moment - rotation angle diagram for limestone particles modelled as smooth mono-disperse spheres. Both the non-linear elastic curves by partially sticking and microslip within the flattened contact plane [12] and the straight lines of elastic secant stiffness are demonstrated. But the non-linear elastic hysteresis curves are not drawn here. Again, one has to consider the strongly increasing level of friction limits due to the adhesion within the flattened contact plane.

2.6 Essential Constitutive Particle Parameters

From these elastic-plastic and frictional force - displacement laws, force - force equations and moment - angle models one can conclude that six independent, physical material parameters are necessary to describe the micromechanics of particle adhesion. The following material data of ideally assumed, smooth mono-disperse particles with the mechanical properties of limestone are used:

1. Median particle diameter $d_{50,3} = 1.2\mu m$ and solid density $\rho_s = 2740\text{kg/m}^3$,
2. Hamaker constant $C_{H,sls} = 3.810^{-20}\text{J}$. The characteristic adhesion force of rigid sphere-sphere contact $F_{H0} = -2.64\text{nN}$ was back calculated from powder shear tests.
3. The plastic micro-yield strength $\sigma_p = 300\text{N/mm}^2$, equilibrium centre separation for dipole interaction $\alpha_0 = 0.336\text{nm}$, elastic-plastic contact area coefficient $\kappa_A = 5/6$, plastic repulsion coefficient $\kappa_p = 0.153$, elastic-plastic contact consolidation coefficient $\kappa = 0.224$,
4. modulus of elasticity $E = 150\text{kN/mm}^2$,
5. Poisson ratio $\nu = 0.28$, shear modulus $G^* = 34\text{kN/mm}^2$ and
6. contact friction coefficient $\mu_i = 0.76$.

These material data of ideally assumed, smooth mono-disperse particles with the mechanical properties of limestone are used to calculate all the curves of Fig. 1 to Fig. 7.
Figure 5: Force and moment - normal force diagram of limestone particles to compare the load dependent elastic-plastic adhesion limit $F_H$ as positive force and the load dependent elastic-plastic friction limits of tangential force $F_{T,C,H}$, rolling moment $M_{R,C,H}$ and torsional moment $M_{to,C,H}$. The microscopic normal load $F_N$ is equivalent to macroscopically moderate average pressures $\sigma_{M,st} = 1$ to $25\text{kPa}$ (or major principal stresses $\sigma_1 = 2$ to $40\text{kPa}$), frequently applied in powder handling.

3 Comparison of load dependent adhesion and friction limits

It is worth to note here that the load dependent adhesion and the friction limits determine the energy absorption within the contact plane. Thus, diagram Fig. 5 is shown to compare the sensitivity of load dependent adhesion $F_H(F_N)$ on the friction limits of sliding, rolling and torsion of these four stressing modes.

The tangential force or maximum resistance $F_{T,C,H}(F_N)$ to let the contact begin to slide is larger than to pull-off and separate the particles by maximum adhesion force $F_H(F_N)$. The microscopic rolling moment or maximum resistance $M_{R,C,H}(F_N)$ to let roll the contact is larger than to let rotate or twist the particles by maximum torsional moment $M_{to,C,H}(F_N)$.

4 Energy absorption of adhesive elastic-plastic and frictional contact

All necessary force-displacement and moment-angle relations are derived in form of algebraic functions so that they can be analytically integrated to obtain the mechanical work [13]. Next, the load dependent specific hysteresis and friction work
Figure 6: Particle mass related hysteresis work - normal force diagram. The single contact behaviour is shown to compare the load dependent maximum work of elastic hysteresis of normal deformation $W_{m,N,diss}$, tangential microslip $W_{m,T,max}$, rolling friction $W_{m,R,max}$ and torsional microslip $W_{m,to,max}$.

The smallest values of energy absorption are calculated for the direct contact of the four stressing modes of one particle contact are compared and briefly discussed for normal forces from 3 to 130 nN.

4.1 Comparison of the specific hysteresis work of the four stressing modes

First, the sensitivity of load dependent adhesion $F_H(F_N)$ on the maximum specific work of elastic-dissipative hysteresis (during unloading and reloading) of normal loading, sliding, rolling and spinning (torsion) is demonstrated for the four stressing modes in Fig. 6. The specific energy input that is required to compensate the energy absorption within one loop of the elastic hysteresis for unload/reload in the normal and tangential direction is nearly in the same order $W_{m,N,diss} \approx W_{m,T,max}$. But in contrast to this, the maximum specific hysteresis work necessary for one loop torsion $W_{m,to,max}$ is much larger than for rolling $W_{m,R,max}$.

4.2 Comparison of the specific detachment and friction work of the four stressing modes

The influence of normal load and load dependent adhesion on the work of contact detachment and friction work during sliding, rolling and spinning is shown for the four stressing modes in Fig. 7.

The smallest values of energy absorption are calculated for the direct contact
Figure 7: Particle mass related friction work - normal force diagram. The single contact behaviour is shown to compare the load dependent maximum work of contact detachment in the normal direction $W_{m,N,A}$, tangential sliding $W_{m,T,C}$, rolling friction $W_{m,R,C}$ and spinning $W_{m,to,C}$ [12, 13]

approach and separation in the normal direction, i.e. the specific detachment work $W_{m,N,A} = 2 - 50 \mu J/g$. If one compares maximum (or selected) specific friction work of sliding $W_{T,C}$, rolling $W_{R,C}$, and torsion $W_{T,C}$, only the factors are different, namely $2 \cdot \mu_i$, 1 and $2/3 \cdot \mu_i$ [12, 13]. These comparatively small differences in the mass related energy absorption of different loading/unloading procedures are compared in Fig. 7 with respect to tangential sliding, rolling and spinning (torsion).

### 4.3 Comparison of the local energy densities of surface activation

The logical consequence of the model *stiff particles with soft contacts* is that only the mass fraction of the deformed contact matter is considered to describe the local intensity of energy absorption during mechanical stressing of two particles. For the sake of simplicity, the averaged mass of the locally deformed contact zone is geometrically approximated by the caps of spheres 1 and 2 with their heights or displacements $h_{K,1} = h_{K,2} = h_{K,1}/2$ [13]. The same factors $2 \cdot \mu_i$, 1 and $2/3 \cdot \mu_i$ are found as well when one compares the characteristic (maximum) local energy densities of surface activation by contact sliding, particle rolling and torsion, Eqs. (35), (36) and (37) in Table 5.

The enormous local energy densities of these various stressing modes are found to be in the orders of magnitude of 0.02 to 3MJ/mol. These theoretically estimated molar energies are directly compared with the lattice enthalpies of various ionic crystals of 0.7 – 15MJ/mol. The values are also located within the range of the
energy accumulated in lattice dislocations of about $100 - 1000\text{kJ/mol}$ and are more then the sublimation (evaporation) enthalpies of solids of about $200 - 500\text{kJ/mol}$. It is worth to note here that the local activation energy of tribochemical reactions within the contact zone nearly amounts to the same orders of magnitude and varies from 62 to 744kJ/mol [15, 16].

This local energy consumption is meaningful for surface activation, particle conversion, product formulation, macroscopic non-rapid frictional shear flow of cohesive ultrafine powders and the agglomerate disintegration in powder processing and handling. Thus, the micromechanical approach is qualitatively and quantitatively consistent and conclusive concerning the constitutive force-displacement and moment-angle laws and the estimated maximum specific energy absorption.

5 Conclusions and outlook

By the model stiff particles with soft contacts and the contact force equilibrium, universal models have been graphically demonstrated that include the elastic-plastic particle contact behaviour, load-unload hysteresis and a history dependent adhesion force function. The microscopic load dependent adhesion effect on the friction limits of single particle contacts macroscopically leads to the significant influence of pre-consolidation stress on the frictional flow of ultrafine cohesive powders that is well known in powder handling practice. Thus, the physical models are used for the advanced data evaluation of various powder product properties concerning particle size distribution (nanoparticles to granules), moisture content (dry, moist and wet) and material properties (minerals, chemicals, pigments, waste, plastics, food etc.). The contact models are very meaningful to describe the frictional shear flow of cohesive and compressible ultrafine powders. For this purpose, all the normal and tangential forces as well as angular and trajectorial moments of particles have to be balanced to simulate their dynamics with physically realistic material data by the discrete element method (DEM), see Tykhoniuk et al. [14].

The consequences of elastic-dissipative as well as elastic-plastic, frictional unloading and reloading paths of normal and tangential forces and rolling and torsional moments for the load dependent energy absorption and the friction work have been discussed and compared. The different quantities between the averaged and local intensity of the energy absorption have been explained for single stressing events of contact compression, sliding, rolling and torsion. The averaged energy densities of these various stressing modes have been found to be in the orders of magnitude of about $0.4 - 6\text{mJ/g}$. But the enormous local energy densities amount to $0.2 - 30\text{kJ/g}$, or in molar units $0.02 - 3\text{MJ/mol}$.

In this context, the light emission due to mechano-luminescence effects by elastic, elastic-plastic contact deformations and, consequently lattice dislocations, crystal phase conversions and particle breakages can be explained qualitatively at intensive and multiple stressing of particles in grinding processes with large local energy densities, see Aman and Tomas [17].

This microscopic energy absorption macroscopically leads to the significant influence of pre-consolidation stress on the non-rapid frictional flow of ultrafine cohesive powders and to the remarkable macroscopic energy consumption that is well-known
in powder storage and handling practice. This is also meaningful for the agglomerate disintegration in powder processing and generates inelastic contact and particle deformations, surface defects, surface asperity abrasion, particle-wall abrasion and micro-cracking up to particle breakage. Those agglomerate disintegration effects are undesired and cause product damage and quality reduction, see Antonyuk et al. [18].

The micromechanical interaction rules of particle adhesion are necessary to describe the pre-consolidation dependent, mechanical flow and consolidation behaviour of ultrafine cohesive powders and to simulate the dynamics of packed particle beds in powder processing, i.e. at agglomeration, disintegration, size reduction, powder storage and flow. At present, with this advanced knowledge an improved apparatus design is accomplished for industrial partners in process industries.

References


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<table>
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<th>Approach</th>
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<th>Equation</th>
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<td>$-\infty &lt; h_K \leq 0$</td>
<td>sphere-sphere model</td>
<td>$F_N = -F_{H0} = -\frac{C_{H1+H2}}{6(a_0-h_K)^2}$</td>
<td>(1)</td>
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<td>Elastic</td>
<td>Hertz and DMT</td>
<td>$F_N = \frac{3}{2}E^*\sqrt{r_{1,2}}h_K^2 - F_{H0}$</td>
<td>(2)</td>
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<tr>
<td>Yield limit</td>
<td>displacement</td>
<td>$F_N = \pi r_{1,2}p_f(\kappa_A - \kappa_p)h_K - F_{H0}$</td>
<td>(3)</td>
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<tr>
<td>$h_{K,f} \leq h_K \leq h_{K,U}$</td>
<td></td>
<td>$\kappa_A = \frac{2}{3} + \frac{1}{3}\frac{A_{p1}}{A_{p1}+A_{el}} = 1 - \frac{1}{3}(\frac{h_K}{h})^3$</td>
<td>(4)</td>
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<tr>
<td></td>
<td></td>
<td>$\kappa_p = \frac{p_{VdW}}{p_f} = \frac{C_{H1+H2}}{6\alpha_0 p_f} = \frac{p_{VdW}}{a_0 p_f}$</td>
<td>(5)</td>
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<td>Unload $h_{K,A} \leq h_K \leq h_{K,U}$</td>
<td>Elastic recovery, U-A</td>
<td>$F_N = \frac{2}{3}E^*\sqrt{r_{1,2}}(h_K - h_{K,A})^3 - F_{H0}$</td>
<td>(6)</td>
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<td></td>
<td>contact detachment</td>
<td>$h_{K,A(0)} = h_{K,U} - (h_{K,A} - h_{K,U})^2$</td>
<td>(7)</td>
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<tr>
<td></td>
<td></td>
<td>$F_N = -\frac{2}{3}E^*\sqrt{r_{1,2}}(h_{K,U} - h_K)^3$</td>
<td>(8)</td>
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<td>Adhesion limit</td>
<td>Plate-plate model</td>
<td>$F_N = -\pi r_{1,2}p_{VdW}h_K - F_{H0}$</td>
<td>(9)</td>
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<tr>
<td>Detachment $-\infty &lt; h_K \leq h_{K,A}$</td>
<td>Plate-plate model</td>
<td>$F_N(h_K) = -\frac{F_{H0} a_0^3}{(a_0 + h_{K,A} - h_K)}$</td>
<td>(10)</td>
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<td></td>
<td></td>
<td>$\pi r_{1,2}p_{VdW}h_K A_{el} a_0^3 (a_0 + h_{K,A} - h_K)^3$</td>
<td>(11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$F_H = F_{H0} + \kappa (F_N + F_{H0})$</td>
<td>(12)</td>
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Table 1: Normal force - displacement laws of contact normal loading $F_N(h_K)$ and van der Waals adhesion force. The essential symbols are explained in section 2.6 (median particle radius of surface curvature $r_{1,2} = \frac{d_{50}}{4}$ and $r_{1,2} = \left(\frac{1}{r_1} + \frac{1}{r_2}\right)^{-1}$, respectively, averaged stiffness $E^* = 2 \cdot \left[\frac{(1-\nu_1^2)}{E_1} + \frac{(1-\nu_2^2)}{E_2}\right]^{-1}$) [6, 12].
Table 2: Tangential force - displacement laws $F_{\gamma} (\delta)$ with load dependent adhesion [12] (averaged shear modulus $G^* = 2 \left[ \frac{2 - \nu_1}{G_1} + \frac{2 - \nu_2}{G_2} \right]^{-1}$, shear modulus $G_i = \frac{E_i}{2(1 + \nu_i)}$, $i = 1, 2$).

Table 3: Rolling resistance force - rolling angle laws $F_R(\gamma)$ with load dependent adhesion [12]
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Table 4: Torsional moment-rotation angle laws $M_{to}(\phi)$ with load dependent adhesion [12].

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<td>Contact stiffness</td>
<td>load dependent</td>
<td>$k_{to,H} = \frac{dM_{to}}{d\phi}$</td>
<td>(27)</td>
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<td>Initial stiffness</td>
<td>Load dependent</td>
<td>$k_{to,H0} = \frac{dM_{to}}{d\phi}</td>
<td>M_{to}=0 = 2(1 - \frac{8Gr^3}{3K^3}[2(1 - M_{to,C,H}) - 1]^{-1} - 1)(27)$</td>
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<td>Friction limits</td>
<td>Torsional moment</td>
<td>$M_{to,C,H} = \frac{2\mu}{3\sqrt{3}}[\frac{(1 + \kappa)r_1,2(F_{H0} + F_N)}{\pi \kappa A_p f}]^3$</td>
<td>(29)</td>
</tr>
<tr>
<td>Loading</td>
<td>Moment-angle</td>
<td>$\phi_{C,H} = \frac{3\mu i\kappa A_p f}{4G}$</td>
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<td>$0 \leq \phi \leq \phi_{C,H}$</td>
<td></td>
<td>$M_{to} = 4M_{to,C,H} \left[ \sqrt{\frac{3}{4\phi_{C,H}}} + 1 - \frac{3}{4\phi_{C,H}} - 1 \right]$</td>
<td>(31)</td>
</tr>
<tr>
<td>Unloading</td>
<td>frictional behaviour</td>
<td>$M_{to} = 8M_{to,C,H} \left[ \sqrt{\frac{3}{2\phi_{C,H}}} + 1 - \frac{3}{2\phi_{C,H}} - 1 \right]$</td>
<td>(32)</td>
</tr>
<tr>
<td>$-\phi_{C,H} \leq \phi \leq \phi_{U,C,H}$</td>
<td></td>
<td>$M_{to} = \frac{3(M_{to} - \phi)}{2\phi_{C,H}} + 1 - \frac{3(M_{to} - \phi)}{8\phi_{C,H}} - 1$</td>
<td>(32)</td>
</tr>
<tr>
<td>Reloading</td>
<td>frictional behaviour</td>
<td>$M_{to} = 8M_{to,C,H} \left[ \sqrt{\frac{3}{2\phi_{C,H}}} + 1 - \frac{3}{2\phi_{C,H}} - 1 \right]$</td>
<td>(33)</td>
</tr>
<tr>
<td>$-\phi_{C,H} \leq \phi \leq \phi_{Y,C,H}$</td>
<td></td>
<td>$M_{to} = -\frac{M_{to,LI} - \phi}{\phi_{Y,C,H}} + \frac{3(M_{to} + \phi)}{2\phi_{C,H}} + 1 - \frac{3(M_{to} + \phi)}{8\phi_{C,H}} - 1$</td>
<td>(33)</td>
</tr>
</tbody>
</table>

Table 5: Activation energy of locally deformed contact zone ($\tilde{M} = 100$ g/mol molecular mass of CaCO$_3$).
Thermomicromechanical continuum modeling of granular materials

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Abstract

Presented here is a method for the development of thermomicromechanical constitutive laws that are expressed solely in terms of particle scale properties, and thus engenders physical transparency across micro-meso-macro scales. The focus of this study is on dense granular media under quasi-static loading. Micromechanical relations for the internal variables, tied to nonaffine deformation, and their evolution laws are derived from a structural mechanical analysis of a particular mesoscopic event: confined, elastic-plastic buckling of a force chain. The resulting constitutive law can reproduce the defining behavior of strain-softening under dilatation, and strain localization in the context of bifurcation theory. The thickness and angle of, and the distributions of particle rotation and the emergent normal contact force anisotropy inside the band are consistent with DEM simulations.

1 Introduction

The gauntlet thrown down to Micromechanics has been the development of constitutive laws for heterogeneous materials, without need for any phenomenological parameters above the microscopic length scale [9]. From the standpoint of mathematical modeling alone, this challenge is fraught with many difficulties, not least of which is that mechanisms governing bulk behavior are inherently multiscale [2, 5, 8, 15, 6, 7]. Thus, if and when such mechanisms are identified and quantitatively characterized, there arises an even greater problem of establishing a purely micromechanical formulation that engenders ‘physical transparency’ in the transition from particle to bulk, i.e. one that results in a constitutive law that is entirely in terms of particle scale properties. Key to this problem is the formulation for energy dissipation or plastic response of the material. Unlike classical plasticity theory in which dissipative mechanisms are all lumped into one variable, i.e. the plastic strain, a purely micromechanical formalism demands that the fundamental origins of dissipation be
explicitly identified in order for internal variables to be given clear physical meaning [6, 15, 2, 5, 8]. A promising approach lies in the study of foams and amorphous solids, where considerable attention has been paid to the kinematics of mesoscopic structural rearrangements that result in irreversible loss of elastic energy, i.e. T1 events [2, 5] and STZs [3, 8, 7]. Although there is still the pressing need to consider kinetics along with the kinematics to fully characterize material behavior [2] – the direct consideration of internal events that involve loss of connectivity in the material domain – from which to build constitutive laws is a compelling avenue for micromechanical advancement.

In the case of granular materials, rotational degrees of freedom lead to a richness in kinematics that significantly complicates rheological behavior. For these systems, no clear rearrangement event prevails throughout deformation [11, 7]. However, recent experiments and discrete element (DEM) studies lend considerable credence to Oda’s hypothesis that confined buckling of force chains is a governing event for dissipation and failure of dense granular systems [11, 10]. In this Letter, we present a new approach for constitutive development, focussing on this key dissipative mechanism. A novel result is a constitutive law that has physical transparency across micro-meso-macro scales. Well established techniques, along with recent advances, underpin this new development: Thermomicromechanics of Micropolar continua [16, 17]; use of Discrete Element Method (DEM) along with recently developed local measures of kinematics and kinetics to establish key internal mechanisms and their relative contributions to dissipation [12]; and use of Structural Mechanics to model the kinetics of the dissipative event of confined buckling of a force chain [13].

The thermomicromechanical formulation in [17] was developed for a micropolar continuum representation of a granular material, and is based on a homogenization scheme on the scale of a particle and its first ring of neighbors. It proceeds in three steps. Step 1 relates the continuum micropolar deformation quantities of strain, $\varepsilon_{ij}$, and curvature, $\kappa_{ij}$, to the motions of the particle centers. Step 2 links the particle motions to the forces and moments at their contacts via a contact law. Step 3 connects these forces and moments to the stress, $\sigma_{ij}$, and couple stress, $\mu_{ij}$, via the stored free energy $\psi = \psi(\varepsilon_{ij}, \kappa_{ij}, \alpha^1, ..., \alpha^n)$: $\sigma_{ij} = \partial \psi / \partial \varepsilon_{ij}; \mu_{ij} = \partial \psi / \partial \kappa_{ij}$ where $\alpha^1, ..., \alpha^n$ are a set of internal variables (tensors, vectors, or scalars). The $\alpha^i$ represent dissipative mechanisms responsible for the loss of stored free energy: to close the governing system of equations, each requires an evolution law that satisfies $\partial \psi / \partial \alpha^i \otimes \delta \alpha^i \leq 0$ in accordance with the 2nd Law of Thermodynamics. Complete details of this approach can be found in [16, 17] and the references cited therein.

The central challenge lies in Step 1. The majority of continuum models, including those constructed using micromechanical techniques, employ the assumption of an affine deformation (e.g. [14]). Here, the relative contact displacement is expressed in terms of a single strain tensor: $\Delta u = 2R e_{ij} n_j + 2R^2 e_{ij\kappa} n_j n_k$ in two dimensions, where $R$ is the particle radius, $n_i$ the contact normal vector and $e_{ij\kappa}$ the permutation symbol. However, past studies have shown that this is inadequate for granular materials (e.g. [12, 1]). To capture nonaffine deformation, we decouple the relative normal and tangential displacements [16]; with rotations, we get:

$$
\Delta u^{en} = 2R(e_{ij} - e_{ij}^{pn}) n_j n_i; \\
\Delta u^{et} = 2R(e_{ij} - e_{ij}^{pt}) t_i n_j + 2R^2(\kappa_i - \kappa_i^{p}) n_i; \\
\Delta w^e = 2R(\kappa_i - \kappa_i^{p}) n_i
$$

(1)
where three internal variables have been introduced: \( \epsilon_{ij}^{pn} \) is the normal plastic strain, \( \epsilon_{ij}^{pt} \) the tangential plastic strain, and \( \kappa_i^p \) the plastic curvature. These represent nonaffine deformation associated with normal, tangential, and rotational motion respectively. Using these internal variables, the constitutive laws are:

\[
\begin{align*}
\sigma_{ij} &= \frac{NR^2}{4V} \left\{ k_n (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) (\epsilon_{kl} - \epsilon_{kl}^{pn}) \\
&\quad + k_t (3\delta_{ik}\delta_{jl} - \delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk}) (\epsilon_{kl} - \epsilon_{kl}^{pt}) \right\}, \\
\mu_i &= \frac{NR^4}{V} (k_t^i + k_r^i)(\kappa_i - \kappa_i^p),
\end{align*}
\]

where \( N \) is the number of contacts per particle, \( V \) is the area of the Delaunay polygon for the particle, \( k_n, k_t, k_r \) spring stiffness constants associated with normal and tangential forces and contact moment (rolling resistance) respectively, and \( \delta_{ij} \) the Kronecker delta [16]. With the exception of the internal variables and their corresponding evolution laws which are yet to be defined, the material parameters in the constitutive relations in Eq. 2 are entirely expressed in terms of particle scale properties. In [16], the recourse to a curve-fitting analysis of DEM data on bulk properties to obtain relations for the internal variables and their evolution laws resulted in a phenomenological constitutive law. However, the deviation from the micromechanical formulation is now isolated and confined to the internal variables and their evolution laws: thus a clear focal point for subsequent analysis and model development is now firmly in place.

For the next step, we adopt the approach initially pursued for foams and amorphous solids, which focuses on the kinematics of key nonaffine rearrangement events: T1 events [5, 2], and STZs [3, 8]. More recent studies, however, emphasize the need to consider kinetics along with the kinematics to fully characterize material behavior [2]. Indeed, in preparation for the constitutive development proposed here, we have quantitatively characterized both kinetics and kinematics at multiple length scales (i.e. interparticle contact-, meso- and macro-scales), via a series of DEM studies on two-dimensional densely packed granular systems under biaxial compression and punch penetration tests. For brevity, we briefly summarize relevant findings: details can be found in [12] and references cited therein. Global averages of energy dissipation and nonaffine deformation (i.e. micropolar strain and curvature, on the scale of a particle and its first ring of neighbours) were found to be strongly correlated. Quantitative characterization of the evolution of force chains, and their failure via buckling and associated kinematics, showed that, locally, a strong spatial and temporal correlation exist between particle rotations, nonaffine deformation, dissipation, and confined buckling of force chains [12].

We begin our construction of the constitutive model with a proper analysis of the kinetics and kinematics of the confined buckling of force chains. Techniques of Structural Mechanics are employed. In a companion paper, we presented a structural analysis of the elastic-plastic buckling of a three-particle force chain with lateral support from weak network particles; model development was guided by and validated against DEM data [13]. Given the correlation between dissipation, nonaffine deformation and buckling events [12], we assume that the nonaffine deformation in Eq. 1 is governed by the kinematics of confined buckling of force chains. Thus we now use
the structural mechanics model of force chain buckling to derive expressions for the nonaffine deformation and their evolution laws in terms of particle scale properties, subject to the 2nd Law of Thermodynamics.

To do this, we first briefly summarize key aspects of the force chain buckling model in [13]. This model yielded explicit expressions for the positions and rotations of, and hence contact forces and moments between, the particles in the model, in terms of the degree of buckling, or ‘buckling angle’ $\theta$ (Fig. 1). As schematically illustrated in Fig. 1, these functions are: $\Delta(\theta)$, the amount of vertical compression of the force chain; $x(\theta)$, the $-x_1$ position of particles 4 and 5; $\Delta n(\theta)$, the relative normal displacement magnitude between particles 2 and 3; $f^s(\theta)$, the total lateral supporting force magnitude from particles 4 and 5; and $w(\theta)$, the rotation of particle 1.

For brevity, we express the continuum nonaffine deformation in terms of these functions: the exact equations for which may be found in Ref. [13]. In addition, we will use the elastic rotation of particle 1, $w_e(\theta)$.

Due to the symmetry about the $x_1$ axis of the buckling motion, the total and elastic rotations of particle 3 are equal and opposite to those of particle 1; the central particle does not rotate (Fig. 1). The only parameters appearing in these functions are particle scale properties. Thus, these parameters can either be directly compared with DEM: $R, k^n, k^t, k^r$ (previously defined), and $\mu_r$ (friction coefficient for contact moment between force chain particles); or, can be measured via DEM: $\mu_s, \sigma_s$ (limiting or maximum stress the weak network particles can exert on a force chain particle); or, can be derived via limiting the maximum particle overlap: $k_{t FC}^t, k^s$ (spring constants related to resistance to lateral motion of the force chain).

To derive explicit expressions for the nonaffine deformation $\epsilon_{pn}^{ij}, \epsilon_{pt}^{ij}, \kappa_i^p$ in Eqs. 1, we start by defining a continuum strain and curvature for the structure. We define strains in principal strain space so that shear strains are 0. By considering deformation of a continuum element through the centers of the outer ring of particles (Fig. 1), principal strains are expressed as

$$\epsilon_1(\theta) = \frac{\sqrt{3}R + x(\theta) - 2\sqrt{3}R}{2\sqrt{3}R} = \frac{x(\theta) - \sqrt{3}R}{2\sqrt{3}R}. \tag{4}$$

Curvature measures gradient in rotation ($\kappa_i = \frac{\partial w}{\partial x_i} \approx \delta w/\delta x_i$). The change in rotation $\delta w$ along the $x_2$ direction is $-2w(\theta)$, occurring over $\delta x_2 = 4R - \Delta(\theta)$. Hence $\kappa_2(\theta) = -2w(\theta)/(4R - \Delta(\theta))$. Relative rotations between particle 2 and weak network particles are 0, so there is no rotation gradient in the $x_1$ direction: $\kappa_1(\theta) = 0$.

Next, we rewrite Eqs. 1 in a simpler form. We express the contact normal and tangential unit vectors as $n_i = (-\sin\Theta, \cos\Theta)$, and $t_i = (\cos\Theta, \sin\Theta)$. Note that $\Theta$ measures the contact angle of contacts with particle 2: this is different to the buckling angle $\theta$, which varies throughout deformation (Fig. 1). Assuming contact forces and moments (and hence relative elastic displacements and rotations) are

\[ Prior \text{ to } the \text{ point when the contact moment becomes plastic, } w_e(\theta) = w(\theta). \text{ After this point, } w_e(\theta) = \mu_r k^n \Delta n(\theta)/(Rk^r) \text{ (see [13] for a full discussion).} \]
well-fitted by a 2nd-order Fourier series, Eqs. 1 become

$$\Delta u^e_n = 2R((\epsilon_v(\theta) - \epsilon_v^m(\theta)) - (\epsilon_d(\theta) - \epsilon_d^m(\theta))\cos2\Theta);$$
$$\Delta u^e_t = -2R(\epsilon_d(\theta) - \epsilon_d^m(\theta))\sin2\Theta;$$
$$\Delta \omega^e = 2R((\kappa_2(\theta) - \kappa_2^m(\theta))\cos\Theta - (\kappa_1(\theta) - \kappa_1^m(\theta))\sin\Theta)$$

(5)

where $\epsilon_v = \frac{1}{2}(\epsilon_{11} + \epsilon_{22}) = \frac{1}{2}(\epsilon_1 + \epsilon_2)$, $\epsilon_d = \frac{1}{2}(\epsilon_{11} - \epsilon_{22}) = \frac{1}{2}(\epsilon_1 - \epsilon_2)$ are the volumetric and deviatoric components of a tensor $\epsilon_{ij}$. Note that there is no contribution to volumetric strain by relative elastic tangential displacements.

Consider the first of Eq. 5. To find the two unknown functions $\epsilon_v^m(\theta)$ and $\epsilon_d^m(\theta)$, we use knowledge of the two distinct relative elastic normal displacements $\Delta u^e_n$ and their corresponding contact angles $\Theta$ from the force chain buckling model. The first of these has magnitude $\Delta n$, and acts at a contact angle $\Theta = -\theta$. Hence, $\Delta u^e_n$ has magnitude $\sqrt{3}\epsilon_s(\theta)$. We then substitute the two $\Delta u^e_n$ values and their corresponding contact angles into the first of Eqs. 5; solving the resulting equations gives

$$\epsilon_d^m(\theta) = \epsilon_d(\theta) - \frac{4k_n\Delta n(\theta) - \sqrt{3}\epsilon_s(\theta)}{4Rk_n(1 + 2\cos2\Theta)};$$
$$\epsilon_v^m(\theta) = \epsilon_v(\theta) + \frac{\sqrt{3}\epsilon_s(\theta)\cos2\Theta + 2k_n\Delta n(\theta)}{4Rk_n(1 + 2\cos2\Theta)}.$$  

(6)

Now consider the second of Eq. 5. There is only one unknown function, $\epsilon_d^m(\theta)$: hence, we can choose either of the two contact angles $-\theta$, $\frac{\pi}{3}$ used for the derivation of $\epsilon_v^m(\theta)$, $\epsilon_d^m(\theta)$. But $\Delta u^e_t \approx 0$ from the second of Eq. 5 when $\Theta \approx 0$: thus we use the interactions at $\Theta = \frac{\pi}{3}$. With $\Theta$ given above, the tangential force is $\frac{\epsilon_s(\theta)}{2}\cos\frac{\pi}{3}$. Hence, $\Delta u^e_t = -\frac{\epsilon_s(\theta)}{2}\cos\frac{\pi}{3}$, where the minus sign arises because deviatoric strains $\epsilon_d(\theta) - \epsilon_d^m(\theta)$ in the second of Eq. 5 for this mechanism must be positive. Substituting $\Delta u^e_t$ and $\Theta = \frac{\pi}{3}$ into the second of Eq. 5, we obtain

$$\epsilon_d^m(\theta) = \epsilon_d(\theta) - \frac{\epsilon_s(\theta)}{4\sqrt{3}Rk_t}.$$  

(7)

Last, consider the third of Eq. 5. There are two unknown functions $\kappa_2^m(\theta), \kappa_2^m(\theta)$. From earlier $\kappa_1(\theta) = 0 \forall \theta$: this implies $\kappa_2^m(\theta) = 0 \forall \theta$ for compliance with the 2nd Law of Thermodynamics. Hence, we only need one relative elastic rotation to obtain $\kappa_2^2(\theta)$. As relative rotations with weak network particles are all 0 [13], we use the relative elastic rotation with particle 3. This is $-\omega^e(\theta)$, since particle 2 does not rotate, and acts at a contact angle of $\Theta = \theta$. Substituting this into the third of Eq. 5 yields:

$$\kappa_2^m(\theta) = \kappa_2(\theta) + \omega^e(\theta)/(2R\cos\Theta); \kappa_1^m(\theta) = 0.$$  

(8)

Eqs. 3 and 4 are numerically solved for $\theta(\epsilon_{ij})$ to eliminate $\theta$ from the nonaffine deformation equations. This results in a set of strain evolution laws for $\epsilon_v^m, \epsilon_d^m, \kappa_i^m$.
as a function of the particle scale parameters, $R, k^n, k^t, k^r, \mu_s, \mu_r, k_{FC}, k^s$. Substitution of Eqs. 6-8 into Eq. 2 yields the micromechanical constitutive law:

$$\sigma_v(\theta) = \frac{-NR(\sqrt{3}f^v(\theta)\cos2\theta + 2k^n \Delta^n(\theta))}{16V(1 + 2\cos2\theta)},$$

$$\sigma_a(\theta) = \frac{NR(\frac{4k^n \Delta^n(\theta)}{1 + 2\cos2\theta} - \sqrt{3}f^a(\theta) + k_{FC} f^s(\theta))}{32V},$$

$$\mu_2(\theta) = \frac{NR^3(k^t + k^r)w^e(\theta)}{2V\cos\theta}, \mu_1(\theta) = 0. \tag{9}$$

The constitutive law (Eq. 9) successfully captures strain-softening under dilatation – a defining feature of densely packed granular materials – as well as unloading behavior (Fig. 2a). The nonaffine component $(\varepsilon_{pn})$ is shown, demonstrating the model’s behavior at all stages of deformation: the model captures an elastic regime, occurring during the pre-buckling phase, where nonaffine deformation is negligible. Essentially, nonaffine deformation takes effect with the onset of buckling (i.e. after the critical buckling load [13]).

The constitutive law (Eq. 9) is of the form of equation 1 in [14]; as such, the bifurcation theory developed therein for modelling the shear band evolution applies. As shown in Fig. 2b-c, the band thickness, distribution of rotation and the emergent evolution of normal contact force anisotropy are in good agreement with those from DEM biaxial compression tests displaying a single shear band [12, 14, 4]. Compared to the DEM, the bifurcation analysis underestimates the degree of rotations: a check of the rotations in the buckling model in [13] showed this to be due to the assumption of zero rotations prior to shear banding in the bifurcation analysis rather than a shortcoming of the constitutive law (Eq. 9). The shear band angle from the bifurcation analysis (i.e. $46^\circ$), is consistent with that from the DEM (i.e. $45^\circ$) [12].

To conclude, we have presented a new method for constructing constitutive laws, focussing on dense granular materials, that obviates the need for phenomenological parameters above the particle scale. Internal variables and their evolution laws were
Figure 2: (color online) (a) $\sigma_d$ (Eq. 9), $\epsilon_v$ (from Eqs. 3 and 4) and $\epsilon_{pn}^v$ (Eq. 6) against $|\epsilon_2|$ (Eq. 3). (b) Shear band (SB) width, measured in particle diameters (D) against axial strain magnitude $|\epsilon_{22}|$. Inset: rotation, symmetric about the central axis of the SB, with lines and stars respectively showing analytical results and data from DEM simulation with identical parameters (see [12]). (c) Angular distribution of normal contact force for systems in (b). Additional model parameters for (a): $\mu_s \sigma_s = 0.022k^n, k_{FC}^t = 0.004k^n, k_s = 0.03k^n$; and (b-c): $\mu_s \sigma_s = 0.0028k^n, k_{FC}^t = 0.31k^n, k_s = 0.024k^n$.

tied to the nonaffine deformation of confined buckling of force chains, giving these clear physical meaning. The resulting constitutive law reproduced the defining behavior of strain-softening under dilatation and strain localization. The thickness and angle of, and the distributions of particle rotation and normal contact force distribution inside, the band are consistent with DEM simulations. Whether this model can robustly predict behavior under more complex boundary conditions (e.g. penetration tests) in finite element simulations is a matter for future research. Finally, the method for constitutive development presented here is general, and may be applicable to other forms of complex materials.

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Solving inverse kinematics task for redundant robotic hand with constrains in coordinates

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Abstract

In this article is considered a method for solving the inverse kinematics task (IKT) based on iterative algorithm for minimizing the errors of hand gripper positioning by repeating solving the forward kinematics task (FKT).

1 Introduction

There are a lot of works [1],[3] for solving IKT, but there is no comparison between them; there are no comparison of these methods difficulty; conjugation speed and solution behavior near the constrains are not clear. In this cases it is needed to be engaged in research the characteristics of iterative methods for solving the IKT when there are fixed constrains in a way of range for system coordinates corrections. To be defined the most perspective algorithm for solving the task with view points in real time. The kinematics of a manipulator with seven degrees of freedom can be described with matrix homogeneous coordinates transformations. The position of the robotic hand gripper can be described with seven variables: position coordinates in Cartesian coordinate system and corresponding orientation angles (Euler angels) [1]. On fig. fig:1 is shown the general mode of a seven degrees of freedom robotic hand, where:

\[ x, y, z \] directions of global axes ;
\[ \alpha, \phi, \theta \] rotation angles around axes \( x, y, z \) respectively ; \( x_1, x_2, x_3 \) the length of the corresponding link.

However the robot hand has seven degrees of freedom, so there are seven rotation angles for each link and the IKT in this case will have six equations with seven unknown variables [2]. Obviously, the solution for IKT for all random points that belong to the distance the mechanical gripper can reach will have infinity multitude. In general, the FKT can be described with matrix homogeneous coordinates transformations.
Solving inverse kinematics task for redundant robotic hand with constrains in coordinates

Figure 1: Kinematics scheme of a seven degrees of freedom robot hand and its VRML model.

Let $\alpha, \phi, \theta$ be the corresponding rotation angles around axes $x, y, z$ and the hand is oriented along the length of axe $x$. Since there are three degrees of freedom for the shoulder articulation of the robot, for the first robot hand link the following rotation matrixes around axes $x, y, z$ and translation matrix along the axe $x$ can be written:

$$
R_x^1 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \alpha & -\sin \alpha & 0 \\
0 & \sin \alpha & \cos \alpha & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}, \\
R_y^1 = \begin{pmatrix}
\cos \alpha & 0 & -\sin \alpha & 0 \\
0 & 1 & 0 & 0 \\
-\sin \alpha & 0 & \cos \alpha & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}, \\
R_z^1 = \begin{pmatrix}
\cos \alpha & -\sin \alpha & 0 & 0 \\
\sin \alpha & \cos \alpha & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
$$

(1)

where $T_1$ is the translation matrix for the first robot link; $x_1$ the length of the first link.

The second link of the robotic hand, fore arm, has two degrees of freedom: rotation around axes $x$ and $y$. The rotation and translation matrixes for this link $R_x^2, R_y^2, R_z^2$, have corresponding variables $\alpha_2, \phi_2, \theta_2, x_2$ and have the following form (1). The third robotic hand link, hand, also has two degrees of freedom rotation around axes $y$ and $z$. The coordinates transformation for this link can be represented $R_y^3, R_z^3, T_3$ with variables $\phi_3, \theta_3, x_3$. The matrixes for coordinate transformation have the following form (1). The general equation for the forward kinematics task can be written as $T_{end} = R_x^1 R_y^1 R_z^1 T_1 R_x^2 R_y^2 R_z^2 R_y^3 R_z^3 T_3$ or

$$
f(\alpha_1, \phi_1, \theta_1 \alpha_2, \phi_2, \theta_2, \phi_3, \theta_3) = \begin{pmatrix}
r_{1,1}^2 & r_{1,2}^2 & r_{1,3}^2 & X \\
r_{2,1}^2 & r_{2,2}^2 & r_{2,3}^2 & Y \\
r_{3,1}^2 & r_{3,2}^2 & r_{3,3}^2 & Z \\
0 & 0 & 0 & 1
\end{pmatrix},
$$

(2)

where X,Y,Z are the coordinates of the last link of the robotic hand (mechanical gripper).
All the elements \[ r_{1,1} \ldots r_{3,3} \] from equation (2) are depending on each other and represent the orientation angles of the mechanical gripper in relation to global coordinate system. Using the coefficients of the rotation matrix it is always possible to turn into Euler angles using the following representations:

\[
\begin{align*}
\alpha_{\text{end}} &= -\arctan 2 \left( \frac{r_{2,3}}{r_{3,3}} \right) \\
\phi_{\text{end}} &= \arcsin (r_{1,3}) \\
\theta_{\text{end}} &= \arctan 2 \left( \frac{r_{2,1}}{r_{1,1}} \right)
\end{align*}
\]

where the \( f(x) = \arctan 2 (x) \) function is the arctan with quadrant report. With the FKT equation all angles mean in each articulation are known and the position and orientation of the mechanical gripper in base coordinate system can be defined as \( (\alpha_1, \phi_1, \theta_1)_{\text{end}} = f(r_{1,1} \ldots r_{3,3}) \). Translation coordinates is calculated with equation (2). Shortly the IKT can be written in the form:

\[
f^{-1} \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & X \\ r_{2,1} & r_{2,2} & r_{2,3} & Y \\ r_{3,1} & r_{3,2} & r_{3,3} & Z \\ 0 & 0 & 0 & 1 \end{pmatrix} = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3).
\]

The IKT in case of constrains can be summarized as follows: Find such values for rotation angles around each axe \( q = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3) \), so coordinate transformations from the set point to be equal to transformed coordinates of all points, determine the position and orientation of the last link in global coordinates. That way \( T_{\text{end}} = T_{\text{end}}' \) where \( T_{\text{end}} \) is the set position and orientation and \( q = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3) \) ∈ \( S \), where \( q \) is multitude of all permissible values for robotic hand degrees of freedom; \( S \) - region of permissible values, defined by the restrictions in inequality form for the robotic hand degrees of freedom. The simplest constrains have the form and they are mostly used in practice [3]. All constrains for the anthropomorphic robotic hand are shown in table 1.

<table>
<thead>
<tr>
<th>grad</th>
<th>( \alpha )</th>
<th>( \phi )</th>
<th>( \theta )</th>
<th>( \alpha_2 )</th>
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</tbody>
</table>

In general all constrains have the form \( q_1 \leq g(q) \) and they can be linear or non-linear dependencies. To find the most suitable decision usually the initial (starting) position and orientation of the manipulator are set and using iterative optimization method in order to find the most closer to the initial \( (\text{in terms of the distance between the coordinates in the homogeneous transformation matrix} (T_{\text{end}}' \rightarrow T_{\text{end}})) \) configuration of the manipulator satisfying the fixed constrains. The fastest and the simplest methods is the gradient-based methods, but there are some disadvantages: \textit{Failing in local minimum and finding a decision without any constrains of coordinates.}

The problem with local minimum is not important, because by default the IKT has countless solutions with arbitrary small error. Also in practice it is required not
only to cover from point A to point B but to follow a trajectory. In this case the trajectory is sampled on small sections and the distance between the start point A and the final point B could be relatively little so as the variation of rotation angles in all degrees of freedom to realize the transition from A to B. In this case there is failing in an area of determinate local minimum and because of the small distance between points A and B, the IKT will have only one minimum determined by the initial value \( q_0 \). If the distance between points A and B is relatively large, the IKT could have several minimums at the same time and the solution will be the closest to the initial point \( q_0 \) local minimum. Finding the closest local minimum allows covering the distance from point A to point B with minimum variation of the manipulators degrees of freedom. Discarding the obvious incomplete solutions of the IKT is realized with including constrains in the optimization algorithm. The method for determine the position error plays an important role. This error can be defined in open way reporting on equation (3) and it can be written as mean square error:

\[
E = \frac{1}{2} \left( (X - X')^2 + (Y - Y')^2 + (Z - Z')^2 +
\right.
\]

\[
+(\alpha - \alpha')^2 + (\phi - \phi')^2 + (\theta - \theta')^2 \right),
\]

(5)

where \( X, Y, Z, \alpha, \phi, \theta \), are the current position and orientation of the mechanical gripper; \( X', Y', Z', \alpha', \phi', \theta', \), are the desired position and orientation of the mechanical gripper.

Such a method for describing the error requires additional computations and differencing (3). This can be avoided by presenting the position error as elements \( r_{1,1} \ldots r_{3,3} \) of the rotation matrix. In this case, equations (3) and (5) won’t be used. Calculation of the position error can be written in the form:

\[
E = \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} (r_{ij} - r'_{ij})^2 + \frac{1}{2} \left( (X - X')^2 + (Y - Y')^2 + (Z - Z')^2 \right),
\]

(6)

Calculation of (6) doesn’t depend on the difficult calculation of reverse trigonometric functions and that makes all calculation easier. The solutions of gradient methods are given in general scheme. At first some initial values for all degrees of freedom are chosen \( q_0 \). Solving the FKT gives transformation matrix from mechanical gripper to global coordinate system. This allows calculating the error using (6). After that equation (6) is differenced for all degrees of freedom angles and the result is finding the correction of all angles \( q \), which are subtracting the error. Since the expressions for the IKT are analytical, it is possible to calculate the Jacobian \( J = \frac{\partial T_{\text{end}}}{\partial q} \), where \( J \) calculate about position elements \( [X, Y, Z] \) and rotation elements \( [r_{1,1} \ldots r_{3,3}] \) preliminarily. Because of special (singular) points, in which some constituent of the Jacobian can incline to infinity, the Newton-Gauss method cannot be used [3], [4]. In Levenberg-Marquardt method [3], [4] dempfering of all inclining to infinity elements is made which allows optimization near the singular point [2], [3]. Coordinates corrections is made following the rule:

\[
q_{i+1} = q_i + \Delta q_i,
\]

(7)
After correction of all angles degrees of freedom is done next step of the iteration procedure is made until reaching the stop criteria. To analyze how the algorithm is processing with simple coordinate constrains which are always between the lower and upper constrain line is necessary
\[ q = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3) \in [\text{min}..\text{max}] \]

2 Experiments

Algorithm 1. Equalization gradient method. The simplest method which doesn’t add corrections to the coordinates at the end if at some of the iteration steps is placed on constrain line. This can be written in the form:

\[ \text{if}(q_{i+1} < \text{min}) \text{or}(q_{i+1} > \text{max}), \text{then } q_{i+1} = q_i; \]  

(8)

This is quite simple method for realization. The disadvantage is sticking of the solution near the border of permissible values area and that leads to high number of iterations.

Algorithm 2. Gradient reflection method. The coordinates correction is made by formula (7). Processing constrains conditions can be written as:

\[ \text{if}(q_{i+1} < \text{min}) \text{or}(q_{i+1} > \text{max}), \text{then } \Delta q_{i+1} = -\Delta h q_i; \]  

(9)

where \(h\) is the reflection factor \(\in [0..1]\). If \(h = 0\), then algorithm 2 is converting to algorithm 1. In case of nonlinear constraining conditions \(g(q) < 0\) gradient reflection method will have more difficult formula, reporting on the gradient reflection of inequality constrain. Advantage of this algorithm is simple realization for simple constrains \(q = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3) \in [\text{min}..\text{max}]\) and high conjugating speed compared to algorithm 1. Disadvantage is selection of the factor \(h\). This is very important when the permissible values area is little and the value of \(h\) is large.

Algorithm 3. Lagranges multipliers method. The main idea of this method is substituting the functional of the decision function in the way:

\[ E(q, \lambda) = E(q) + \lambda g(q), \]  

(10)

which is own sum of target function and multiplication of Lagranges multipliers \(\lambda\) and constrains functions \(g(q)\). In this case the necessity to minimize the function \(E(q)\) with constrains presence \(g(q)\) can be written as follows:

\[
\begin{align*}
\frac{\partial F(q, \lambda)}{\partial q} &= \frac{\partial F(q)}{\partial q} + \lambda \frac{\partial g(q)}{\partial q} = 0 \\
\frac{\partial F(q, \lambda)}{\partial q} &= g(q) = 0,
\end{align*}
\]

(11)

The optimum point for criteria (ref10) in fact is the solution of system equations (11), where \(q = q_{\text{opt}}, \lambda = \lambda_{\text{opt}}\) are the decisions in optimum point [4], [5]. In case of searching the decision functional minimum reporting on Lagranges multipliers the adaptation algorithm can be written in the form below:
\[
\begin{pmatrix}
q_{i+1} \\
\lambda_{i+1}
\end{pmatrix} = q_i + \left( \frac{H(q_i, \lambda_i), A(q_i)}{A^T(q_i) \ldots 0} \right)^{-1} \ast \left( \frac{\frac{\partial f(q_i)}{\partial q_i} - A(q_i) \lambda_i}{g(q_i)} \right)
\]  
(12)

Where \( A(q_i) \) - is active constrains vector, \( H(q_i, \lambda_i) \) - Hessian or second derivative matrix. In case of using Levenberg-Marquardt method \( H(q_i, \lambda_i) = (J'J + \mu I) \) where reporting on constrains Jacobian can be written as:

\[
J = \left( \frac{\frac{\partial f(q_i)}{\partial q_i} - A(q_i) \lambda_i}{g(q_i)} \right).
\]  
(13)

Lagranges multipliers method can be written step by step by the way:

1. Initialization \( q, \lambda \), initialization \( a, b \) method parameters;
2. Computation of "penalty" function \( P = \left\| \frac{\partial f(q_i)}{\partial q_i} - A(q_i) \lambda_i \right\|^2 + \|g(q_i)\|^2 \).
3. If \( P < \varepsilon \) where \( \varepsilon > 0 \) then calculate \( \left( \frac{q_{i+1}}{\lambda_{i+1}} \right) \) and go to step 5. Else:
   4. Calculation of \( \left( \frac{q_{i+1}}{\lambda_{i+1}} \right) \) if \( P \left( \frac{q_i + a\Delta q_i}{\lambda_i + a\Delta \lambda_i} \right) \leq (1 - ba)P \left( \frac{q_i}{\lambda_i} \right) \) then go to step 5, else \( a = a/4 \) and go to step 4.
5. \( \left( \frac{q_{i+1}}{\lambda_{i+1}} \right) = \left( \frac{q_i}{\lambda_i} \right) + \left( \frac{a\Delta q_i}{a\Delta \lambda_i} \right) \)

**Algorithm 4. Opposite limited functions method.** The decision functional \( E = f(q) \) is replased by the functional

\[
E = f(q) + R \frac{1}{g(q)},
\]  
(14)

where \( R > 0 \), then as near we are closing to the limit, as fast the additional functional term increases. In the adaptation algorithm the parameter \( R \) gradually decreases thus, so \( \lim_{i \to \infty} R = 0 \).

**Algorithm 5. Logarithmic limited functions method.** In this case the quality criteria are written as follow:

\[
E = f(q) + R \log (g(q))
\]  
(15)

The advantages of algorithm 5 compared to algorithm 4 consist in limited function, which increases the error sense by closing the limits. As written in algorithm 4, it is important to notice that \( g(q) \neq 0 \).

On fig. 2 are shown how the position error is changing in function from optimization epochs(left). The numbers on fig. 2 left and fig. 2 right, show the corresponding algorithm number 1-5. The correction character of separate manipulator coordinates \( q_2 \) in the optimization techniques reporting on constrains can be written as \( q = (\alpha_1, \phi_1, \theta_1, \alpha_2, \phi_2, \phi_3, \theta_3) \in [\min .. \max] \) when \( q_{2\text{max}} = 1 \). It is obvious from fig. 2 left, the fastest conjugating algorithm is algorithm 5, algorithm with logarithmic limit functions. The slowest conjugating algorithm is Lagranges method, although its
first iteration shows a good result. Moreover, as it is notable from fig. 2 right, Lagranges method also comes out of border of permissible values during iterations, but disadvantage can be avoided by setting up additional conditions for coordinates correction, which can be reduced to the algorithm by 1 equalization gradient for every conditions in the algorithm; 2 gradient descent method. Results of using all the methods 1-5 for solving the IKT for the robotic hand are also given in table 2.

All presented methods reach low enough error level at tenth and further iteration and after that the error is monotone decreasing. The equalization gradient method, gradient reflection methods and limited function method type $\log(g(q))$ show approximately equal error level. The best result is given by logarithmic limited function, and the worse by Lagranges method, but it is known by very high computing complexity.

Table 2. Comparison of optimization methods in case of constrains based on Levenberg-Marquardt optimization method for 50 adaptation epochs.

<table>
<thead>
<tr>
<th>Constraining</th>
<th>Reached error</th>
<th>Execution time,sec</th>
<th>Relative time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Equalization</td>
<td>1.83-005</td>
<td>0.016681</td>
<td>1</td>
</tr>
<tr>
<td>2 Reflection</td>
<td>1.4004e-005</td>
<td>0.016416</td>
<td>0.9841</td>
</tr>
<tr>
<td>3 Lagrange</td>
<td>6.2976e-005</td>
<td>0.045967</td>
<td>2.7557</td>
</tr>
<tr>
<td>4 Limit $\frac{1}{g(q)}$</td>
<td>1.644e-004</td>
<td>0.020461</td>
<td>1.2266</td>
</tr>
<tr>
<td>5 Limit $\log(g(q))$</td>
<td>2.1e-0.07</td>
<td>0.026842</td>
<td>1.6091</td>
</tr>
</tbody>
</table>

Conclusion: Based on the results, shown at fig. 2 and in table 2, the method, combining in them high conjugation speed and relatively low complexity, is the logarithmic limited function. Practical the number of epochs can be reduced to 10 without substantial quality loss and in this case the execution time is reduced to 5 times. The most perspective application with view points in real time can be specified the gradient reflection method, which combines in itself high enough conjugation speed and simple realization.
References


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Simulation of heat propagation from deepen pipeline with accounting filtration and solar radiation

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Abstract

A new mathematical model of heat propagation from an underground source is considered with accounting of physical factors such as filtration of water and a solar radiation. Such problem arises, for example, in studying heat propagation from a damaged deepen pipeline.

1 Introduction

Measuring of temperature is useful in many types of diagnostics. For example, it is used in non-destructive monitoring of wholeness of underground pipelines. In Fig. 1 a real temperature field on earth surface is shown. The white spots and lines are thermal trace of underground pipelines.

Figure 1: Temperature on the earth surface over two pipelines.
One of methods of investigation of thermal fields in different media is direct numerical simulation of thermal diffusivity processes. Soil is a complex structure which includes solid particles, water and air with water vapor (fig. 2). We will consider two basic ways of heat transfer: thermal conductivity in solids and groundwater flow which filtrates through pores in soil. Purpose of this work is elaboration of models, computational algorithms and codes to investigate temperature distribution with taking into consideration humidity of soil, water flow through soil and also solar radiation and evaporation on earth surface.

![Figure 2: Structure of soil.](image)

2 Heat distribution with accounting solar radiation on earth surface

In [1] thermal diffusivity processes was considered in 3D origin where the heat source is a pipeline with a constant temperature. It is supposed that heat flow from the earth (upper) surface is caused by solar energy and difference of temperatures between earth and air.

Let us consider two components of heat propagation processes: thermal diffusivity and filtration of water in soil.

This problem is described by a linear thermal diffusivity equation:

$$\frac{\partial T}{\partial t} = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right),$$  \hspace{1cm} (1)

where $T = T(t, x, y, z)$ — heat distribution, $\lambda = \kappa/\rho c_v$ — thermal conductivity coefficient, $\kappa$ — heat conductivity, $\rho$ — density, $c_v$ — specific heat.

Suppose that heat flow from the pipeline is proportional to difference of ground and pipeline temperatures, and the coefficient is essentially increased at places where
the isolating shell has wear. Boundary condition at the pipeline has the form:

\[ \lambda \frac{\partial T}{\partial n} = \epsilon(x) \left( T_{\text{pipe}} - T_{\text{media}} \right) n, \]

where \( n \) is normal vector to the surface.

Let the pipeline is inside of a parallelepiped (Fig. 3). At the time moment \( t = 0 \) the following initial conditions are fulfilled

\[ T(0, x, y, z) = T_0(z) = T_{\text{air}} + (T_{\text{bot}} - T_{\text{air}})z, \]

where \( T_{\text{air}} \) is temperature of air, \( T_{\text{bot}} \) is temperature at the bottom of the parallelepiped. Assume that at the lateral area heat flow equals to zero and at the bottom temperature is fixed. Consider flows balance condition at the upper surface.

Let \( V_{\text{sol}} = (x_{\text{sol}}, y_{\text{sol}}, z_{\text{sol}}) \) be a vector of solar radiation. A part of energy for the ground is \( \gamma_{\text{sol}} q_{\text{sol}} v_{\text{sol}} \left[ \text{Wt/m}^2 \right] \), where \( \gamma_{\text{sol}} \) is a part of absorbed solar radiation, \( q_{\text{sol}} \) is a solar power, \( v_{\text{sol}} \) is a sun beam projection, \( v_{\text{sol}} = z_{\text{sol}} / \sqrt{x_{\text{sol}}^2 + y_{\text{sol}}^2 + z_{\text{sol}}^2} \), \( w_{\text{top}} \) is a thermal exchange coefficient between soil and air, \( \sigma \) is Boltzmann constant, \( \kappa \) is thermoconductivity coefficient. Then

\[ \gamma_{\text{sol}} q_{\text{sol}} v_{\text{sol}} + w_{\text{top}} (T_{\text{air}} - T|_{z=0}) = \sigma (T|_{z=0})^4 + \kappa \frac{\partial T}{\partial z} \bigg|_{z=0}. \]

The term \( \sigma T^4 \) included to the model corresponds to emission of a heated body. Condition (4) makes the considered problem be nonlinear.

Figure 3: Model of heat distribution.
3 Heat propagation with accounting water filtration in ground

Equation system of groundwater flow which filtrates through pores in soil has the form

\[
\begin{align*}
\frac{\partial h}{\partial x} + \frac{V_x}{k} + \frac{1}{q} \frac{\partial V_x}{\partial t} &= 0, \\
\frac{\partial h}{\partial y} + \frac{V_y}{k} + \frac{1}{q} \frac{\partial V_y}{\partial t} &= 0, \\
\frac{\partial h}{\partial z} + \frac{V_z}{k} + \frac{1}{g} \frac{\partial V_z}{\partial t} &= 0,
\end{align*}
\]

where \( \vec{V} = (V_x, V_y, V_z) \) is flow rate, \( h = h(x, y, z) \) is a potential. Let Darcy low be used for the considered soils (for example, sand, clay and others).

\[
\vec{V} = k \vec{J} = -k \frac{dh}{dt},
\]
or

\[
V_x = -k \frac{\partial h}{\partial x}, \quad V_y = -k \frac{\partial h}{\partial y}, \quad V_z = -k \frac{\partial h}{\partial z}.
\]

It was shown [2], that for small values of filtration coefficient \( k = \frac{1}{100} \text{ m/day} \) it is possible to use quasistationary model instead of (5). Let assume that the flow is incompressible and the soil is uniform, then we obtain

\[
\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = 0.
\]

For heat distribution in soil we have

\[
\frac{\partial T}{\partial t} + \text{div}(\vec{V}T) = \lambda \Delta T.
\]

Boundary and initial conditions for \( T(t, x, y, z) \) are the same as (2)–(4). Boundary conditions at upper surface is

\[
\gamma_{\text{sol}} q_{\text{sol}} v_{\text{sol}} + w_{\text{top}} (T_{\text{air}} - T|_{z=0}) = \sigma (T|_{z=0})^4 - k m \rho_f (Q + c_v T) \frac{\partial h}{\partial z} + \frac{\partial T}{\partial z} \bigg|_{z=0},
\]

where \( m \) is porosity of soil, \( \rho_f \) is density of flow, \( Q \) is thermal capacity of evaporation. Boundary condition for \( h(x, y, z) \) at upper and lower surfaces of the considered parallelepiped include evaporation at the soil surface, are proportional to absorbed solar radiation, and have the form

\[
\frac{\partial h}{\partial z} = -\frac{\gamma}{k} T(t, x, y, 0).
\]

At the lateral surfaces it is assumed that

\[
\frac{\partial h}{\partial x} = \frac{\partial h}{\partial y} = 0.
\]
Boundary condition at the pipeline has the form ($\nabla = 0$):

$$\frac{\partial h}{\partial x} = \frac{\partial h}{\partial y} = \frac{\partial h}{\partial z} = 0,$$

(12)
or

$$\frac{\partial h}{\partial x} n_x + \frac{\partial h}{\partial y} n_y + \frac{\partial h}{\partial z} n_z = 0, \quad \frac{\partial \nabla_x}{\partial \n} = 0,$$

(13)

where $\n = (n_x, n_y, n_z)$ is an unit normal, $\nabla_x$ is projection on tangential surface to the pipeline surface.

Thus the problem of simulation of heat propagation in soil with taking into account flow which filtrates through pores in soil leads to solution of the problem (6)–(8) with initial conditions (3) and boundary conditions (2), (9)–(13). It is expected that taking into consideration water filtration in soil allows to describe heat distribution more effectively.

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**References**


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Discrete Limit Analysis for Plate Bending Problems by Using Hybrid-type Penalty Method

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Abstract

In present paper are given investigations of plate bending problem by numerical treatment using hybrid-type penalty method (HPM). The HPM assume linear and nonlinear displacement field with rigid displacement, rigid rotation, strain and its gradient in each subdomain and introduce subsidiary condition about the continuity of displacement into the framework of the variational expression with Lagrange multipliers. For this purpose accepted the Kirchhoff theory, which takes no into account the transversal shear deformation. In first step of work we are giving the equilibrium equations for deformable body in 3D case and as boundary conditions we are giving geometrical (for displacement field) and kinetic (for surface force) boundary conditions. Secondary we apply Kirchhoff theory to make the displacement field for plate bending problem into the 3D case. For this purpose we use quadratic form which includes rigid, linear and nonlinear parts of displacements. The parameters used in this displacement field are independently defined in each subdomain. We introduce penalty function which presents strong spring connecting each subdomain. Then we obtain stiffness matrix by analytically integration by area of contact surface of each subdomain. We apply nonlinearity in penalty function such as spring system, which allow us to calculate hinge line. If hinge line makes mechanism then we can calculate limit load. We used load incremental method which is called r-min method as a material nonlinear analysis. We can calculate growing hinge line step by step using this algorithm for the nonlinear analysis. Finitely we calculate simple problems to check accuracy of elastic solution and limit load.

1 Introduction

As mentioned in abstract in this paper used hybrid-type penalty method (HPM), which applied the concept of the penalty method to the principle of hybrid type virtual work. HPM applies the concept of the spring of RBSM (Rigid Bodies-Spring
Model) in Lagrange multiplier and assume independent displacement field to each subdomain and because compatibility requirements of the intersection boundary on adjacent sub-domain are secured by using the penalty method, the displacement field can be assumed regardless of the shape of sub-domain. However, excellent accuracy was not obtained when shape other than the triangle were used at the linear displacement field, and the division of arbitrary shape was difficult. To solve such a problem, it proposes the method of applying the second-order displacement field where the inclination of the strain was added to HPM. In the first part of paper is given brief analytical formulation of model, and in second part are given numerical results.

2 Governing Equation and Hybrid-Type Virtual Work

1. Governing equation. Let $\Omega \subset \mathbb{R}^{n_{\text{dim}}}$, with $(1 \leq n_{\text{dim}} \leq 3)$, be the reference configuration of a continuum body with smooth boundary $\Gamma := \partial \Omega$ and closure $\overline{\Omega} := \Omega \cup \partial \Omega$. Here is the ndim dimensional Euclidean space.

![Figure 1: Reference configuration $\Omega$ and smooth boundary $\partial \Omega$](image)

The local form of the equilibrium equation for a deformable body can be written by

$$\text{div} \sigma + f = 0 \text{ in } \Omega$$  \hspace{1cm} (1)

$$\sigma = \sigma^t \text{ in } \Omega$$  \hspace{1cm} (2)

where $f : \Omega \rightarrow \mathbb{R}^{n_{\text{dim}}}$ is the body force per unit volume, $\sigma : \overline{\Omega} \rightarrow S$ is the Cauchy stress tensor respectively. Here $S = \mathbb{R}^{(n_{\text{dim}}+1) \cdot n_{\text{dim}}/2}$ is the vector space of symmetric rank-two tensor and $e_i$ is the standard base vector of $\mathbb{R}^{n_{\text{dim}}}$, so that the stress tensor becomes $\sigma = \sigma_{ij} e_i \otimes e_j$, where $\otimes$ denotes a tensor product. $u : \Omega \rightarrow \mathbb{R}^{n_{\text{dim}}}$ is a displacement field of particles with reference position $x \in \Omega$. We write $u(x)$ and denote the infinitesimal strain tensor by
\[
\varepsilon = \nabla^s u \overset{\text{def.}}{=} \frac{1}{2} [\nabla u + (\nabla u)^t],
\]

where \(\nabla := (\partial/\partial x_i)e_i\) is the differential vector operator, \(\nabla^s\) shows the symmetry part of \(\nabla\).

In what follows, we assume that the boundary \(\Gamma = \Gamma_u \cup \Gamma_\sigma\).

\[
\Gamma = \Gamma_u \cup \Gamma_\sigma, \Gamma = \Gamma_u \cap \Gamma_\sigma = \emptyset.
\]

Here \(\Gamma_u := \partial_u \Omega \subset \partial \Omega\) where displacements are prescribed as

\[
u |_{\Gamma_u} = \hat{u} \text{ (given)},
\]

where as \(\Gamma_\sigma := \partial_\sigma \Omega \subset \partial \Omega\) where tractions \(t := \sigma n\) are prescribed as

\[
\sigma |_{\Gamma_\sigma} \hat{n} = \hat{t} \text{ (given)}.
\]

Here \(\hat{n}\) is the field normal to the boundary \(\Gamma_\sigma\). The constitutive equation to the elastic body is provided as follows by the use of the elasticity tensor \(C\).

\[
\sigma = C : \varepsilon.
\]

2. **Virtual work equation (weak forms).** Let denote by \(U\) the space of admissible displacement field, defined as

\[
U \overset{\text{def.}}{=} \{u : \Omega \rightarrow \mathbb{R}^{\text{dim}} | u|_{\Gamma_u} = \hat{u}\}.
\]

And, let denote by \(V\) the space of admissible virtual displacement field, defined as

\[
V \overset{\text{def.}}{=} \{\delta u : \Omega \rightarrow \mathbb{R}^{\text{dim}} | \delta u|_{\Gamma_u} = 0\}.
\]

We can now use Equation (1) and integrate volume of the body to give a weak statement of the static equilibrium of the body as

\[
\delta W := \int_\Omega (\text{div} \sigma + f) \cdot dudV = 0 \forall \delta u \in V.
\]

A more common and useful expression can be derived to give the divergence of the vector \(\sigma \delta u\) as

\[
\text{div}(\sigma \delta u) = (\text{div} \sigma) \cdot du + \sigma : \text{grad} \delta u.
\]

Using this equation together with the Gauss theorem enable Equation (10) to be rewritten as

\[
\int_\Omega \sigma : \text{grad} \delta u dV = \int_\Omega f \cdot dudV - \int_{\Gamma_\sigma} \hat{t} \cdot \delta u dS = 0 \forall \delta u \in V
\]

This equation is virtual work equation. If \(u\) is the weighing function, this is a weak forms. It is \(U \subset H^1(\Omega)\) and \(V \subset H^1(\Omega)\) where denotes the Sobolev space \(H^1(\Omega)\) of function possessing space integrable derivatives.

3. **Hybrid-type virtual work equation.** Let \(\Omega\) consist of \(M\) sub-domains \(\Omega^{(e)} \subset \Omega\) with the closed boundary \(\Gamma^{(e)} := \partial \Omega^{(e)}\) as shown in Figure 2.
Figure 2: Sub-domain $\Omega^{(e)}$

Figure 3: Common boundary $\Gamma^{(ab)}$ of sub-domain $\Omega^{(a)}$ and $\Omega^{(b)}$

That is

$$\Omega = \bigcup_{e=1}^{M} \Omega^{(e)} \text{ here } \Omega^{(r)} \cap \Omega^{(q)} = 0 \ (r \neq q). \quad (13)$$

In what follows, we assume that the closure $\Omega^{(c)} := \Omega^{(e)} \cup \delta \Omega^{(e)}$.

We denoted by $\Gamma^{(ab)}$ the common boundary for two sub-domain $\Omega^{(a)}$ and $\Omega^{(b)}$ adjoined as shown in Figure 3, and which is defining as

$$\Gamma^{(ab)} \overset{\text{def.}}{=} \Gamma^{(a)} \cap \Gamma^{(b)}. \quad (14)$$

The relation for $\tilde{u}^{(a)}$ and $\tilde{u}^{(b)}$ are following:

$$\tilde{u}^{(a)} = \tilde{u}^{(b)} \text{ on } \Gamma^{(ab)}, \quad (15)$$

they are the displacements on the $\Gamma^{(ab)}$ intersection boundary in $\Omega^{(a)}$ and $\Omega^{(b)}$ sub-domain.

This subsidiary condition is introduced into the framework of the variational equation (12) with Lagrange multipliers $\lambda$ as follows:

$$H_{ab} \overset{\text{def.}}{=} \delta \int_{\Gamma^{(ab)}} \lambda \cdot (\tilde{u}^{(a)} - \tilde{u}^{(b)}) dS, \quad (16)$$

where $\delta (\bullet)$ shows the variation of $\bullet$. Physical meaning of the Lagrange multiplier $\lambda$ is equal to the surface force on the intersection boundary $\Gamma^{(ab)}$

$$\lambda = t^{(a)}(\tilde{u}^{(a)}) = -t^{(b)}(\tilde{u}^{(b)}) \quad (17)$$
where \( t^{(a)} \) and \( t^{(b)} \) are the surface force on the intersection boundary \( \Gamma_{<ab>} \) in sub-domain \( \Omega^{(a)} \) and \( \Omega^{(b)} \). The hybrid type virtual work equation can be described as follows about \( M \) subdomain and \( N \) intersection boundary:

\[
\sum_{e=1}^{M} \left( \int_{\Omega^{(a)}} \sigma : \text{grad}(\delta u)\,dV - \int_{\Omega^{(a)}} f \cdot (\delta u)\,dV \right)
- \sum_{s=1}^{N} (\delta \int_{\Gamma_{<s>}} \lambda(\tilde{u}^{(a)} - \tilde{u}^{(b)})\,dS) - \int_{\Gamma_{\text{v}}} \hat{t} \cdot \delta u\,dS = 0 \quad \forall \delta u \in V \quad (18)
\]

### 3 Independent Displacement Field and Relative Displacement

1. **3D displacement field.** In the following work is considered three-dimensional displaced field. \( u \in U \) with \( n_{\text{dim}} = 3 \) is considered. Taylor’s expansion of displacement \( u(x) \) is carried out for \( x_p = (x_p, y_p, z_p) \in \Omega^{(e)} \) from point \( \Omega^{(e)} \) arbitrary domain. So that the second-order displacement field in the arbitrary sub-domain \( \Omega^{(e)} \) by matrix form will be:

\[
\begin{align*}
\mathbf{u}^{(e)} &= \mathbf{N}_d^{(e)} \mathbf{d}^{(e)} + \mathbf{N}_e^{(e)} \mathbf{e}^{(e)} + \mathbf{N}_{g_x}^{(e)} \mathbf{\epsilon}^{(e)}_x + \mathbf{N}_{g_y}^{(e)} \mathbf{\epsilon}^{(e)}_y + \mathbf{N}_{g_z}^{(e)} \mathbf{\epsilon}^{(e)}_z \\
\end{align*}
\]

where

\[
\begin{align*}
\mathbf{N}_d^{(e)} &= \begin{bmatrix} 1 & 0 & 0 & 0 & Z & -Y \\ 0 & 1 & 0 & -Z & 0 & X \\ 0 & 0 & 1 & Y & -X & 0 \end{bmatrix}, \\
\mathbf{N}_e^{(e)} &= \begin{bmatrix} x^2 & -Y^2 & -Z^2 & 0 & -Yz & 0 \\ 0 & xY & 0 & 0 & Zx & 0 \\ YX & 0 & Z & 0 & 0 & -X^2 \end{bmatrix}, \\
\mathbf{N}_{g_x}^{(e)} &= \begin{bmatrix} x & 0 & 0 & -Y^2 & 0 & -Z^2 \\ 0 & 0 & ZX & 0 & 0 & x^2 \\ Z & 0 & 0 & 0 & -Y^2 & 0 \end{bmatrix}, \\
\mathbf{N}_{g_y}^{(e)} &= \begin{bmatrix} x^2 & 0 & 0 & Y^2 & 0 & Z^2 \\ 0 & 0 & YZ & 0 & 0 & -X^2 \\ -Y & 0 & 0 & 0 & Y^2 & 0 \end{bmatrix}, \\
\mathbf{N}_{g_z}^{(e)} &= \begin{bmatrix} x^2 & 0 & 0 & -Y^2 & 0 & -Z^2 \\ 0 & 0 & YZ & 0 & 0 & -X^2 \\ -Z & 0 & 0 & 0 & Y^2 & 0 \end{bmatrix}, \\
\mathbf{d} &= [u_p, v_p, w_p, \theta_x, \theta_y, \theta_z]^t, \quad \mathbf{e} = [\mathbf{\epsilon}_x, \mathbf{\epsilon}_y, \mathbf{\epsilon}_z, \mathbf{\gamma}_{xy}, \mathbf{\gamma}_{yz}, \mathbf{\gamma}_{zx}]^t, \\
\mathbf{\epsilon}_x &= [\mathbf{\epsilon}_{x,x}, \mathbf{\epsilon}_{y,x}, \mathbf{\epsilon}_{z,x}, \mathbf{\gamma}_{xy,x}, \mathbf{\gamma}_{yz,x}, \mathbf{\gamma}_{zx,x}]^t, \quad \mathbf{\epsilon}_y = [\mathbf{\epsilon}_{x,y}, \mathbf{\epsilon}_{y,y}, \mathbf{\epsilon}_{z,y}, \mathbf{\gamma}_{xy,y}, \mathbf{\gamma}_{yz,y}, \mathbf{\gamma}_{zx,y}]^t, \\
\mathbf{\epsilon}_z &= [\mathbf{\epsilon}_{x,z}, \mathbf{\epsilon}_{y,z}, \mathbf{\epsilon}_{z,z}, \mathbf{\gamma}_{xy,z}, \mathbf{\gamma}_{yz,z}, \mathbf{\gamma}_{zx,z}]^t, \\
X &= x - x_p, \quad Y = y - y_p, \quad Z = z - z_p
\end{align*}
\]
2. Displacement for Mindlin plate. The Mindlin plate is defining as follows:

\[ \Omega := \{(x, y, z) \in \mathbb{R}^3 | z \in [-t/2, t/2], (x, y) \in A \subseteq \mathbb{R}^2 \} \]  \hspace{1cm} (20)

where \( t \) is plate thickness and \( A \) is plate area.

![Figure 4: Mindlin plate](image)

Since for Mindlin plate we have following assumptions:

\[ \varepsilon_z = \gamma_{yz} = \gamma_{zx} = 0 \]  \hspace{1cm} (21)

we will obtain deflection for mindlin plate as follows:

\[ w = w_p + \theta \mathbf{p} - \frac{1}{2} X^2 \varepsilon_{x,z} - \frac{1}{2} Y^2 \varepsilon_{y,z} - \frac{1}{2} XY \varepsilon_{x,y,z} \]  \hspace{1cm} (22)

And displacement at arbitrary point will be:

\[ \mathbf{u}^{(e)} = Z_M N_{Md}^{(e)} d_M^{(e)} + Z_M N_{Mq}^{(e)} \varepsilon_M^{(e)} \]  \hspace{1cm} (23)

where

\[ Z_M = \begin{bmatrix} -z & 0 & 0 \\ 0 & -z & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad N_{Md}^{(e)} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & Y & -X \end{bmatrix}, \quad N_{Mq}^{(e)} = \begin{bmatrix} -X & 0 & -Y \\ 0 & -Y & -\frac{X}{2} \\ -\frac{X^2}{2} & -\frac{Y^2}{2} & -\frac{XY}{2} \end{bmatrix}, \quad d_M^{(e)} = \begin{bmatrix} w_p \\ \theta_{x}^{p} \\ \theta_{y}^{p} \end{bmatrix}, \quad \varepsilon_M^{(e)} = \begin{bmatrix} \varepsilon_{x,z}^{p} \\ \varepsilon_{y,z}^{p} \\ \varepsilon_{x,y,z}^{p} \end{bmatrix}, \quad \mathbf{u}^{(e)} = \begin{bmatrix} u^{(e)} \\ v^{(e)} \\ w^{(e)} \end{bmatrix} \]

(23) we can write by matrix form:

\[ \mathbf{u}^{(e)} = Z_M N_{Md}^{(e)} U^{(e)} \]  \hspace{1cm} (24)

where

\[ N_{Md}^{(e)} = \begin{bmatrix} N_{Md}^{(e)} & N_{Mq}^{(e)} \end{bmatrix}, \quad U^{(e)} = \begin{bmatrix} d_M^{(e)} & \varepsilon_M^{(e)} \end{bmatrix}^t \]
3. Relative displacement  Now we have to do transformation from global coordinate system to local. The local coordinate system matrix form is follows:

\[ \mathbf{\tilde{u}}(e) = \mathbf{R}^{(e)} \mathbf{u}(e) \]  

(25)

where \( \mathbf{R}^{(e)} \) is:

\[ \mathbf{R}^{(e)} = \begin{bmatrix} l & m & 0 \\ -m & l & 0 \\ 0 & 0 & 1 \end{bmatrix} \]

where

\[ l = \frac{y_{43}}{L}, \quad m = -\frac{x_{43}}{L}, \quad L = \sqrt{x_{43}^2 + y_{43}^2}, \quad x_{ij} = x_i - x_j \]

The relative displacement on the intersection boundary will be:

\[ \delta_{<ab>} = \sum \mathbf{R}^{(e)}_{<ab>} \mathbf{U}^{(e)}_{<ab>} \]  

(26)

and the matrix form for relative displacement is:

\[ \delta_{<ab>} = \mathbf{Z}_M \mathbf{B}_{<ab>} \mathbf{U}_{<ab>} \]  

(27)

where

\[ \mathbf{B}^{(e)}_{<ab>} = \left[ \mathbf{R}^{(a)}_{<ab>} \mathbf{N}^{(a)}_{<ab>} \mathbf{R}^{(b)}_{<ab>} \mathbf{N}^{(b)}_{<ab}> \right], \quad \mathbf{U}_{<ab>} = [\mathbf{U}^{(a)}_{<ab>} \mathbf{U}^{(b)}_{<ab>}] \]

4. Discretization for HPM

1. Lagrange multiplier and penalty function. Physical meaning of the Lagrange multiplier \( \lambda \) is equal to the surface force on the intersection boundary. Generally, in a hybrid-type variational principle, this multiplier is dealt with as an unknown parameter. Since it has the meaning that Lagrange multiplier \( \lambda \) is the surface force on the boundary \( \Gamma_{<ab>} \) in sub-domain \( \Omega^{(a)} \) and \( \Omega^{(b)} \), the surface force is defined as follows:

\[ \lambda_{<ab>} = k \cdot \delta_{<ab>} \]  

(28)

Here \( \delta_{<ab>} \) shows relative displacement on the sub-domain boundary \( \Gamma_{<ab>} \), and it is shown in three dimensional problem (also plate bending problem) as follows:

\[ \begin{bmatrix} \lambda_{n<ab>} \\ \lambda_{sx<ab>} \\ \lambda_{sy<ab>} \end{bmatrix} = \begin{bmatrix} k_n & 0 & 0 \\ 0 & k_{sx} & 0 \\ 0 & 0 & k_{sy} \end{bmatrix} \begin{bmatrix} \delta_{n<ab>} \\ \delta_{sx<ab>} \\ \delta_{sy<ab>} \end{bmatrix} \]  

(29)

where

\[ k_n = k_{sx} = k_{sy} = p \]

where \( p \) is a penalty function.

2. Discretization for subsidiary condition The (16) expression we can write by following way:
\[ H_{<ab>} = -\delta \int_{\Gamma_{<ab>}} \lambda^t_{<ab>} (u_{<ab>}^{(a)} - u_{<ab>}^{(b)}) d\Gamma \]
\[ = -\delta \int_{\Gamma_{<ab>}} \delta^t_{<ab>} k_{<ab>} \delta_{<ab>} d\Gamma \]
\[ = -\delta U_{<ab>}^{(a)} \int_{\Gamma_{xy<ab>}} B^t_{<ab>} \tilde{k}_{<ab>} B_{<ab>} d\Gamma_{xy} U_{<ab>} \]

where \( U_{<ab>} = M_{<ab>} U \)

here \( M \) is a matrix which relates the total degree of freedom and the degree of freedom of each sub-domain. It is similar for virtual displacement:

\[ \delta U_{<ab>} = M_{<ab>} \delta U \]

Then we obtain following equation:

\[ H_{<ab>} = -\delta U^t K_{<s>} U \] (31)

where

\[ K_{<s>} = M_{<s>}^t \int_{\Gamma_{xy<ab>}} B^t_{<s>} \tilde{k}_{<s>} B_{<s>} d\Gamma_{xy} M_{<s>} \]

where

\[ \tilde{k}_{<s>} = \int_{-t/2}^{t/2} Z^t M k Z M dZ = \begin{bmatrix} \frac{t^3}{12} k_n & 0 & 0 \\ 0 & \frac{t^3}{12} k_{sx} & 0 \\ 0 & 0 & tk_{sy} \end{bmatrix} \]

3. Discretization virtual work equation for each sub-domain. For Mindlin plate theory a reduced form of the constitutive relations is obtained by making \( \sigma_z = 0 \) and subsequently eliminating \( \varepsilon_z \). Strains in Mindlin plate are:

\[ \varepsilon_x = \frac{\partial u}{\partial x} = -z \frac{\partial^2 w}{\partial x^2}, \quad \varepsilon_y = \frac{\partial v}{\partial y} = -z \frac{\partial^2 w}{\partial y^2}, \]
\[ \gamma_{xy} = \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} = -2z \frac{\partial^2 w}{\partial x \partial y}, \quad \gamma_{xz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} = 0, \quad \gamma_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} = 0 \] (32)

After application of Mindlin plate strains we obtain \( \tilde{D} \) matrix for an elastic isotropic material:

\[ \tilde{D} = \frac{E}{1-\nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix} \] (33)

Next is bringing strain vector into the matrix using displacement field.

\[ \tilde{\varepsilon}^{(e)} = L u^{(e)} = \tilde{Z} B^{(e)} U^{(e)} \] (34)

where

\[ B^{(e)} = L N^{(e)} \]

we will have:

\[ \int_{\Omega^{(e)}} [L \delta u]^t \sigma d\Omega = \int_{\Omega^{(e)}} \delta \tilde{\varepsilon}^{(e)} \tilde{D}^{(e)} \tilde{\varepsilon}^{(e)} d\Omega = (\delta U^{(e)})^t \int_{\Omega^{(e)}} B^{(e)\top} k^{(e)} B^{(e)} d\Omega_{xy} U^{(e)} \]

(35)
We have:
\[ U^{(e)} = A^{(e)} U, \quad \delta U^{(e)} = A^{(e)} \delta U \]
Taking into account we will obtain:
\[ \int_{\Omega^{(e)}} [L \delta u]^t \sigma d\Omega = \delta U K^{(e)} U \]  
(36)
here \( A \) is a matrix which relates the total degree of freedom and the degree of freedom of each sub-domain.

\[ K^{(e)} = \int_{\Omega^{(e)}_{xy}} B^{(e)} k^{(e)} B^{(e)} d\Omega_{xy} \]
here
\[ k^{(e)} = \int_{-t/2}^{t/2} Z^t \bar{D}^{(e)} Z dZ = \frac{t^3}{12 (1-\nu^2)} \left[ \begin{array}{ccc}
1 & \nu & 0 \\
\nu & 1 & 0 \\
0 & 0 & \frac{1-\nu}{2}
\end{array} \right] \]  
(37)
The body and surface force discretization is given below:
\[ \int_{\Omega^{(e)}} \delta u^t f d\Omega + \int_{\Gamma^{(e)}} \delta u^t T d\Gamma = \delta U^t P^{(e)} \]  
(38)
where
\[ P^{(e)} = (A^{(e)})^t \int_{\Omega^{(e)}} (N^{(e)})^t Z_M f d\Omega + \int_{\Gamma^{(e)}} (N^{(e)})^t Z_M T d\Gamma \]
Finally we obtain following discretized equation:
\[ \delta U^t \left( \sum K^{(e)} + \sum K_{<s>} \right) U - \delta U^t \left( \sum P^{(e)} \right) = 0 \]  
(39)
The (39) equation we can write by the (40) form, because \( \delta U \) is arbitrary:
\[ KU = P \]  
(40)
where
\[ K = \sum K^{(e)} + \sum K_{<s>}, \quad P = \sum P^{(e)} \]
The discretization equation of this model becomes a simultaneous linear equation shown in equation (40). Left coefficient matrix \( K \) consists of stiffness in the sub-domain and subsidiary condition on the intersection boundary for the adjacent sub-domain. The discontinuous phenomenon of hinge etc. can be expressed without changing degree of freedom by changing the value of \( k \) of equation (28) to zero.

5 Numerical Example
As a numerical example we present some simple problems. At first is given cantilever beam with concentrated load. The beam has following material properties and geometrical properties: Young’s Modulus = 1x10^6 kN/m^2, Poisson’s ratio = 0,
Length=4m, width=1m and thickness=0.1m, line-load=1kN/m.
For this case are obtained deflection and moments by exact treatment and by HPM.
In the figure 5 is given comparision between exact solution and numerical solution
by HPM. And as shown in figure 5 the numerical solution for moments exactly equal
to the analytically solution. Also as shown in figure 6 high accuracy deflection can
be obtained.

![Figure 5: Moments](image)

![Figure 6: Ratio of deflections by exact and HPM](image)

Has done also calculations for both-end fixed beam with uniform distributed
load. The beam has the same characteristics as in cantilever beam, only uniform-
distributed-load=1kN/m$^2$. As for cantilever beam case here also given comparison
between exact treatment and HPM results. Results for this case have given by the figures 7 and 8. Here also for moment analytical and numerical solutions are equal.

The next example is simple supported plate with concentrated load. Plate material and geometrical properties are following:
Young’s Modulus = $1\times10^6$ kN/m$^2$,
Poison’s ratio = 0,
length = 4m,
width = 4m,
thickness = 0.1m,
concentrated-load=4kN.
In figure 9 and 10 given results obtained for this case.
Here we obtain high accuracy between exact and HPM results for moment calculations, but not exactly the same solutions.

![Figure 9: Moments](image)

The last example is again simple-supported plate, but with uniform distributed force, which is equal 1kN/m². Material and geometrical characteristics are the similar with previews example. Results for this case are given in figures 11 and 12.

![Figure 10: Ratio of deflections by exact and HPM](image)
Discrete Limit Analysis for Plate Bending Problems by Using Hybrid-type Penalty Method

6 Discrete Limit Analysis

1. Constitutive Law. In case of plate bending problems yield function has following forms:

$$f(M) = \left( \frac{M_n}{M_{pn}} \right)^2 - 1$$  \hspace{1cm} (41)

It’s assumed that the plastic hinge will occur if the bending moment on intersection boundary will be zero:

$$f(M_n) = 0$$
For this case we can obtain incremental bending moment:

$$\Delta M_n = k^{ep} \Delta \delta$$  \hspace{1cm} (42)

where $\Delta \delta$ is the relative displacement and

$$k^{ep} = \left(k^e - k^e \frac{\partial f}{\partial \lambda} \frac{\partial k^e}{\partial \lambda} \frac{\partial Q}{\partial \lambda} \right)$$ \hspace{1cm} (43)

2. Load Incremental Method. Load at the (i+1)-th step can be calculated by using the load at the i-th step:

$$P^{(i+1)} = (1 - r_i)P^{(i)}$$ \hspace{1cm} (44)

where $r_i$ is a rate of load increment. Which we can calculate using this equation:

$$f(M_n + r\Delta M_n) = 0$$ \hspace{1cm} (45)

After solving following equation:

$$\left( \frac{M_n + r\Delta M_n}{M_{pn}} \right)^2 - 1 = 0$$

we will obtain $r$:

$$r = \frac{M_{pn} - M_n}{\Delta M_n}$$ \hspace{1cm} (46)

In case of bending moment residual load at the n-th step will be:

$$P^{(n)} = \prod_{i=0}^{n-1} [(1 - r_i)]P$$ \hspace{1cm} (47)

Cumulative rate of load increment:

$$r_{TOTAL} = \sum_{k=1}^{n} \left( \prod_{i=0}^{k-1} [(1 - r_i)] \right) r_k$$ \hspace{1cm} (48)

When $r_{TOTAL} = 1$ iteration is finish.

7 Numerical Example for Discrete Limit Analysis

In case of Discrete-Limit Analysis has done numerical calculations when we have simple supported plate with distributed load. The plate has following geometrical and material properties:

Young’s Modulus = 1x10^6 kN/m^2, Poison’s ratio = 0, Yield Moment: $M_{pn} = 0.1$ Nm,

Length=2m, width=2m and thickness=0.1m,

Distributed Load=1kN/m^2.
As a result of calculations has obtained Load-Displacement curve, which has compared with exact solution and as we can see above in the graph numerical and exact solutions are the same:

Also has done comparison between numerical, analytical and experimental results and we can see bellow for two cases obtained the same results:

Next example is again simple supported plate with same properties, only now applied concentrated load, which is equal 4kN. For this case also has done the same calculations and the same comparisons and in this case also theoretical, experimental and numerical results are congruent. Below given Load-Displacement curve obtained
analytically and numerically. Next is given Hinge Lines obtained analytically and numerically.

Figure 15: Load-Displacement Curve Ratio of deflections by exact and HPM

Figure 16: Theoretical and Numerical Hinge-lines
Conclusions

In this paper proposed new approach for solving plate bending problem by using HPM. After comparison of analytical solution and HPM results for deflection and bending moment in case of several examples we can see that we have high accuracy between them. As a result we can conclude that HPM corresponds to all requirements for solving problems such as plate bending.

References


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Modeling coupled interaction between crack growth, stress-assist diffusion and chemical reactions

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Abstract

The model is suggested to describe the oxidation zone formation in front of a crack and the interconnection between the zone and the crack growth in a polycrystalline silicon film. The simplest realization of the model within the framework of Barenblatt-Dugdale cohesive zone approach is suggested. The crack growth description is based on the critical crack opening criterion. It is shown that the crack will not grow until the oxide size reach a certain value. Then the crack begins to grow and reaches the oxide boundary after some time. If there is a gap between critical crack opening values in polysilicon and silicon-oxide then the further crack growth rate is determined by the velocity of the chemical reaction front until the critical crack opening for polysilicon is reached.

1 Statement of the problem.

It is known that micron-scale polycrystalline silicon thin films as used in microelectromechanical systems (MEMS) can fail in cyclic fatigue in ambient atmospheres [1, 2, 3, 4]. Studies by the authors have established that the mechanisms associated with such fatigue failures involves sequential oxidation and environmentally-assisted crack grows solely within SiO$_2$ layer (Fig.1).

In the present paper we consider a polycrystalline silicon film with a small crack and present a model directed to the description of crack growth due to the oxidation of silicon. Following Muhlstein et al we divide a body into three zones: we divide a body into three zones: a fracture zone (a crack itself), a diffusion (transport) zone of oxide trough which chemically active components are delivered, and a chemical reactions zone near the interface between polysilicon Si and silicon-oxide SiO$_2$. We suppose that chemical reactions are localized at the chemical reactions front.
Modeling coupled interaction between crack growth, stress-assist diffusion and chemical reactions

The growing oxide area represents a transport zone for an oxidant. Recent experiments (see [5] and reference therein) have shown that oxidizing species which diffuse through the oxide to the boundary with polysilicon may be different, in dependence on temperature and atmosphere in which the oxide growth happens (for example, $O_2$ or $H_2O$ atmosphere, room or high temperature). In one case the diffusion of molecular oxygen $O_2$ is a limiting process. In other cases oxidizing species may be ions $O^-$ or radicals $OH$ (ions $OH^-$) which, on one hand are much more mobile than $O_2$, and, on the other hand, can suffer recombination processes in the transport zone on the way to the chemical reaction front.

Further consider a straight line crack in a thin specimen. A plastic zone near the crack tip is represented by the Dugdale model [6]. Note that polycristaline silicon is much more plastic material then silicon monocrystals. We assume that chemical reactions and diffusion are also localized in a thin layer in front of crack. The motivation is a chemical activity increase of a plastically deformed material.

As a result the diffusion problems becomes a one-dimension problem. The diffusion equation takes the form

$$\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} - q c^\alpha, \quad J = -\beta c \frac{\partial \mu}{\partial x} \quad (1)$$

where $c$ is the partial molar concentration of oxidizing species, $J$ is the flux, $\mu$ is a chemical potential, $\beta$ is the molar mobility, the term $q c^\alpha$ represents the loss reaction (recombination) of oxidizing component ($\alpha$ is the order of the bulk recombination, $q$ is the rate coefficient of the recombination).

We assume that the oxidizing component concentration is given at the external oxide surface and coincides with the concentration at the crack tip, i.e.

$$c = c_0 \quad \text{at} \quad x = l(t) \quad (2)$$

The oxidizing component concentration on the interface $x = x_s(t)$ between $SiO_2$ and $Si$ is controlled by the balance of the diffusion influx and the “deflux” due to
oxidation reaction. The last is accepted to be proportional to the concentration. Then neglecting recombination processes we have
\[ \beta c \frac{\partial \mu}{\partial x} = -k c \text{ at } x = x_*(t) \quad (3) \]
where \( k \) is a parameter of the reaction.

The velocity \( V \) of the chemical reactions front is determined by the mass balance
\[ \beta c \frac{\partial \mu}{\partial x} |_{x_*} = -n V g \quad (4) \]
where \( g \) is the concentration of soluble components, i.e. the concentration of Si which participates in the reaction equal to the concentration of \( \text{SiO}_2 \). Note that silica formation first of all takes place in the inter-crystallite space. The multiplier \( n \) equal to the number of oxidizing units for forming one \( \text{SiO}_2 \) units. In a case of the oxidation by radicals \( \text{OH} \) or ions \( \text{OH}^- \) \( n = 2 \).

In the steady-state approximation
\[ \frac{\partial c}{\partial t} = -\dot{l} \frac{\partial c}{\partial x} \equiv -\dot{l} \frac{\partial c}{\partial \xi}, \quad \xi = x - l \quad (5) \]
where \( l = l(t) \) is the crack length, \( \dot{l} \) is the crack growth rate.

If the problem \((1)-(5)\) is solved, given \( l \), we know the lengths \( \xi_* = x_* - l \) of the oxide zone.

Since the oxide formation is accompanied by the volume increase, the oxide zone is under the action of compression acting from the side of a surrounding material. This compression is proportional to \( g \) and volume mismatch of \( \text{Si} \) and \( \text{SiO}_2 \). On the other hand oxide formation produces tension stresses in front of the diffusion zone. We do not have experimental evidence of crack initiation in front of oxide zone. This motivates that oxide induced stresses relax in front of the oxide zone because of plastic deformations.

To complete the statement we have to formulate the fracture criterium. Various local fracture criterions, including the entropy criterion and energy balance/release criteria can be examined, the demonstration given below is based on widely used critical crack opening criterion \([6]\).

2 Results

To simplify the consideration we assume that the stress on the oxide segment is a known constant \( t_* \) in the absence of external stress. This means that we relate these stresses only with the concentration of the oxide and do not discuss how elasticity moduli changes due to chemical reactions effect the stress state. The distribution of the oxidant concentration \( c(\xi) \) effects only the size \( \xi_* \) of the oxide zone.

The next simplification is related with the chemical potential. One of the opportunities would be to take \( \mu \) as the trace of the partial Eshelby stress tensor. Suspending this opportunity, we accept now Fick’s first law of diffusion:
\[ J = -D \frac{\partial c}{\partial x} \]
where $D$ is the diffusion coefficient. Then the problem (1)–(5) takes the form

$$D \frac{\partial^2 c}{\partial \xi^2} - qc^\alpha = -l \frac{\partial c}{\partial \xi}, \quad \xi \in [0, \xi_*]$$

(6)

$$c = c_0 \quad \text{at} \quad \xi = 0, \quad D \frac{\partial c}{\partial \xi} = -kc \quad \text{at} \quad \xi = \xi_*$$

$$-D \frac{\partial c}{\partial \xi}|_{\xi_*} = kc|_{\xi_*} = nVg$$

![Figure 2: A crack with oxide and plastic zones in Barenblatt-Dugdale model](image)

To calculate stresses and the crack opening we use Barenblatt-Dugdale cohesive zone model (Fig. 2). In the case of a crack $(-l, l)$ under external uniform tension $\sigma_0$ the stress is calculated as the superposition of uniform tension $\sigma_0$ and stresses in a body with a crack $x \in (-l - a, l + a)$ loaded at $y = 0, x \in (-l - a, l + a)$ by normal stress $-p(x)$,

$$p(x) = \begin{cases} 
\sigma_0, & x \in (-l, 1), \\
\sigma_0 + t_*, & |x| \in (1, 1 + \xi_*), \\
\sigma_0 - \sigma_s, & |x| \in (1 + \xi_*, l + a)
\end{cases}$$

(7)

where $\sigma_s$ is the yield limit of polysilicon, $\pm (l + a)$ are coordinates of the plastic zones ends. The size $a$ depends on $l$ and $\xi_*$. The dependence is to be found from the condition that stress is not infinite (stress intensity factor for the segment $x \in (-l - a, l + a)$ equals zero), $\xi_*$ is found from the solution of (6).

The crack growth description is based on the critical crack opening criterion. The opening $\delta(x) = 2v(x), x \in (-l + a), l + a)$, where $v$ is a vertical displacement, is given by known formulae. We assume that

$$\delta(x = l) = \delta_c$$

(8)

where $\delta_c$ is a critical opening for silicon-oxide $\text{SiO}_2$. We also believe in the fact that $\delta_c < \delta^c$ where $\delta^c$ is the fracture parameter for polysilicon $\text{Si}$. Note that oxide layer is
compressed by stresses induced by chemical reactions. Then the crack propagation
in oxide is a result of competition between external and internal stresses.

The stress non-singularity condition

\[
\int_{-(l+a)}^{l+a} p(x) \sqrt{\frac{l + a + x}{l + a - x}} \, dx = 0
\]

(9)

with \(p(x)\) given by (7) takes the form of the equation

\[
\psi(l, a|\xi_*, \sigma_0) = 0
\]

(10)

where \(\sigma_0\) is given by boundary conditions, and \(\xi_*\) can be considered as a time parameter. The dependence of \(\xi_*\) on time is found independently from the solution of the diffusion problem (6)

The criterion (8) takes the form of the equation

\[
\delta(l|l + a, \xi_*, \sigma_0) = \delta_c
\]

(11)

The solution of the system of two equations (10) and (11) gives the dependencies \(l(x_*)\) and \(a(x_*)\) where the position \(x_*\) of the chemical reaction front act as time.

![Figure 3: Crack opening \(\delta(x = l_0)\) in dependence on the oxide zone size at various crack lengths \(l_0\). Given \(\delta_c\) and \(l_0\), the incubation time corresponds to \(\xi_*\) at which the dotted line crosses the solid line.](image1)

![Figure 4: The oxide and plastic zones growth during the incubation period](image2)

The model predicts that the crack will not grow until the oxide size reach a
certain value. Indeed, Fig.3 represents the dependencies of the opening \(\delta(x = l_0)\) at
the crack tip on the size of the diffusion zone \(\xi_*\) at various initial crack lengths \(l_0\).
One can see that incubation time \(t_{in}\) must pass before crack starts if \(\delta(x = l_0) < \delta_c\).
Oxide size must reach a value such that the opening at \(x = l_0\) will reach the critical
value \(\delta_c\). Fig.4 represents the moving of the oxide boundary \(x_*(t) = l_0 + \xi_*(t)\) and
the plastic deformations front \(l_0 + a(t)\) during the incubation period.

Fig.5 represent the dependencies of of the crack length and plastic deformation
front on \(x_*\). The point \(A\) corresponds to \(x_* = x_*^{in}\) at \(t = t_{in}\). The critical state (poin
Modeling coupled interaction between crack growth, stress-assist diffusion and chemical reactions

![Figure 5: Crack and plastic zone growth due to the oxidation process](image)

B) corresponds to \( l = x_\ast \) when the line of the solution \( l = l(x_\ast) \) crosses the straight line \( l = x_\ast \). Then \( \delta(x = l) > \delta_c \) if the crack grows. If there is a gap between \( \delta_c \) and \( \delta^0_c > \delta_c \) then the crack growth rate is determined by the velocity \( V \) of the chemical reaction front until the final instability moment \( \delta(x = l) = \delta^0_c \).

The above calculations are made at the following relationships between stresses:
\[
t_\ast = \sigma_s / 4, \quad \sigma_0 = \sigma_2 / 2.
\]

3 Concluding remarks

Note that the diffusion and stress problems are uncouple unless the dependencies of chemical potential and parameters of (1) on stress/strain are taken into account. This may be a reason to return to more general equations (1)–(4).

We also understand that chemical reactions and diffusion are localized in intergranular layers. In fact, we have the oxidant diffusion with respect to deformed skeleton made of the mix of silica oxide and polysilicon that did not participate in the reactions. The effective diffusion coefficient depends on the skeleton structure and deformation.

Addition chemical reactions in the oxide zone will give a distribution of \( \text{SiO}_2 \) concentration. In particular, this will affect the stress distribution in the oxide zone.

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Prediction of the Mechanical Behavior of Collagen Fibrils

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Abstract

The aim of this paper is to apply a new constitutive equation based on macromolecular theories of rubber elasticity to predict experimental data from collagen fibrils. The new model is based on two material parameters that have full physical meaning. The prediction of the provided experimental data from the literature was fitted accurately enough with the proposed model.

1 Introduction

Collagen is a triple helix formed by three extended protein chains that wrap around one another. The Mechanical response of these molecules is similar to rubber hyperelastic materials. Many rodlike collagen molecules are cross-linked together are cross-linked together self-assemble in the extracellular space to form unextendable collagen fibrils. of the collagen fibril is caused by the repeating arrangement of the collagen molecules within the fibril. The architecture of these molecules is similar with the rubber hyperelastic materials. Collagen fibrils are evolutionary molecular assemblies of collagen molecules, brought together by covalent bonds. Actually, ninety per cent of the driving energy for this assembly of collagen molecules comes from hydrogen bonding of water associated with hydrophobic domains on the collagen molecules. Covalent bonds play a role in stabilizing the assembled structure. The collagen fibrils are extremely slender with lengths ranging from one to several hundred nanometers while diameters stay within the nanometer scale. Biological materials are virtually often composites utilizing different proportions of the basic components and a variety of hierarchical structural architectures. While microscopic studies reveal biological composites including as many as few distinct substructures, such as protein interlayers, fibrils, fibers and lamella etc [1]. The influence of these small features in their mechanical properties is not well understood. The influence of these small features in their mechanical properties is not well understood. This
lack is reflected in the limited knowledge of the mechanics under nanoscale confinement, leading to the routine use of bulk properties. The meso-scopic character of the relevant processes in organic nano-materials cannot be simulated adequately by conventional atomistic or continuum techniques a multiscale modeling approach should be adopted. Laser tweezers and atomic force microscopy are used to probe structures at the molecular scale; an experimental gap exists between these smallest length scales and the micron and larger scales.

The scope of this paper is to demonstrate, by using published stress-strain response of a single collagen fibril that previously proposed mathematical model for rubber materials fits the data equally well. The proposed model is based on two materials parameters that have full physical meaning presenting the shear modulus of elasticity and the maximum extensibility of chain. Its application to simple tension data from collagen is remarkable and can be used for other modes of deformations as well.

2 Theoretical background

A new approach has been proposed [2] for the development of a constitutive equation that is appropriate for rubber materials. This new constitutive equation is based on the concepts of statistical mechanics, thermodynamics and rubber elasticity [3]. The partition function for a random walk of the chain of macromolecules can be written as a function of the Langevin function and the Helmotz free energy was estimated. The strain energy function, which expresses the Helmotz free energy per unit volume, was expressed as a function of the maximum extensibility of the chain. The proposed model was based only on two physical parameters of the macromolecule, which are the shear modulus of the material and the maximum extensibility of the chain. Is was proved that the engineering stress is equal to:

\[
s = D \left( G; l_M \right) \left[ \frac{1}{1 - \frac{3}{5} \left( \frac{1}{l_M} \right)^2 - \frac{1}{5} \left( \frac{1}{l_M} \right)^4 - \frac{1}{5} \left( \frac{1}{l_M} \right)^6} - \frac{1/2}{1 - \frac{3}{5} \left( \frac{1}{l_M} \right)^2 - \frac{1}{5} \left( \frac{1}{l_M} \right)^4 - \frac{1}{5} \left( \frac{1}{l_M} \right)^6} \right] \]  

(1)

where the function \( D \left( G; l_M \right) \) has the form:

\[
D \left( G; l_M \right) = \frac{G \left( 1 - \frac{3}{5 l_M^2} - \frac{1}{5 l_M^4} - \frac{1}{5 l_M^6} \right)^2}{\left( 1 + \frac{1}{5 l_M^2} + \frac{2}{5 l_M^4} \right)}.
\]  

(2)

The parameters \( G \) and \( l_M \) define the shear modulus of the material and the maximum extensibility of the chain, that must be determined by non-linear fitting with the experimental data from uniaxial tension experiments in collagen fibrils material. The left hand side of equation (1) defines the engineering stress, which by multiplication with the principal stretch \( l \), is converted to true stress. For more details for the proposed model one can consult reference [2]. Since the behavior of
collagen fibril materials is like rubber solids, one can apply this constitutive equation for the prediction of the stress-strain response of this type of materials too.

3 Comparison of published experimental data and with the proposed theoretical model

The testing materials are single type I collagen fibrils isolated from the sea cucumber [4]. This nanoscale structures are several dozen microns long and have cross-sectional dimensions 10-500 nm. The employed labeling technique provided staining along the fibril axis, which should allow for intrinsic strain measurements. In this experiment three collagen fibrils are measured via SEM (UIUC). The device displacement is measured using an integrated Venier scale, labeled V, with 0.25 mm resolution. Figures 1-4 show the fitting process of the true stress vs. stretch of the experimental points from the experimental tested collagen fibrils material under simple tensile loading. The black square points represent the experimental data, the red line the fitting of the data with the proposed constitutive equation, based on the maximum extensibility of the chain. The continuum black line shows the fitting process with respect to Xu-Aifantis model based on the logarithmic strain approach [5].

![Graph showing comparison of data and models](image)

Figure 1: (Sample A)

The model based on the maximum extensibility of the chain predicts the data well with only two parameters that are listed in each plot. The parameters were estimated using a typical non-linear fitting process. All the experimental data were fitted well up to break. Both unknown parameters can also be determined, just by looking the graph even without fitting them. The determined Young's modulus calculated by fitting is in the range of values that is determined experimentally too [4], [6]. The prediction of the stress-strain response, of the experimental data by
Xu-Aifantis theory, was on logarithmic strain, while here the data were plotting on the direct principal stretch of the macromolecules.

4 Conclusions

Using the proposed model for fitting the uniaxial tension experimental data from collagen fibrils one can conclude that: (1) the model fits the data well up to break with a nonlinear fitting procedure; (2) for low strain the prediction is accurate enough so that the prediction of the shear modulus is almost exact; (3) assuming that the collagen fibrils behave as a rubber material the modulus of elasticity can be computed from dividing the derived shear modulus by three.
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Investigation of dynamic processes in vibration machine with unbalanced vibro-exciters and asynchronous electric motor

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Abstract

The results of simulation of the process of acceleration and stationary regime of motion of vibrating machine with unbalanced vibro-exciter put in rotation by three-phase asynchronous motor with the use of dynamic and static characteristics are presented.

1 Posing the problem

Oscillations in many vibration machines and devices are exited by power-driven unbalanced vibro-exciters which are set into rotation by electric motors of asynchronous type. Vibration machines with inertial excitation are, as a rule, transresonance ones. Consequently, intensive resonant oscillations arise during the coincidence of natural and forced frequencies in the proceses of acceleration and deceleration in vibration machines with unbalanced exciters. The amplitudes of these oscillations greatly exceed the ones of the stationary regime of motion. Dynamic loads on the members of vibrating machine structure grow up correspondingly. Besides, it is necessary to sufficiently increase the power of electric motor for the transition of resonance zone by its rotor.

Motors of existing vibration machines usually are of limited power and therefore, may be referred to imperfect sources of energy. Hence, an interaction of oscillatory movements of vibrating body and rotational motion of electric motor rotor may take place.

Machines with electric drive should be considered as electromechanical systems. To investigate their dynamics it is methodically correct to use Lagrangian-Maxwell’s equations of motion of mechanical part or the system and bound up to them equations of electrical part. However, by reason of complicacy of mathematical models and the problem of determination of coefficients of its nonlinear differential equations, static characteristics of engine is mostly used for the investigation of machine
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dynamics [1-3]. In this case only the maker’s data sheet of electric motor is needed for the realization of the model. They usually recommend to neglect transient processes and use static characteristics [1-3]. Moreover, linear model of motor static characteristic is used most often [3, 4]. At the same time more complicated models are recommended in some works, [5, 6] for example, to investigate the processes of acceleration deceleration and even steady-state motion in case of oscillatory load.

2 Analysis of the latest investigations and publications

Fundamental theoretical investigations of vibratory systems with account of their interaction with imperfect power source are presented in the works of V.O. Kononenko and his followers [1]. Most complete bibliographic data concerning investigations in this direction, covering the corresponding period are presented in the work [7,8] and in the reference book [9]. The works [4, 10] present the results of numerical simulation of the problem of acceleration of unbalanced rotor installed on elastically fixed platform with one degree of freedom. The most notable among the latest investigations is article [11] where the problem of unbalanced rotor motion at passing over the resonance zone is solved by method of direct separation of motions. Nevertheless the need of more detailed analysis of dynamic processes taking place at passing over the resonance zone by rotor of unbalanced vibro-excitor still remains.

The object of the work

is a comparative analysis of the processes of acceleration and steady-state regime of motion of transresonance vibration machine with unbalanced drive for the cases of use of both static and dynamic characteristics of three-phase asynchronous engine. The scheme of the vibratory system under consideration is given in Fig. 1. Vibrating body is connected to the fixed base by means of elastic and damping elements and may shift with respect to the fixed base along some fixed direction Ox. Unbalanced vibro-excitator activated by three-phase asynchronous engine is installed on the vibration body. Let the unbalanced mass of the vibro-excitator rotate in horizontal plane. Generalized coordinates of the system under consideration are angle of rotation of the vibro-excitator rotor \( \phi \) and horizontal shift of the vibrating body \( x \). Resistance to oscillation of vibration body is taken into account in the form of linear force \( \beta \ddot{x} \).

The motion of such vibratory system is described by equations [1-3].

\[
I\ddot{\phi} = L - R + m\varepsilon \ddot{x}\sin\phi \tag{1}
\]

\[
M\ddot{x} + \beta_x \dot{x} + c_x x = m\varepsilon (\ddot{\phi}\sin(\phi) + \dot{\phi}^2\cos(\phi)) \tag{2}
\]

where \( I \) is a moment of rotor inertia; \( m, \varepsilon \) are, correspondingly, the mass of the vibro-excitator and its eccentricity; \( M \) is the mass of vibrating body; \( \beta_x \) is the damping factor; \( c_x \) is the longitudinal rigidity of the spring; \( L, R \) are correspondingly, the electromagnetic moment of engine and the moment of resistant to motion forces.
Hence, the system under consideration belongs to the class of dynamic systems for the investigation of steady-state and unsteady oscillations of which static characteristic of the electric motor may be taken as \( L \).

Such assumption is quite justified, inasmuch the period of acceleration (deceleration) during which Sommerfeld’s effect manifests itself is the most interesting and thoroughly investigated for vibration machines with unbalanced drive. The velocity of rotor acceleration grows slowly during this time period, that is \( \frac{\partial \phi}{\partial t} \) does not change much during the period of oscillations. So, we have to do with motion regime which is close to steady-state one. We used the linear model of static characteristic. Function \( L \) in the working section is approximated by a straight line through points \((\omega_n, L_n)\) and \((\omega_s, 0)\) where \( \omega_s, \omega_n \) are synchronous and nominal angular velocities of the engine, \( L_n \) is a nominal moment of the engine. On the other hand, an approach based on joint solution of differential equations of the motion of mechanical part of the system (1), (2), and the equation of electromagnetic conditions in asynchronous motor [6, 12],

\[
T_D^2 \ddot{\xi} \ddot{L} + T_D \ddot{\xi}(2 - \frac{T_D}{s} \dot{s}) \ddot{L} + (1 - \frac{T_D}{s} \dot{s})L = 2\xi L_{max} s_r \tag{3}
\]

where \( T_D = \frac{1}{100 \pi \text{cr}} \) is electromagnetic time constant; \( \xi = \frac{1}{1+\text{cr}} \); \( s_r = \frac{\omega_s - \dot{\phi}}{\omega_s} \) is slip ratio; \( s = \omega_s - \dot{\phi} \) is running slip; \( s_{cr} = \frac{s_n + \sqrt{s_n^2 - \lambda_{cr}}}{1 + \sqrt{1/s_n}} \) is critical slip; \( s_n = \frac{\omega_s - \omega_n}{\omega_s} \) is nominal slip; \( A = \lambda_n (\lambda_{max} - \lambda_n), \lambda_n = \frac{L_A}{L_n}, \lambda_{max} = \frac{L_{max}}{L_n}, L_{max}, L_s \) are maximal and starting torques of the engine.

The moment of forces resistant to rotation is brought about mainly by resistance in bearings and is determined by formula \( R = R(\dot{\phi}) = 0,5 f^* m \varepsilon \dot{\phi}^2 d \), where \( f^* \) is a friction coefficient in the bearing and \( d \) is its internal diameter.

Simulation of the process of acceleration of unbalanced vibro-exciter is reduced to numerical integration of differential equations of the motion of mechanical part of the system (1), (2), (3) by means of Maple program product at the following parameter values: \( m = 4\text{kg}; \varepsilon = 0,037\text{m}; I = 0,006\text{kg/m}^2; M = 39\text{kg}; c_s = 4,5 \cdot 10^4\text{N/m}; f^* = 0,003; d = 0,02\text{m}; \beta_x = 135\text{kg/s}; p = 33,9\text{s}^{-1} \) - frequency of system own oscillations. Three-phase asynchronous short circuited motors A4 with synchronous
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Figure 2: Time dependences of rotor angular velocity for the period of acceleration (a) and steady-state regime (b) in case of using: 1 - static characteristic of the engine; 2 - equation of electromagnetic conditions in the engine

frequency of rotation \( n_s = 1500 \text{rot/min} \) and nominal powers \( N = 0.09 \text{kw} \) and \( N = 0.12 \text{kw} \) were used.

Results of the investigation

It is determined that minimal power of engine at which its acceleration and operation in steady-state regime is possible makes \( N = 0.09 \text{kw} \) both in case of simulation by means of static characteristic of asynchronous motor (second variant). It should be noted that if nominal power of engine would acquire any values in the range of standard electric motors power \( N = 0.09 - 0.06 \text{kw} \) its starting with further reaching the regime of rotation with angular velocity close to nominal one would be possible at \( N = 0.075 \text{kw} \) in the first and at \( N = 0.074 \text{kw} \) in the second variant. So, both investigated variants give rather close results.

Fig. 2 shows time dependences of rotor angular velocity of vibro-exiter. Comparison of two graphs testifies to qualitatively similar reproduction of the process of rotor acceleration in both investigated cases.

According to presented graphs, both curves practically coincide in the first stage of acceleration - from the moment of engine starting to reaching by rotor angular velocity equal to critical one in the case under consideration \( \omega_{cr} = 100.08 \text{s}^{-1} \). There are small divergences in the second stage of rotor acceleration (from the moment of reaching the critical value of velocity to the moment to reaching a steady-state motion).

In general they are reduced to some lag of rotor acceleration velocity for the model with dynamic characteristic of the engine and, as a result, to somewhat lesser velocity of steady-state rotation. It is seen from the presented graphs that most substantial differences between the rotor angular velocities occur in the section...
Figure 3: Time dependences of generalized coordinate of vibrating body shift for the period of acceleration (a) and for steady-state regime (b) in case of using: 1 - static characteristic of the engine; 2 - equation of electromagnetic conditions in the engine.

which corresponds to the discontinuity point of piecewise linear function of electric motor static characteristic. Rotor angular velocities in steady-state regime of motion in both investigated cases equal \( \omega_{\text{stat}} = 133, 8s^{-1} \), \( \omega_{\text{dyn}} = 126, 9s^{-1} \) the difference being near 5%. Along with this practically similar oscillations of velocity take place.

Fig. 3 shows time dependencies of generalized coordinate of vibrating body shift for the most interesting period of acceleration - transition of resonance zone. According to presented graphs the amplitudes of vibrating body oscillations are practically the same for both investigated cases both by value and by the character of change. This conclusion refers both to transient and steady-state regimes of motion (Fig. 3 b).

Fig. 4 shows time dependencies of motor torque and vibrational moment acting on rotor for the cases of using static characteristic and equation of electromagnetic conditions in the engine. Vibrational moment is regarded as additional moment acting on rotor in case of its axle oscillations and causing to various vibrational effects [3, 7].

It should be noted that vibrational moment is practically equal to zero in the first stage of acceleration (engine starting without load takes place). It grows rapidly at the beginning of the second stage. So long as vibrational moment is practically breaking one, rotor acceleration is relatively small in that period of time. After running out of resonance zone vibrational moment becomes mostly rotary and grows down fast, but frequency and amplitude of its oscillation increase incessantly up to reaching the steady-state regime of motion. Difference in values acquired by vibrational moment in both compared variants does not exceed 5..7% both in the process of rotor acceleration and the period of steady-state motion.

Similar small divergence may be established between the values of motor torque for the cases of using different mechanical characteristics. It explains the fact that the results of simulation of dynamic processes with the use of both characteristics
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Figure 4: Time dependencies of the motor torque (1, 2) and vibrating moment (3, 4) for the period of acceleration (a) and steady-state regime (b) in case of using: 1, 3 static characteristic of the engine; 2, 4 - equation of electromagnetic conditions in the engine

are close enough. Oscillations of motor torque in steady-state regime of motion are observed somewhat bigger for the first investigated variant.

These oscillations are small as compared with those of vibrating moment because of high frequency of load change and availability of considerable mass inertia of vibro-exciter and rotary parts of electric motor and they a depicted in Fig.4 in the form of practically straight line.

It should be noted that similar results were obtained as a result of conducted investigation of rotor acceleration of vibro-exciter set into rotation by motor of higher power \( (N = 0,12 \text{kw}) \) only somewhat smaller divergence between the values of investigated parameters is observed. Practically the same result may be obtained if function \( L \) in the working section would be approximated by parabola through points \( (\omega_n, L_n) \) and \( (\omega_s, 0) \).

It is connected, first of all, with the fact oscillations of vibration moment are by an order of magnitude greater than those of motor torque, so the effect of that motor torque is levelled.

Taking into account numerical simulation of the process of acceleration and steady-state regime of motion of vibro-exciter rotor for the cases of using static and dynamic characteristics of the electric motor and the obtained results of analytical and experimental investigations we may draw a conclusion that models with both characteristics describe the motion of the vibration machine adequately and, practically, in the same way.

Thus, both static and dynamic engine characteristics may be used for simulation the dynamics of vibration machines with unbalanced vibro-excitor driven by three-phase asynchronous motor for both the steady-state period of motion and the process of acceleration.
References


1 Abstract

There are different approaches to and various accuracy degrees of study of different aspects of heterogeneous environments behavior. One may generalize the experimental data of mechanical testing of certain sample of material with heterogeneous structure or one may search for analytical expression of properties of such materials, thus developing a theoretical basis for studying of thermomechanical behavior of heterogeneous environments.

Generally in a composite one of the components is commonly known as matrix (filling or bonding agent) and the rest of the components are inclusions. Composites may vary in types of forms of inclusions: granular, fibrous, layered or other forms.

If the operator relation, for instance the relation between the heat flow vector and the temperature gradient or the relation is the periodic function of coordinates:

\[ \Phi((\nabla T), R + n_1 a_i + n_2 b_j + n_3 c_k) = \Phi((\nabla T), R), \]

(1.1)

where \( a_i \) are constant vectors and \( n_i \) are arbitrary integral numbers, then the composite is called the composite with periodic structure. The vectors \( a_i, b_j \) and \( c_k \) determine the periods of such structure.

In this study we shall consider the composite with periodic structure as a special kind of composite materials. We shall represent it as a solid consisting of a large quantity of identical cells with the sizes \( a, b \) and \( c \) respectively along the coordinate axes \( Ox, Oy \) and \( Oz \) (sizes of cells \( a, b \) and \( c \) are the projections to the coordinate axes of \( a_i \) vectors from representation (1.1)). Each of the cell face is closely adherent to the face of the neighboring cell so the temperature and vector of the heat flow will be uninterrupted while passing from one cell to another.

With the aid of the so called ”basic solutions” and regular variable factorization in the form of linear combination of basic solution we shall be looking for solution of the thermomechanical problem for periodic composite.

Heat conduction equation has the form:

\[ h = - K \cdot (\nabla T), \]

(1.2)
where $K$ is the tensor heat conduction coefficient, the value of which is explicitly
dependent on the coordinates, i.e. to solve the equation (1.2) the tensor should be
determined for each point of the composite.

$$K(R + n_1 a_1 + n_2 b_2 + n_3 c_3) = K(R)$$

(1.3)

In this study we shall consider a new method of composite homogenization which
consists in a special mode of formulation for effective heat conduction coefficient
using the so called basic solutions and regular variable factorization in the form
of linear combination of basic solutions. They provide accurate values of effective
heat conduction coefficients for the spatially constant average temperature gradient
and heat flux vector. As an example we shall consider the application of the above
method to isotropic material.

For greater definition we shall consider that the composite material under study
consists of two cells, the bars of equal size. To simplify the analysis we shall also
consider that each cell has three planes of symmetry passing through the geometrical
center of the cell and parallel to its side faces.

2 The three basic problems for periodic composites

Let us select one cell with the edge sizes $a$, $b$ and $c$ and consider it the central cell. Its
geometrical center will obviously coincide with the origin of coordinates. Cartesian
coordinates $x$, $y$ and $z$ of this cell will vary within the corresponding limits:

$$\frac{-a}{2} \leq x \leq \frac{a}{2}, \quad \frac{-b}{2} \leq y \leq \frac{b}{2}, \quad \frac{-c}{2} \leq z \leq \frac{c}{2}$$

(2.1)

Let us consider the three problems of heat conduction for the selected cell:
1. Let on side edge $x = \frac{-a}{2}$ and $x = \frac{a}{2}$ constant temperatures $-T_0$ and $T_0$ respectively
are specified. The rest of the edges have the condition of heat insulation. Then the boundary conditions for this problem will be expressed as follows:

\[
\begin{align*}
  x &= -\frac{a}{2}, \quad T = -T_0; \\
  x &= \frac{a}{2}, \quad T = T_0; \\
  y &= \pm \frac{b}{2}, \quad z = \pm \frac{c}{2}, \quad n \cdot h = 0. 
\end{align*}
\]  

(2.2)

It is easy to note that the distribution of temperature relative to the plane ZOY is antisymmetrical and the temperature on the very plane equals 0 respectively.

2. Similarly to the first problem let on side edge \( y = -\frac{b}{2} \) and \( y = \frac{b}{2} \) certain constant temperatures \(-T_0\) and \(T_0\) respectively are specified. The rest of the edges have the condition of heat insulation. Then the boundary conditions for this problem will be expressed as follows:

\[
\begin{align*}
  y &= -\frac{b}{2}, \quad T = -T_0; \\
  y &= \frac{b}{2}, \quad T = T_0; \\
  x &= \pm \frac{a}{2}, \quad z = \pm \frac{c}{2}, \quad n \cdot h = 0. 
\end{align*}
\]  

(2.3)

3. Let on side edge \( z = -\frac{c}{2} \) and \( z = \frac{c}{2} \) certain constant temperatures \(-T_0\) and \(T_0\) respectively are specified. The rest of the edges have the condition of heat insulation. Then the boundary conditions for this problem will be expressed as follows:

\[
\begin{align*}
  z &= -\frac{c}{2}, \quad T = -T_0; \\
  z &= \frac{c}{2}, \quad T = T_0; \\
  y &= \pm \frac{b}{2}, \quad x = \pm \frac{a}{2}, \quad n \cdot h = 0. 
\end{align*}
\]  

(2.4)

3 Formation of periodic basic solutions for a composite

The solutions above were formed for one cell. They allow formation of a certain periodic solution of certain boundary problems for the whole composite\(^1\).

Distribution of temperature in the central cell was determined in basic problems. In order to define the temperature in the series of immediate cells having common border with the central one it is necessary to add translation temperature to the temperature field of the given cell (bordering the central). Having determined the temperature field in the cell bordering the central one it is possible, acting by analogy, to define temperature fields for all the rest of the composite cells, thus

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\(^1\) V.A. Palmov, Basic solutions and regular factorization in mechanics of periodic composites, Technical University of St-Petersburg, 2005.
defining the temperature in the whole composite. The operations described above ensure continuity of the temperature field. Naturally it will not be periodic and will vary in different cells. If we measure off a certain distance \( x_1 \) from the central cell, say, along Ox axis, then the temperature at this point may be determined as \((2n - 1)T_0 + T_I\), where \( n \) is a maximum integral number of the half length of the cell edge parallel to OXY plane and may be located in the interval \([0; x_1]\), \( T_I \) being the temperature at point \((x_1 - ma)\), it is easy to note that this point will belong to the central cell and its temperature field has been already determined above. A similar procedure may be repeated in other directions of Cartesian coordinate axes.

According to the above we may conclude that the temperature value at similarly located points of different cells varies by a certain constant value multiple of a specific constant temperature \( T_0 \), of which follows that the temperature gradient will be the same in these cells. That is the temperature gradient will be the periodic function.

Thus we can obtain the so-called periodic solution for composite. Periodicity of the solution will be according to the temperature gradient and the heat flow vector. Their function will be continuous while passing from one cell to another.

Let us assign to the central cell selected above the number 0,0,0 in the complete numbering system of the composite cells. Its coordinates vary within the limits determined by correlation (2.1). It is easy to see that the coordinates of the cell center for numbers \( m, n \) and \( p \) are determined by the following correlations: \( x = ma \), \( y = nb \), \( z = pc \). Coordinates of the set of points of this cell will lie within the following intervals:

\[
\begin{align*}
\frac{ma - a}{2} & \leq x \leq ma + \frac{a}{2}, \\
\frac{nb - b}{2} & \leq y \leq nb + \frac{b}{2}, \\
\frac{pc - c}{2} & \leq z \leq pc + \frac{c}{2}.
\end{align*}
\]

Let us introduce the local coordinates:

\[
\xi = x - ma, \quad \eta = x - nb, \quad \sigma = z - pc.
\]

From the expressions (3.1) and (3.2) the intervals of variation of local coordinates within any cell can clearly be seen:

\[
\begin{align*}
-\frac{a}{2} & \leq \xi \leq \frac{a}{2}, \\
-\frac{b}{2} & \leq \eta \leq \frac{b}{2}, \\
-\frac{c}{2} & \leq \sigma \leq \frac{c}{2}.
\end{align*}
\]

It is easy to note that the limits of variation of local coordinates coincide with the limits of variation of coordinates from (2.1). Therefore if we use local coordinates then in all the cells we shall have identical distributions of heat flow and gradient of temperatures in each of basic solutions.

If we analyze the temperature separately its distribution shall not be periodic. Let us bring the above reasoning a strict formal expression. Let us consider the first basic solution in which the function \( T_I \) is not a periodic function but it varies as described above.

Let us express the temperature in the following form:

\[
T_I = \frac{2T_0}{a}x + \hat{T}_I, \quad \hat{T}_I = T_I - \frac{2T_0}{a}x, \quad \hat{T}_I = \hat{T}_I(\xi, \eta, \sigma).
\]
where $\hat{T}_I$ is a periodic function; it is easy to check that its value at the end of the interval (2.1) (i.e. when $x = \frac{a}{2}$) coincides with the value at the beginning of the interval (when $x = -\frac{a}{2}$). On the left side of this cell there will be:

$$\hat{T}_I = -2T_0, \quad \frac{a}{2a} = -T_0. \quad (3.5)$$

We can see that the function $\hat{T}_I$ tolerates periodic extension onto the second, third and the following cells in the direction to Ox axis necessarily using the local coordinates (3.2).

Similarly we shall obtain the expressions for temperatures in the second and third basic solutions:

$$T_{II} = \frac{2T_0}{b}y + \hat{T}_{II}, \quad \hat{T}_{II} = T_{II} - \frac{2T_0}{b}y, \quad \hat{T}_{II} = \hat{T}_{II}(\xi, \eta, \sigma) \quad (3.6)$$

$$T_{III} = \frac{2T_0}{c}z + \hat{T}_{III}, \quad \hat{T}_{III} = T_{III} - \frac{2T_0}{c}z, \quad \hat{T}_{III} = \hat{T}_{III}(\xi, \eta, \sigma) \quad (3.7)$$

4 Linear combination of solutions of basic problems

Due to linearity of equations and boundary conditions the solution of any of the three problems considered above multiplied by a certain constant factor will also make up a solution, and the linear combination of solutions that represents a sum of solutions with certain constant factors will also be a solution for this problem:

$$T = \sum_{k=1}^{3} \alpha_k T_k, \quad (4.1)$$

where $T_k$ is the temperature for $k^{th}$ problem and $\alpha_k$ are certain constant factors.

Let us introduce the following designation for the temperature gradient:

$$\Gamma = (\nabla T), \quad \Gamma = \sum_{k=1}^{3} \alpha_k \Gamma_k; \quad (4.2)$$
where $\Gamma_k$ is the temperature gradient for $k^{th}$ problem.

For the heat flow vector we shall then obtain:

$$ h = \sum_{k=1}^{3} a_k h_k, $$

(4.3)

where $h_k$ is the heat flow vector for $k^{th}$ problem.

Let us call the representations of solutions of the forms (4.1), (4.2), (4.3) the "regular factorizations" of solutions of heat conduction equations for composite. They are the accurate periodic solutions of the heat conduction problem for periodic composite. It is necessary to note that we speak about the accuracy of solutions from the assumption that the solutions of basic problems obtained are accurate.

5 Application of "regular factorizations" to the problem of composite homogenization

Let us determine the averaging operator according to the volume of cell in the following way:

$$ < M > = \frac{1}{V} \int_V M dV. $$

(5.1)

It was stipulated above that all the cells of the composite have identical shape and size and therefore the integral (5.1) may be expressed as a triple integral within the integration (2.1).

$$ V = abc. $$

(5.2)

Let us consider averaged vector of heat flux; by analogy with (5.1) it will be:

$$ < h > = \frac{1}{V} \int_V h dV. $$

(5.3)

Taking into account the form of regular factorization (4.3) we shall have:

$$ < h > = \frac{1}{V} \int_V \sum_{k=1}^{3} a_k h_k dV = \\
= \sum_{k=1}^{3} a_k \frac{1}{V} \int_V h_k dV = \sum_{k=1}^{3} a_k < h_k > = \\
= \sum_{k=1}^{3} a_k(< h_x^k > i + < h_y^k > j + < h_z^k > k). $$

(5.4)

The expression (5.4) in the coordinate form will be expressed as follows:

$$ < h_x > = \alpha_1 < h_x^I > + \alpha_2 < h_x^II > + \alpha_3 < h_x^III >, $$

$$ < h_y > = \alpha_1 < h_y^I > + \alpha_2 < h_y^II > + \alpha_3 < h_y^III >, $$

$$ < h_z > = \alpha_1 < h_z^I > + \alpha_2 < h_z^II > + \alpha_3 < h_z^III >. $$
\[ < h_y > = \alpha_1 < h^1_y > + \alpha_2 < h^II_y > + \alpha_3 < h^III_y >, \]
\[ < h_z > = \alpha_1 < h^1_z > + \alpha_2 < h^II_z > + \alpha_3 < h^III_z >. \]

Let us introduce the following designation: \( H \) is the matrix of average values of heat flux:
\[
H = \begin{pmatrix}
< h^I_x > & < h^II_x > & < h^III_x > \\
< h^I_y > & < h^II_y > & < h^III_y > \\
< h^I_z > & < h^II_z > & < h^III_z >
\end{pmatrix},
\]
\[ h = \begin{pmatrix}
< h_x > \\
< h_y > \\
< h_z >
\end{pmatrix}, \]
\[ \alpha = \begin{pmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3
\end{pmatrix}. \]

The above may also be represented in matrix form:
\[ h = H \alpha. \]

Averaging for the temperature gradient will be as follows:
\[ < \Gamma > = \frac{1}{V} \int_V \Gamma dV. \]

Considering the form of regular factorization (4.2) we shall obtain:
\[ < \Gamma > = \frac{1}{V} \int_V \sum_{k=1}^3 a_k \Gamma_k dV = \]
\[ = \sum_{k=1}^3 a_k \frac{1}{V} \int_V \Gamma_k dV = \sum_{k=1}^3 a_k < \Gamma_k >, \]
\[ = \sum_{k=1}^3 a_k ( < \Gamma^k_x > + < \Gamma^k_y > + < \Gamma^k_z >). \]

The expression (5.9) in coordinate form will be as follows:
\[ < \Gamma_x > = \alpha_1 < \Gamma^I_x > + \alpha_2 < \Gamma^II_x > + \alpha_3 < \Gamma^III_x >, \]
\[ < \Gamma_y > = \alpha_1 < \Gamma^I_y > + \alpha_2 < \Gamma^II_y > + \alpha_3 < \Gamma^III_y >, \]
\[ < \Gamma_z > = \alpha_1 < \Gamma^I_z > + \alpha_2 < \Gamma^II_z > + \alpha_3 < \Gamma^III_z >. \]

The matrix form of record will be:
\[
\Gamma = \begin{pmatrix}
< \Gamma^I_x > & < \Gamma^II_x > & < \Gamma^III_x > \\
< \Gamma^I_y > & < \Gamma^II_y > & < \Gamma^III_y > \\
< \Gamma^I_z > & < \Gamma^II_z > & < \Gamma^III_z >
\end{pmatrix}, \quad \gamma = \begin{pmatrix}
< \Gamma_x > \\
< \Gamma_y > \\
< \Gamma_z >
\end{pmatrix}. \]
Let us introduce the following designation:

\[ \gamma = \Gamma \alpha. \]  \hspace{1cm} (5.12)

From the record (5.12) we shall express the vector of constant coefficients \((\alpha_1, \alpha_2, \alpha_3)\):

\[ \alpha = \Gamma^{-1} \gamma. \]  \hspace{1cm} (5.13)

Let us express the temperature gradient in vector form:

\[ \Gamma = \nabla T = \frac{\partial T}{\partial x} \mathbf{i} + \frac{\partial T}{\partial y} \mathbf{j} + \frac{\partial T}{\partial z} \mathbf{k}. \]  \hspace{1cm} (5.14)

The desired elements of matrix \(\Gamma\) will be nonzero in general case.

Let us calculate the inverse matrix to matrix \(\Gamma\) and designate it as \(\Gamma^{-1}\); let us substitute the constant values \((\alpha_1, \alpha_2, \alpha_3)\) obtained above for the expressions for averaged vectors of heat flux (5.6):

\[ h = H \Gamma^{-1} \gamma. \]  \hspace{1cm} (5.15)

Formula (5.15) connects the averaged values of the elements of temperature gradient vector in the composite with averaged values of elements of the heat flux vector.

Let us introduce the following designation:

\[ K_E = -H \Gamma^{-1}. \]  \hspace{1cm} (5.16)

Then the equation of heat conduction (1.2) may be represented as follows:

\[ h = -K_E \gamma. \]  \hspace{1cm} (5.17)

or taking into account the designations (4.2) earlier introduced the expression will be as follows:

\[ < h >= -K_E < \nabla T >. \]  \hspace{1cm} (5.18)

6 Average meanings of the temperature, gradient and vector of the heat flux and their deviations

Let us average the regular decomposition of the heat conduction equation solutions, which have been introduced in (4.1), (4.2) and (4.3), within the limits of one element, thus we will have:

\[ < T >= \sum_{k=1}^{3} \alpha_k < T_k >, \]  \hspace{1cm} (6.1)

\[ < \Gamma >= \sum_{k=1}^{3} \alpha_k < \Gamma_k >, \]  \hspace{1cm} (6.2)

\[ < h >= \sum_{k=1}^{3} \alpha_k < h_k >. \]  \hspace{1cm} (6.3)
Let us subtract the corresponding parts of the average expressions derived above, from the left and right parts of the regular decomposition (4.1), (4.2) and (4.3); the result of these mathematical operations will be the following:

\[ T - \langle T \rangle = \sum_{k=1}^{3} \alpha_k (T_k - \langle T_k \rangle), \]  

\[ h - \langle h \rangle = \sum_{k=1}^{3} \alpha_k (h_k - \langle h_k \rangle), \]  

\[ \Gamma - \langle \Gamma \rangle = \sum_{k=1}^{3} \alpha_k (\Gamma_k - \langle \Gamma_k \rangle). \]

(6.4) (6.5) (6.6)

It is not difficult to see, that the right parts of the expressions (6.4)-(6.6) are deviations of the temperature field in (6.4), the vector of the heat flux in (6.5) and the temperature gradient in (6.6).

Taking into account the values of the constants \((\alpha_1, \alpha_2, \alpha_3)\), which have been defined earlier, we can get the following deviations from the average values of temperature, temperature gradient and vector of the heat flux:

\[ T - \langle T \rangle = \frac{a}{2T_0} < \Gamma_x > (T_I - \langle T_I \rangle) + \frac{b}{2T_0} < \Gamma_y > (T_{II} - \langle T_{II} \rangle) + \frac{c}{2T_0} < \Gamma_z > (T_{III} - \langle T_{III} \rangle). \]

\[ h - \langle h \rangle = \frac{a}{2T_0} < \Gamma_x > (h_I - \langle h_I \rangle) + \frac{b}{2T_0} < \Gamma_y > (h_{II} - \langle h_{II} \rangle) + \frac{c}{2T_0} < \Gamma_z > (h_{III} - \langle h_{III} \rangle). \]

\[ \Gamma - \langle \Gamma \rangle = \frac{a}{2T_0} < \Gamma_x > (\Gamma_I - \langle \Gamma_I \rangle) + \frac{b}{2T_0} < \Gamma_y > (\Gamma_{II} - \langle \Gamma_{II} \rangle) + \frac{c}{2T_0} < \Gamma_z > (\Gamma_{III} - \langle \Gamma_{III} \rangle). \]

(6.7) (6.8) (6.9)

Calculations of the average meanings of the temperature gradient and vector of the heat flux are trivial, because they have got only periodic (concerning the coordinates) summands; whereas the calculation of average meanings of the temperature is more difficult, since it has got periodic (concerning the coordinates) and non-periodic summands. It is not difficult to express from (6.8) and (6.9) exactly actual values of the temperature gradient and vector of the heat flux. In practice we need just actual values.

\[ \langle T \rangle = \langle \Gamma_x \rangle x + \langle \Gamma_y \rangle y + \langle \Gamma_z \rangle z \]

\[ T = \langle T \rangle + \frac{a}{2T_0} < \Gamma_x > \hat{T}_I + \frac{b}{2T_0} < \Gamma_y > \hat{T}_{II} + \frac{c}{2T_0} < \Gamma_z > \hat{T}_{III}. \]

(6.10) (6.11)

From the above mentioned, we can make the following conclusion: the temperature’s deviation is considerably smaller than it’s average meaning, and the deviations
of temperature gradient and vector of the heat flux are of the same degree as their averaged values.

And so, we have got the real meanings of the temperature field, temperature gradient and vector of the heat flux, which are expressing using the average meanings. It is very important addendum for solution of the problem composites homogeneity.

References

Specialty description for the solution problems dynamical thermoelasticity for heat-conducting medium

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Abstract

Experimental results and theoretical analysis of the stress response thermo-introduced by short pulse heating of laser are presented. Analysis of thermo-elasticity problems has been carried out. Solution of the differential equations of the dynamical thermoelasticity is proposed by the sum of quasistatic stresses $\sigma_s$ and dynamical stresses $\sigma_d$. It is shown evaluation of the quasistatic stresses $\sigma_s$ for heat-conducting medium. Experimental results showed significant inertia of thermomechanical response stress for heat-conducting medium. This phenomenon for dielectric and semiconductive material wasn’t found.

1 Stress due to thermal shock

Dynamical thermo-elasticity problems were considered in the many articles [2, 3]. Nevertheless there is interest to the dynamical thermo-elasticity problem connected with laser shock loading of duration $\tau_{lm} > 10^{-9}$ s. As pointed out by many investigators, the uncoupled theory of thermoelasticity is a good model by using if parameter of connectivity $\leq 2 \cdot 10^{-2}$.

Consider an elastic semi-space $x_3 = z \geq 0$. For our purpose, the study of wave propagation is one space dimension, the system eqs. with initial and boundary condition can be written

\[
\frac{\partial^2 \sigma_z}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 \sigma_z}{\partial t^2} = \frac{s}{c^2} \frac{\partial^2 T}{\partial t^2}
\]

\[
\frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial z^2} + W_0 f(t) e^{-\alpha z}
\]  

(1)
\[ T(z, 0) = 0; \quad \frac{\partial T}{\partial z} \bigg|_{z=0} = 0 \]

\[ \frac{\partial \sigma_z}{\partial z} \bigg|_{z=0} = 0; \quad \sigma_z(z, 0) = 0; \quad \sigma_z(\infty, t) = 0 \]

where

\[ \frac{(3\lambda + 2\mu)\alpha_T}{\lambda + 2\mu} - \rho = \frac{1 + \nu}{1 - \nu} \alpha_T \rho = \frac{s}{c^2}; \quad s = (3\lambda + 2\mu)\alpha_T \]

(2)

where \( \sigma_z \) - stress, \( T = T(z, t) - T_0 \), \( T_0 \) - initial temperature, \( \nu, \mu \) - Lame's constants, \( \alpha_T \) - the coefficient of the thermal expansion, \( \rho \) - density, \( c = \sqrt{\frac{\lambda + 2\mu}{\rho}} \) - longitudinal velocity of wave propagation an elastic medium, \( W_0 = \frac{I_0}{\rho c_p} \), \( \chi = \frac{\lambda}{\rho c_p} \), \( \lambda_q \) - thermal conductivity, \( c_p \) - thermal capacity, \( I_0 \) - the part of intensity heating puls taken up by medium, \( \alpha \) - absorption for light.

The methods of mathematical analysis used here are based on the Fourier integral transformation

\[ \tilde{T}^\omega(\omega, z) = \int_{-\infty}^{\infty} T(t, z)e^{i\omega t} dt \]

The solution of the equation (1) for \( T \) can be written

\[ \tilde{T}^\omega = \frac{W_0}{i\omega + \alpha^2\chi} \left[ \frac{\alpha}{\sqrt{-i\omega / \chi}} \exp \left( -\sqrt{-i\omega / \chi} z \right) - e^{-\alpha z} \right] \tilde{f}(\omega) \]

(3)

When \( \omega << \alpha^2\chi = \omega_T \), the temperature field \( T \) depends on heat conducting

\[ \tilde{T}^\omega = \frac{I_0}{\rho c_p} \exp \left[ -(-i\omega / \chi)^{1/2} z \right] \tilde{f}(\omega) \]

(4)

When \( \omega >> \omega_T \), the temperature field \( T \) depends on production heat:

\[ \tilde{T}^\omega = \frac{W_0 \tilde{f}(\omega)e^{-\alpha z}}{-i\omega} \]

(5)

Using Fourier transformation we can written equation for \( \tilde{\sigma}_z^\omega \) (1):

\[ \frac{d^2 \sigma_z}{dz^2} + \frac{\omega^2}{c^2} \tilde{\sigma}_z = \frac{s}{c^2} \omega^2 \tilde{T} \]

(6)

The solution for (6)
Specialty description for the solution problems dynamical thermoelasticity for heat-conducting medium

\[ \tilde{\sigma}^\omega = \left( \frac{s \omega}{c} \right) \int_0^z \tilde{T}(z', \omega) \sin \frac{\omega}{c} (z - z') dz' \]  

(7)

On performing a partial integration we find

\[ \tilde{\sigma}^\omega = s \left[ \tilde{T}(z, \omega) - \tilde{T}(0, \omega) \cos \frac{\omega}{c} z - \int \frac{d\tilde{T}}{dz}(z', \omega) \cos \frac{\omega}{c} (z - z') dz' \right] \]  

(8)

Let us define quasistatic part of the solution (6)

\[ \tilde{\sigma}^\omega_{st} = s \left[ \tilde{T}(z, \omega) - \tilde{T}(0, \omega) \cos \frac{\omega z}{c} \right] \]  

(9)

dynamical part of the solution (6)

\[ \tilde{\sigma}^\omega_d = -s \int \frac{d\tilde{T}}{dz}(z', \omega) \cos \frac{\omega}{c} (z - z') dz' \]  

(10)

\[ \tilde{\sigma}^\omega = \tilde{\sigma}^\omega_{st} + \tilde{\sigma}^\omega_d \]  

(11)

The solution \( \tilde{\sigma}_d \) is in accordance with [1, 2]. The rapid changes \( \tilde{T}'_z(z', \omega) \) in temperature fields provoke thermal stresses of dynamical character. Dynamical stress thermoelasticity has been described [1, 2, 3, 4] and corresponds to \( \tilde{\sigma}_d \) (6).

2 Experimental

The entire experimental apparatus is shown schematically in Fig. 3. The pulse thermal stress was done by a heating pulse of duration \( 3 \cdot 10^{-8} \) s, created by the action of laser radiation. A laser apparatus on base YAG-Nd with \( \lambda = 1,06 \) mkm and \( \tau_{im} = 15 \cdot 10^{-9} \) s was used. In our experiments the stress on the back side \( h = 2 \div 10 \) mm were measured. The piezoelectric transducer was used to measure the dynamic stress.
Experimental results showed significant difference of thermomechanical stress for heat-conducting and low-conductivity medium (Fig. 4, Fig.5). Laser heating pulse are shown in Fig. 4. Form of pulse stress is defined by the sum of dynamical and quasistatic (expansion phase) material response under fast heating for heat-conducting medium (Fig. 4).

Fig.3 Schema of the experiment

Fig.4. Stress on the back side in sample wolfram, laser impulse (a) and aluminium (b)
3 Discussion

In the thermoelastic problems, the inertia terms is Lame’s displacement equations are usually taking into consideration. But there are thermal models (slow) correspond to Lame’s equation without the inertia terms. The quantity values dynamical stress and statical stresses depend on heat conducting. Experimental results showed significant inertia of thermomechanical response stresses for heat-conducting medium.

References


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Atomistic mechanisms of plastic deformation initiation in vanadium crystallite under mechanical loading

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Abstract

Atomistic mechanisms of plastic deformation initiation under mechanical loading in vanadium crystallites were simulated with the molecular dynamics method. The influence of loading conditions and temperature on local structural changes was studied. Plastic deformation initiation in face-centered cubic (fcc) and body-centered cubic (bcc) lattices was comparatively analyzed.

1 Introduction

The multilevel description of plastic deformation processes in crystalline materials implies the presence of elementary structural defects. As a rule, the dislocation is considered as an elementary plastic carrier in materials with crystal structure. All stages of plastic deformation are related with the evolution of a dislocation ensemble. In the case of nanostructured materials, the classical dislocation theory of plastic deformation cannot be used due to the smallness of grain sizes. That is why, one of the fundamental problems of solid state physics and materials science is the investigation of possible generation mechanisms of local structural distortions and transformations of the atomic structure. It is obvious that their generation in a stable crystal is related to the local loss of lattice stability [1, 2], which can be due to the action of thermal, mechanical, chemical or radiation forces, or their combinations. The plastic deformation initiation in fcc crystallites has been studied in detail in papers [3, 4]. In the latter characteristic local changes of the structure which precede the generation of conventional structural defects were revealed. These characteristic local structural changes were called protodefects. Using direct molecular dynamics simulation papers [3, 4] showed for the first time the possibility of the thermal fluctuation mechanism of structural defect nucleation under dynamic loading in materials with initially perfect lattice. In this case, there is a threshold
strain value at which the growth of zones with local structural changes is almost avalanche-like. In the considered cases, the character of structural defect nucleation and evolution strongly depends on the specimen temperature and to a lesser extent on the loading conditions. Notice that during relaxation one of the three scenarios is possible: 1) a protodefect breaks down with energy release, 2) it remains a nonequilibrium structural formation, or 3) protodefects coalesce, condense with the formation of one of the conventional structural defects.

The present paper is aimed at the investigation of atomistic mechanisms responsible for plastic deformation initiation in a bcc vanadium crystallite at different temperatures.

2 Model

The nucleation of various structural defects on the atomic level is rather difficult to investigate experimentally because of the need for high temporal ($10^{-14}$ s) and spatial ($10^{-9}$ m) resolution. Computer simulation is therefore an effective way to study both the mechanisms of structural defect generation and dynamics of their evolution. The problems posed in the paper are solved on the basis of molecular dynamics simulation. Interatomic interaction in vanadium crystallites is described using the interatomic potential derived by Mendeleev and calculated within the FinnisSinclair approximation. The potential allows a quite accurate description of characteristics essential in the simulation of atomic collision cascades, such as the lattice parameter, elastic moduli, energy of point defect nucleation and migration, etc.

The simulated vanadium crystallite was a parallelepiped in shape. Its orientation was the following: one parallelepiped edge was oriented along the [100] crystallographic direction, the second along [010], and the third along [001]. It is known that under uniform compression of a bcc crystal by $\sim 11\%$ along two directions and simultaneous tension by $\sim 26\%$ along the third direction the initial bcc structure transforms to fcc.

3 Simulation results

The influence of temperature on the response of the simulated crystallite structure was studied at 100, 300 and 500K. The calculation results for the dependence of potential energy per atom on strain degree for different temperatures is given in Fig.1. As evident from the figure, the transformation of the initial bcc vanadium crystallite into an fcc crystallite by the above-described loading scheme is characterized by constant growth of the potential energy. According to the pattern of initial structure transformation, the variation of potential energy per atom makes up about two tenths of an electron volt.

Note that like in the case of crystallites with fcc structure the final temperatures radically change the deformation pattern in the bcc crystallite.

To analyze the integral influence of temperature on the nucleation and evolution of structural defects under high-rate deformation of the vanadium crystallite,
Figure 1: Potential energy per atom versus tension degree of the crystallite. Calculations at: 1 — T = 0 K, 2 — T = 100 K, 3 — T = 300 K, 4 — T = 500 K

curves 24 in Fig.1 can be arbitrarily divided into three portions. In the first portion potential energy smoothly increases (is injected). In the second the curves have less slope, kink and then drop abruptly. In the third portion potential energy increases much slower and the curves have abrupt drops.

Analysis of the simulation results has shown that the beginning of the second portion directly relates to the beginning of atomic structure distortion in compression planes. In the first and second curve portions in Fig.1 atomic planes in the tension direction are preserved and atoms do not jump from one atomic plane to another in the tension direction. Atomic structure distortions in the compression planes are regular (Fig.2) and begin almost simultaneously in all planes at the achievement of the threshold strain, at which the first characteristic kink appears in the curves. The threshold strain value at which structural distortions begin in the atomic planes subject to compression depends on the crystallite temperature and increases with its growth to higher strain values (Fig.1). This substantiates the thermal fluctuation origin of structural distortion generation in corresponding atomic planes. The increase of the threshold strain value with temperature growth indicates that the atomic thermal fluctuations on the one hand induce structural distortions, while on the other with temperature growth they shift the moment of the distortion generation to higher strains, i.e. favor crystallite accommodation under high-rate loading.

The strain interval corresponding to the second curve portion in Fig.1, when structural distortions are localized only in the atomic planes of compression, reduces with temperature growth. This relates not only to the threshold strain increase with temperature growth, but also to the decrease of strain at which potential energy decrease abruptly (Fig.1).

The main accommodation mechanism leading to the abrupt reduction of potential energy at the end of the second portion under high-rate deformation (Fig.1) is structure rearrangement in the tension direction. In this case, atoms from compres-
Characteristic structural distortions of the atomic plane subject to compression for the second portion of loading $\varepsilon = 7\%$, $T=100K$

Figure 2: Characteristic structural distortions of the atomic plane subject to compression for the second portion of loading $\varepsilon = 7\%$, $T=100K$

The beginning of the third curve portion in Fig.1 corresponds to the end of the abrupt drop in the deformation curves. Analysis of the structure shows that the beginning of the third portion in the curves is characterized both by the presence of additional atomic planes and by the recovery of the initial bcc structure in the greater part of the crystallite (Fig.3). Notice that in the second portion of the deformation curves the initial bcc structure broke down completely. The crystallite structure was analyzed on the basis of a mathematical algorithm accounting for the topological relations of the nearest neighbors [5].

Figure 3: Structure of the simulated crystallite at the beginning of the third portion. Gray color — atoms with bcc topology, black color — atoms belonging to stacking faults

The subsequent kinks in the third portion of the deformation curves are related with the formation of additional atomic planes in the tension direction and with partial recovery of the bcc structure. To study the influence of interfaces on the peculiarities of the crystallite structure response, we have simulated uniaxial tension in the [100] direction at temperature 300K (tension rate was equal to 6.3x10^{9} \text{ s}^{-1}). The interfaces were represented as free surfaces. In the third direction periodic boundary conditions were simulated. The crystallite tension was uniform in the selected direction. The calculation results for potential energy depending on relative
strain are given in Fig.4.

The free surfaces have greatly affected the crystallite response pattern. In particular, the defect structure formation in the material begins near the free surface, and the deformation curve lacks the second portion where structural distortions are generated only in planes perpendicular to the tension direction (Fig.4). The curve in this figure drops abruptly at 9% relative deformation, which is due to the occurrence of structural changes. In this case, the largest atomic displacements take place along the tension directions and free surfaces (Fig.5), gradually propagating throughout the crystallite. Like under the first loading scheme, when intense structural changes stop (after potential energy drop), additional atomic planes are formed in the simulated crystallite and the initial bcc lattice is recovered in the most part of the specimen.

Analysis of the calculation results shows that crystallite deformation at final temperatures essentially changes the atomic distribution pattern on coordination spheres in comparison with zero temperature (Fig.6). For example, at zero temperature the uniaxial uniform tension along the [100] direction increases the distance to the first coordination sphere and causes splitting of the second coordination sphere (Fig. 6). The uniaxial tension at final temperature leads to the splitting of the first coordination sphere and to the displacement of half of the first coordination sphere atoms closer to the central atom. Atoms of the second coordination sphere also have a tendency to displace to the central atom at closer distances. The given atomic rearrangement on coordination spheres is caused by the free surface effect, since structural distortions start near the surface and then propagate throughout the crystallite (Fig.5).

Figure 4: Dependence of potential energy per atom on the uniform tension value at temperature 300 K
4 Summary and Conclusions

We may conclude on the basis of the performed calculations that in crystallites with bcc structure (like in fcc crystallites) under high-rate deformation thermal fluctuations are responsible for the generation of structural defects. In this case, there is a certain threshold strain value at which the structural defect generation becomes avalanche-like. At crystallite deformation with preserving the atomic volume three stages of structural response can be distinguished: 1) injection of additional energy into the crystallite without the violation of regular structure, 2) structural distortions in certain atomic planes with crystalline structure violation, and 3) abrupt structural changes in the whole crystallite and recovery of the initial bcc structure in its most part.

Under deformation of a crystallite with free surfaces, the second stage of structural response is absent. In this case, the account for thermal fluctuations leads to significant atomic redistribution on the first and second coordination spheres of the
Figure 6: Atomic distribution on the first and second coordination spheres for $\varepsilon = 9\%$ for temperatures: a) 0; b) 300 K

vanadium crystallite as compared to zero temperature.

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Experimental investigation into the stability of stationary rupture of the liquid layer on an immiscible fluid surface

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Abstract

The paper is concerned with the analysis of the stationary equilibrium shape of a three-phase liquids/gas system consisting of a horizontal liquid layer with the upper free boundary placed on the immiscible fluid interface. The stability conditions of rupture of the liquid layer surface have been investigated experimentally. The dependencies of rupture parameters on cuvette diameter, layer thickness, values of surface tension of fluids are presented for various pairs of investigated liquids.

1 Introduction

It is generally admitted that in terrestrial conditions there are probable three diverse forms of steady-state three-phase system composed of a gas and two immiscible fluids. In one case, a fluid can form a lens-like drop floating over the surface of another fluid. In the other case, a two-layer system is formed, in which one horizontal liquid layer is overlain the other. The third equilibrium configuration is associated with a stationary concentric rupture of the upper fluid layer, within the limits of which the lower layer comes into contact with gas.

Such a rupture can be observed experimentally in the case when the surface tension $\sigma$ of the upper layer is larger than that of the lower while its thickness is small enough [1, 2]. Then, any local deformation of the upper layer, caused by various reasons (by means of mechanical action, directional jet of air, or application of a small amount of a surfactant on the free layer surface) and propagating nearly through the whole layer thickness, leads to an abrupt growth of its horizontal diameter to some value, which remains constant for an arbitrary long period. The focus of this work is the analysis of stability conditions of a multi-layer fluid system with a rupture and investigation of the dependence of rupture parameters on the cuvette diameter, layer thickness and difference in the values of surface tension of the examined fluids.
2 Experimental procedure

In experiment, an initially two-layer system of horizontal fluid layers was formed in a glass cylindrical cuvette (Petri dish) with the inner diameter $D$ ranging from 2.0 to 29.5 cm. The cuvette was made of chemical glass produced by JENAerGLAS company. This type of glass was chosen for the reason that it is well wetted by the fluids used in the experiment. The thickness of the fluid layer was defined as $h = m / (\rho S)$, where $m$ is the fluid mass, $\rho$ is the fluid density, and $S = \pi D^2 / 4$ is the area of the initial (continuous) layer which is considered to be plane (the volume of the fluid in the meniscus at the cuvette boundary is neglected). The cuvette diameter was measured with slide calliper to within 0.1 mm. The mass of the fluid was defined by regular weighing the cuvette with fluid on AND-EK-610i electronic balance with the scale reading to 0.01 g. In tests, the estimated thickness of the upper layer varied from 1 to 7 mm. The thickness of the liquid substrate was several times greater than the upper layer thickness and varied from 5 to 15 mm.

For a liquid substrate we used tetrachloride carbon $\text{CCl}_4$ ($\sigma = 25.7 \text{ mN/m}$). For an upper layer we used different fluids, such as water ($\sigma = 72.8 \text{ mN/m}$), glycerine $\text{C}_3\text{H}_8\text{O}_3$ ($\sigma = 59.4 \text{ mN/m}$), ethyleneglycol $\text{C}_2\text{H}_6\text{O}_2$ ($\sigma = 46.1 \text{ mN/m}$), aqueous solutions of 1,4-butanediol $\text{C}_4\text{H}_{10}\text{O}_2$ with concentrations $5\% - 100\%$ ($\sigma = 65.0\% - 43.8 \text{ mN/m}$) and isopropyl alcohol $\text{C}_3\text{H}_8\text{O}$ with concentrations $2.5\% - 35\%$ ($\sigma = 61.0\% - 26.2 \text{ mN/m}$) and also solutions of isopropyl alcohol in 1,4-butanediol with concentrations $5\% - 20\%$ ($\sigma = 40.7\% - 34.0 \text{ mN/m}$). In all cases the fluid of the upper layer was lighter than the fluid of the substrate. All fluids were transparent and weakly evaporable except for $\text{CCl}_4$ and isopropanol. The tests were carried out at constant ambient temperature $(23\pm1)\degree\text{C}$.

At the beginning of the experiment the surface of the substrate fluid was overlaid with a horizontal liquid layer of minimal available thickness. After formation of the rupture (in the majority of tests this was accomplished by subjecting the layer surface to short-time actions of a narrow directional air jet, blown out through the syringe needle) the layer thickness started to increase gradually by injecting additional amount of fluid with a pump developing a rather low flow rate. This resulted in a monotonic decrease of the rupture diameter until it approached zero and the rupture disappeared. The evolution of the rupture dynamics and variation of the rupture diameter was traced by filming the layer with the analog video camera having the picture frequency of 25 frames/sec. Simultaneously, the same video camera was used to register the mass of the upper layer taking the digital balance readings. The typical photograph of a steady-state rupture of water layer upon the surface of $\text{CCl}_4$ is shown in Fig.1.

3 Results

The measurements have shown that the rupture diameter depends essentially on the initial thickness of the upper layer, the diameter of the cuvette, and the difference in the values of surface tension of the examined fluids. Fig.2 shows variations of the stationary rupture diameter $d$ with the layer thickness $h$ for several fluids overlaying the carbon tetrachloride substrate in the cuvette with the diameter $D = 7.5 \text{ cm}$.
As it is seen from the plot, with an increase of the layer thickness the diameter of the rupture first monotonically decreases. However after reaching some critical value \( h^* \) there suddenly occurs an abrupt closure of the rupture and, as a result, regeneration of a two-layer system of fluids. At that the critical thickness of the upper layer, above which the existence of rupture is impossible, and the minimum possible diameter of the rupture \( d^* \) differ essentially for various pairs of tested fluids.

Evidently, the diameter of rupture is considerably dependent on the diameter of the experimental cuvette (Fig.3), because as the layer thickness tends to zero the rupture diameter approaches the cuvette diameter. At the same time it can be readily noticed that the maximal thickness of the breaking layer is much more sensitive to the dimensions of the cuvette with small diameters than with large diameters. In Fig.4, the dependence of \( h^* \) on the cuvette diameter \( D \) for the system H\(_2\)O–CCl\(_4\) shows that the zone of marked influence of the boundaries for this particular fluid system is restricted by \( D^* \sim 5 \) cm, so that at larger \( D \) the critical thickness of the layer proves to be practically constant and does not exceed \((6.0 \pm 0.2) \) mm (i.e. comparable with the thickness of the water layer, which spreads freely over the surface of CCl\(_4\)). This is explained by the fact that in cuvettes of small dimensions an increasingly growing contribution is made by the near-wall menisci of the fluids occupying the greater relative area of the fluid layer and specifying the shape of its surface. At the same time the minimal rupture diameter \( d^* \) continues to grow with the cuvette diameter according to polynomial regularity (Fig.5). Thus, in the case of infinitely extended layer \((D \to \infty)\), the existence of such a steady-state rupture of the liquid layer turns to be impossible because closure of the rupture occurs even at arbitrarily large values of its diameter.

The analysis of the obtained experimental relationships supports the view that the critical thickness of the breaking layer is a constant value for any specific pair of fluids and eventually is defined by their physical properties. The basic parameter is found to be the difference \( \Delta \sigma \) between the values of the surface tension of free fluids boundaries, which for the majority of mutually insoluble or weakly soluble fluids is proportional to a high accuracy to the surface tension of their interface according to the known Antonov rule: \( \sigma_{12} = \sigma_2 - \sigma_1 \). To ascertain the dependence of \( h^* \) on \( \Delta \sigma \) in the next series of experiment the surface of carbon tetrachloride was overlaid not with a pure water, but with aqueous solutions of some surface active fluids. This allowed us to vary over a wide range the surface tension of the upper layer, which showed a rather strong non-linear dependence on the solution concentration \( C \). The tests were made for aqueous solutions of isopropyl alcohol and butanediol, and also for solutions of isopropanol in butanediol. Interferometric visualization of the concentration fields near the interface showed that in the time of experiment penetration of CCl\(_4\) into butanediol was rather inessential whereas an inverse penetration of water and butanediol into CCl\(_4\) was not observed at all. In turn, isopropyl alcohol was actively dissolved in CCl\(_4\). Note, however that in the case when its concentration in water was less than 5% and in butanediol was less than 20% the dissolution process was not accompanied by development of solutocapillary phenomena, which significantly accelerated mass transfer.

Typical dependences of rupture diameter versus layer thickness for cuvette with diameter \( D=7.5 \) cm are given in Fig.6 for aqueous solutions of butanediol on the
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carbon tetrachloride substrate. From these plots we can determine the value of $h^*$, corresponding to the solution concentrations. Fig.7 shows the dependence of the maximal layer thickness $h^*$ on the surface tension difference between the upper layer and the substrate layer. It is seen that the experimental points obtained for different fluids and solutions fall on a single curve. The only exception is a few points lying above. These points were obtained from the tests with aqueous solution of isopropyl alcohol whose concentration was more than 10%. However just at these concentrations solubility of isopropanol in carbon tetrachloride begins to play an essential role. In particular, it reduced the actual surface tension at the liquid-liquid interface compared to which the values of the surface tension difference calculated by Antonovs rule proved to be overestimated.

The formation of a steady-state rupture is related to the ability of the liquid system to reduce the total surface energy due to a decrease in the surface area of the upper layer. Conservation of the rupture is mainly due to wetting of the cuvette walls with the fluid of the upper layer. The wetting requirements imply that energetically it is more efficient for a fluid to share the surface with a solid phase than with a gaseous phase. As a result, the rupture is unable to push the fluid away from the walls so that it has to remain in the center of the fluid surface – i.e. at a distance from the solid boundaries. An attempt to create a freely floating rupture in a two-layer liquid system in a cuvette made of non-wettable material, for example, of polyethylene terephthalate, has failed. The rupture shifts to the cuvette periphery, where it comes into contact with the walls. The supplementary factor, stabilizing the rupture, is the effect of hydrostatic pressure of the upper layer under which the height of the rupture area is partially filled with the substrate fluid. The height of the resulting fluid column is defined by the difference between the pressure of the upper layer and the capillary pressure generated by deformation of the free surface of the rupture.

Fig.1. The steady-state rupture of water layer on the surface of CCl$_4$. $D=6.1$ cm
Fig. 2. Rupture radius versus layer thickness for water (1), glycerine (2), ethyleneglycol (3) on the surface of CCl₄.

Fig. 3. Rupture radius versus layer thickness for H₂O–CCl₄ system. $D$, cm: 10.8, 9.4, 7.5, 6.1, 3.8, 2.9, 2.0 (1–7).

Fig. 4. Variation of critical layer thickness with cuvette diameter.

Fig. 5. Variation of critical rupture diameter with cuvette diameter.

Fig. 6. Rupture radius versus layer thickness for butanediol–water solutions with $C$, %: 5, 10, 20, 40, 60, 80, 100 (1–7) and for isopropanol–butanediol solutions with $C$, %: 5, 10, 20 (8–10).

Fig. 7. Critical layer thickness versus surface tension difference for water (1), glycerine (2), ethyleneglycol (3), aqueous solutions of butanediol (4) and isopropanol (5), isopropanol–butanediol solutions (6).
4 Conclusion

The performed experiments were aimed at studying the properties and parameters of steady-state ruptures in a two-layer system of insoluble fluids and determining the conditions of their initiation and closure. The necessary condition for such ruptures is the availability of cavity walls wetted by the fluid of the upper layer. Then, even if the walls are far removed the stationary rupture of the liquid layer continues to ”feel” their presence keeping the dependence of its minimal diameter on the longitudinal dimension of the cavity. Generation of such ruptures is possible only in the case when the thickness of the upper layer does not exceed some critical value (generally ≤6 mm for the examined fluids) defined by the difference in the values of the fluid surface tension between the upper and the substrate layers.

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About existence of second spectrum in Timoshenko beam theory

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Abstract
Per the last decades the Timoshenko beam theory was subjected to a certain revision. In particular, the actual existence of the second spectrum in Timoshenko beam theory is put under doubt. It is confirmed that the second spectrum is a result of specific structure of Timoshenko equations. In the present paper the behavior of Timoshenko beam with different boundary conditions is in details investigated. Many numerical examples presented before were re-examined using the Timoshenko beam theory and the finite element method for a discrete multi-mass modal of the Timoshenko beam. Agreements are excellent for the first and the second spectra. The procedure for dividing of the common spectrum of the Timoshenko beam into two separate spectra is presented. The conclusion indicates the physical existence of the second spectrum of the Timoshenko beam theory.

1. Introduction
The Timoshenko beam theory is widely used in the analyses of the transverse vibrations of beams. In essence, the Timoshenko beam model adds rotary inertia and shearing rigidity to the Bernoulli-Euler beam modal.

It is known, that the simultaneous counting of shearing and rotary inertia of masses leads to the appearance of additional, in contrast to the Bernoulli-Euler’s beam theory, the second spectrum.

The first serious investigations bounded with a possibility of existence of the second spectrum were undertaken by Traill-Nash and Collar [1]. Since that time, two questions have received considerable research interest; the first is bounded with the practical significance of frequencies of the second spectrum of the Timoshenko beam theory and the second is connected with the existence of the second spectrum for beam end conditions other then simply supported. Stephen [2] indicates additionally two boundary conditions for the Timoshenko beam where the Timoshenko frequency equation is divided into two separate equations for the first and second frequency spectra.

It was scored, that the occurrence of the second spectrum is obliged to the presence at the Timoshenko equations of the fourth order time differential term. Dolph [3] has shown that for the simply supported Timoshenko beam two distinct natural frequencies correspond to the same spatial mode shape and that proofs the existence of a second distinct frequency spectrum.
Levinson and Cooke [7] have widened the results obtained by Dolph. It was shown that the vibration modes of the Timoshenko beam include not only the shape of transversal deflections but also the rotation of the cross-section due to bending of a beam. Downs [5] using a discrete beam modal reported the existence of the two spectra for a simple supported beam. Abbas and Thomas [6] after analyzing of a numerical results obtained from the final element modal of the Timoshenko beam concluded that except for the simple supported beam a distinct second spectrum of frequency does not exist. But later Bhashyam and Prathap [7], using also a finite element method, concluded that two distinct spectra exist not only for a beam with simple boundary conditions. Abbas and Thomas [6] also concluded that the lower set of frequencies are bounded upper by the Bernoulli-Euler beam modal, while the upper set of frequencies are bounded below by the pure shear beam modal. It is also shown [1,6,7] that the second set frequencies leads to infinity as the rotary inertia and shear effects of the cross-section go to zero.

The firm conviction about existence of the second spectrum in the Timoshenko beam theory was subjected in the last decades to substantial doubts.

V.V. Nesterenko [8], using the variational approach of M.V. Ostrogradski [9] for differential equations containing the derivatives of the high order made the conclusion that the second spectrum in the Timoshenko beam theory is not realized. This position was supported by N.G. Stephen [10], who comparing of numerical values of the second spectrum frequencies with the frequencies obtained from a solution of the plane problem of the theory of elasticity has come to the conclusion that the frequencies of the second spectrum have no connection with the frequencies obtained from the solution of the theory of elasticity and, therefore, actually the frequencies of the second spectrum are absent. Thus, in the last papers the actual existence of the second spectrum is rejected.

The purpose of this paper is to introduce a complete clearness concerning the existence of the second spectrum of the Timoshenko beam theory.

2. Basic differential associations and their output

Using the Hamilton’s principle

$$\delta \int_{t_0}^{t_1} Ldxdt = 0$$  \hspace{1cm} (1)

where the Lagrangian density is determined by the expression:

$$L = \frac{EI}{2} \left( \frac{\partial \Phi}{\partial x} \right)^2 + \frac{GF}{2} \left( \frac{\partial W}{\partial x} - \Phi \right)^2 - \frac{m}{2} \left( \frac{\partial W}{\partial t} - \frac{\partial \Phi}{\partial t} \right)^2 - \frac{L}{2} \left( \frac{\partial \Phi}{\partial t} \right)^2,$$  \hspace{1cm} (2)

and also supposing, that at $t=t_1$ and $t=t_2$ the position of a mechanical system is assumed as given, the coupled equations free vibration of a uniform Timoshenko beam can be obtained

$$GF \left( \frac{\partial^2 W}{\partial x^2} - \frac{\partial \Phi}{\partial x} \right) - m \frac{\partial^2 W}{\partial t^2} = 0, \quad \frac{EI}{2} \left( \frac{\partial^2 \Phi}{\partial x^2} \right) + GF \left( \frac{\partial W}{\partial x} - \Phi \right) - L \frac{\partial^2 \Phi}{\partial t^2} = 0,$$  \hspace{1cm} (3)

added by the boundary and initial conditions.
Above the following notations were entered: \( W(x,t) \) is the total transverse displacement of the beam; \( \Phi(x,t) \) is the rotation of the cross-section due to bending; \( EI \) is the flexural stiffness of a beam; \( GF \) is the reduced rigidity of a beam on transversal shearing; \( m \) is per unit length mass; \( L \) - per unit length mass moment of inertia; \( x \) is the axial coordinate; \( t \) is the time.

Excluding \( W \) or \( \Phi \) from equations (3) the following two uncoupled differential equations in \( W \) and \( \Phi \) will have

\[
EI \frac{\partial^4 W}{\partial x^4} - \left(L + m \frac{EI}{GF}\right) \frac{\partial^2 W}{\partial x^2 \partial t^2} + m \frac{L}{GF} \frac{\partial^4 W}{\partial t^4} + m \frac{\partial^2 W}{\partial t^2} = 0
\]  

(4)

\[
EI \frac{\partial^4 \Phi}{\partial x^4} - \left(L + m \frac{EI}{GF}\right) \frac{\partial^2 \Phi}{\partial x^2 \partial t^2} + m \frac{L}{GF} \frac{\partial^4 \Phi}{\partial t^4} + m \frac{\partial^2 \Phi}{\partial t^2} = 0
\]  

(5)

Solution of equations (4) and (5) can be presented so

\[
W(x,t) = w(x) \exp(i\omega t), \quad \Phi(x,t) = \varphi(x) \exp(i\omega t),
\]  

(6)

where \( \omega \) is the natural frequency of a beam.

Substituting of (6) into equations (4) and (5) leads to the two uncoupled differential equations for \( w(x) \) and \( \varphi(x) \):

\[
EI \frac{d^4 w}{dx^4} + \omega^2 \left(L + m \frac{EI}{GF}\right) \frac{d^2 w}{dx^2} + \left(m\omega^4 \frac{L}{GF} - m\omega^2 \right) w = 0
\]

\[
EI \frac{d^4 \varphi}{dx^4} + \omega^2 \left(L + m \frac{EI}{GF}\right) \frac{d^2 \varphi}{dx^2} + \left(m\omega^4 \frac{L}{GF} - m\omega^2 \right) \varphi = 0
\]

This set of the two equations can be rewritten in the non-dimensional form:

\[
\frac{d^4 \eta}{d\xi^4} + \phi^2 (\alpha + \beta) \frac{d^2 \eta}{d\xi^2} - \phi^2 (1 - \phi^2 \alpha \beta) \eta = 0,
\]  

(7)

\[
\frac{d^4 \varphi}{d\xi^4} + \phi^2 (\alpha + \beta) \frac{d^2 \varphi}{d\xi^2} - \phi^2 (1 - \phi^2 \alpha \beta) \varphi = 0,
\]  

(8)

Above the additional notations were entered:

\( \eta = w/l, \quad \alpha = L/ml^2, \quad \beta = EI/GFl^2, \quad \phi^2 = \omega^2 ml^4/EI, \quad \xi = x/l \) (\( l \) - length of the beam).

At \( \alpha = 0 \) equation (7) reduces to the shear modal equation, and with \( \alpha = \beta = 0 \) equation (7) is transformed into the Bernoulli-Euler modal equation for the free vibration.

Solution of each equations (7) and (8) can be presented in the form:

\[
\eta_i(\xi) = A_i \exp(\lambda_i \xi), \quad \varphi_i(\xi) = B_i \exp(\lambda_i \xi)
\]

Substituting, for example, particular solution \( \eta_i(\xi) \) in equation (7) the characteristic equation
for definition of four parameters $\lambda_i (i = 1, 2, 3, 4)$ can be obtained:

$$\lambda^4 + \phi^2(\alpha + \beta)\lambda^2 - \phi^2(1 - \alpha \beta \phi^2) = 0. \quad (9)$$

The general solution of equations (7) and (8) are

$$\eta(\xi) = A_1 \cos p\xi + A_2 \sin p\xi + A_3 \cosh r\xi + A_4 \sinh r\xi, \quad (10)$$

$$\varphi(\xi) = B_1 \cos p\xi + B_2 \sin p\xi + B_3 \cosh r\xi + B_4 \sinh r\xi, \quad (11)$$

where the characteristic numbers $p$ and $r$:

$$p(\phi) = \sqrt{\frac{\phi^2(\alpha + \beta)}{2} + \frac{\phi^4(\alpha + \beta)^2}{4} + \phi^2(1 - \alpha \beta \phi^2)}, \quad (12)$$

$$r(\phi) = \sqrt{\frac{-\phi^2(\alpha + \beta)}{2} - \frac{\phi^4(\alpha + \beta)^2}{4} + \phi^2(1 - \alpha \beta \phi^2)} \quad (13)$$

It follows from (13), that at $\alpha \beta \phi^2 = \omega^2 \frac{L}{GF} > 1$ or $\omega > \omega^*$ ($\omega^* = \sqrt{GF/L}$ is the cut-off frequency) parameter $r$ becomes imaginary and hyperbolic functions in (9) and (10) are transformed into trigonometrical functions. Note that all frequencies of the second spectrum are placed after the value $\omega^*$.

The constants in the expressions for $\eta(\xi)$ and $\varphi(\xi)$ are not independent. By usage, for example, one of the equations of (3), the relationship between these constants can be established:

$$B_2 = d_1 A_1, \quad B_1 = -d_1 A_2, \quad B_4 = d_2 A_3, \quad B_3 = d_2 A_4,$$

where $d_1(\phi) = -p + \frac{\beta}{p} \phi^2$, $d_2(\phi) = r + \frac{\beta}{r} \phi^2$.

As a result the expression for $\varphi(\xi)$ takes the form:

$$\varphi(\xi) = -d_1 A_2 \cos p\xi + d_1 A_1 \sin p\xi + d_2 A_4 \cosh r\xi + d_2 A_3 \sinh r\xi. \quad (14)$$

### 3. Dynamic stiffness matrix of Timoshenko beam.

At present for calculation of beam systems the finite element method (FEM) is widely used. The dynamic matrix of a basic finite element $[K]$ bounds the vector of nodal forces $\{Q\}$ with the vector of nodal displacements $\{q\}$

$$\{Q\} = [K] \{q\}, \quad (15)$$

where
The elements of the dynamic matrix are the influence functions of the displacements \( \{q\} \) on the forces \( \{Q\} \). The indexes 1 and 2 in the expressions for \( \{Q\} \) and \( \{q\} \) determine that the considering value belongs to the left or to the right end of the finite element respectively.

The shearing forces and the bending moments at their positive directions, adopted in FEM, are determined by the expressions:

\[
N_1 = -GF \left( \frac{d\eta}{d\xi} - \phi \right)_{\xi=0}, \quad N_2 = GF \left( \frac{d\eta}{d\xi} - \phi \right)_{\xi=1}
\]

\[
M_1 = \frac{EI}{l} \left( \frac{d\phi}{d\xi} \right)_{\xi=0}, \quad M_2 = -\frac{EI}{l} \left( \frac{d\phi}{d\xi} \right)_{\xi=1}
\]

In order to determine the dynamic matrix \( K(\phi) \) the following sequence of computations was used:

a) the constants \( A_i (i=1,2,3,4) \) in (10) and (14) were expressed through the components of \( \{q\} \); b) further, using dependences (17-18), the nodal forces are determined. Then, by using of (15) the elements \( k_{ij} (i,j=1,2,3,4) \) of the dynamic matrix are obtained.

Below, it is supposed to analyze a free vibration of a prismatic Timoshenko beam. The left end of the beam \( (\xi = 0) \) is simply supported and the right end \( (\xi = 1) \) is fully fixed. Let's write out the necessary dependences.

The boundary conditions of the beam:

\[
\xi = 0: \quad \eta = 0, \quad d\phi / d\xi = 0; \quad \xi = 1: \quad \eta = 0, \quad \phi = 0.
\]

Taking into account (16) and (19) the frequency equation and the expressions for the modes of free vibration of the beam \( (\eta(\xi), \phi(\xi)) \) can be derived.

The frequency equation:

\[
\text{Det} \left( \phi \right) = k_{22}(\phi) = d_2(\phi)\sin p(\phi) \cosh r(\phi) + d_1(\phi)\cos p(\phi) \sinh r(\phi) = 0,
\]

or in the simplified form:

\[
\frac{d_2(\phi)}{d_1(\phi)} \tan p(\phi) = -\tanh r(\phi).
\]

The modes of free vibration for a fixed value of the frequency parameter \( \phi \), additionally to the transversal displacements \( \eta(\xi) \), includes the rotary angle of gross-section of the beam \( \phi(\xi) \) or the bending part of the whole transversal deflection \( \eta_b(\xi) \) are:

\[
\eta(\xi) = \left( \sin p\xi - \frac{\sin p}{\sinh r} \sinh r\xi \right) \phi_1,
\]

\[
\eta_b(\xi) = \left( \sin p\xi - \frac{\sin p}{\sinh r} \sinh r\xi \right) \phi_1.
\]
\[ \varphi(\xi) = -\left( \frac{d}{d\xi} p_1 \cos \xi + d_2 \frac{\sin p}{\sinh r} \right) \varphi_1, \quad (22) \]

\[ \eta_h(\xi) = \int_0^\xi \varphi(\xi) d\xi = -\left( \frac{d}{d\xi} \frac{p\sin \xi}{p} + d_2 \frac{\sin p}{\sinh r} \right) \varphi_1. \quad (23) \]

The orthogonality conditions with respect to the potential and kinetic energies can be written respectively so:

\[ \beta \left[ \eta_k(\xi) \eta_i(\xi) d\xi + \int_0^\xi \left( \frac{d\eta_k(\xi)}{d\xi} \varphi_k(\xi) \right) \left( \frac{d\eta_i(\xi)}{d\xi} \varphi_i(\xi) \right) d\xi \right] = \begin{cases} \neq 0 \text{npu} & k = i \\ = 0 \text{npu} & k \neq i \end{cases} \quad (24) \]

\[ \eta_k(\xi) \eta_i(\xi) d\xi + \int_0^\xi \varphi_k(\xi) \varphi_i(\xi) d\xi = \begin{cases} \neq 0 \text{npu} & k = i \\ = 0 \text{npu} & k \neq i \end{cases} \quad (25) \]

In conclusion of this section to consider in more detail V. Nesterenko’s paper [8] that became as a theoretical basis for rejections of actual physical existence of the second spectrum in the Timoshenko beam theory (TBT). The author selected the Lagrangian, from which by the variational way the Timoshenko equation was obtained. In oppose of (2), Nesterenko’s Lagrangian contains derivatives with respect to time both of the first and the second orders.

Further, following to M. Ostrogradski [9] and using the Legendre transformations, instead of the derivatives \( \frac{\partial w}{\partial t}, \frac{\partial^2 w}{\partial t^2} \) the generalized corresponding impulses \( p_1 \) and \( p_2 \) were introduced [11].

The Hamiltonian function was defined by

\[ \Psi = p_1 \frac{\partial w}{\partial t} + p_2 \frac{\partial^2 w}{\partial t^2} - L \left( \frac{\partial^2 w}{\partial \xi^2}, p_1, p_2 \right) \quad (26) \]

The substitution of the expressions for impulses in (26) leads to the expression for the density of some energy, which does not coincide with the density of Timoshenko beam energy [2]. From this it may be concluded that the author of [9] does not have enough arguments and proofs for rejection of the presence the second spectrum in the Timoshenko beam theory.

Let's remark, that usage of the Lagrangian in the form (2) leads to the Hamiltonian function, which is identical to the density of the mechanical energy of Timoshenko beam.

4. Discrete modal of Timoshenko beam

It is marked in some publications that the appearance of the second spectrum is obliged to the presence at equations (4) and (5) the terms with the derivative of the fourth order with respect to the time. And it is supposed that the presence of such terms adds to the Timoshenko equations some specificity which contrasted with the d'Alembert’s dynamic equations that have the time derivatives only of the second order. To refuse or to agree with the conclusion about the reason of
the appearance of the second spectrum it is possible by comparison the behavior of the Timoshenko beam with the behavior of its discrete modal.

Replace the Timoshenko beam by the weightless prismatic beam having the same values for flexural and shearing rigidities. Along the axis of the beam equally spaced concentrated masses are located. Each mass possesses by inertia at the transversal and angular rotation directions. The value of the mass possessing by inertia at the transversal deflection is defined by \( M = ml / N \), and the value of mass with inertia on the rotational deflection of the cross-section of the beam - \( R = L l / N \) ( \( N \) is the number of finite elements on which the beam is divided).

The finite element constructed in the section 3 is used as the basic element but with the approximate value for the dynamic matrix: \([K] = [K^*] - \omega^2 [M^*]\). The stiffness matrix \([K^*]\) and the mass matrix \([M^*]\) are defined by

\[
[K^*] = \frac{EI}{1 + 12 \beta_1} \begin{bmatrix}
2/a & 1 & -(2/a) & 1 \\
1 & 2(1 + 3 \beta_1)/3 & -1 & (1 - 6 \beta_1)/3 \\
-(2/a) & -(1/a) & 2/a & -(1/a) \\
1 & (1 - 6 \beta_1)/3 & -(1/a) & 2(1 + 3 \beta_1)/3 \\
\end{bmatrix},
\]

\[
[M^*] = \begin{bmatrix}
M_1 & 0 & 0 & 0 \\
0 & R_1 & 0 & 0 \\
0 & 0 & M_2 & 0 \\
0 & 0 & 0 & R_2 \\
\end{bmatrix},
\]

where \( a = 1/N \) is non-dimensional length of the basic finite element; \( \beta_1 = EI / GA a^2 \). Let's remark, that the stiffness matrix \([K^*]\) describes precisely the behavior of the non-weighted finite element with taking into account of its bending and shearing rigidities.

The displacements \( \eta(\xi) \) and its flexural component \( \eta_b(\xi) \) for each finite element are determined by

\[
\eta(\xi) = \eta_b(\xi) - \beta_1 \frac{d^2 \eta_b(\xi)}{d\xi^2}, \quad \xi = x / a,
\]

\[
\eta_b(\xi) = \eta_1 E_1(\xi) + \phi_1 E_2(\xi) + \eta_2 E_3(\xi) + \phi_2 E_4(\xi),
\]

where the Hermite functions \( E_i(\xi) \quad (i=1,2,3,4) :\)

\[
E_1(\xi) = \gamma (1 - 3 \xi^2 + 2 \xi^3 + 6 \beta_1),
\]

\[
E_2(\xi) = \frac{\gamma}{n} \left( \frac{\xi}{\gamma} - 2 \xi^2 (1 + 3 \beta_1) + \xi^3 - 4 \beta_1 (1 + 3 \beta_1) \right),
\]

\[
E_3(\xi) = \gamma (3 \xi^2 - 2 \xi^3 + 6 \beta_1),
\]

\[
E_4(\xi) = \frac{\gamma}{n} \left( \xi^2 (6 \beta_1 - 1) + \xi^3 + 12 \beta_1^2 - 2 \beta_1 \right), \quad \gamma = 1/1 + 12 \beta_1
\]

The displacement of the whole beam is determined by combining of the finite element displacements.

The matrix equation for definition of the frequencies and corresponding modes, when the finite element method is used, can be presented so:
\[
\left( [K_\Sigma] - \omega^2 [M_\Sigma] \right) \{ q_\Sigma \} = 0 ,
\]
and the frequency equation:
\[
\left[ K_\Sigma \right] - \omega^2 \left[ M_\Sigma \right] = 0 .
\]

Here \([K_\Sigma]\) and \([M_\Sigma]\) are the global stiffness and mass matrices; \(\{ q_\Sigma \}\) is the vector of
generalized nodal displacements of the discrete modal of Timoshenko beam. Each \(i\)-th node in
the vector \(\{ q_\Sigma \}\) possesses by two components: the transversal deflection \(\eta_i\) and the angular
rotation of the cross-section \(\varphi_i\). The total number of degree of freedom the discrete elastic system
is equal to \(2N\).

Requirements of the orthogonality of free vibration modes of the discrete modal with respect
to potential and kinetic energies are expressed by
\[
\begin{align*}
\{ q \}^T [K] \{ q \} &= \begin{cases} 
0 & \text{for } k = i \\
0 & \text{for } k \neq i
\end{cases} \\
\{ q \}^T [M] \{ q \} &= \begin{cases} 
0 & \text{for } k = i \\
0 & \text{for } k \neq i
\end{cases}
\end{align*}
\]
(26)

The written above in this section dependencies will be used below for numerical calculations.

5. Numerical calculations and analyses.

Let's expose to the analysis of free vibrations of a steel two-tee prismatic beam having the
following parameters: length \(l = 5m\), breadth of upper and lower belts and also the height of the
wall - \(1m\), thickness of the latter elements - \(1cm\), Young's modulus \(E = 200 \cdot 10^9 \text{N/m}^2\),
Poisson's ratio \(\nu = 0.3\), shear modulus \(G = E / 2(1 + \nu) = 77 \cdot 10^9 \text{N/m}^2\), density \(\rho = 7850 \text{kg/m}^3\).
The boundary conditions of the beam are expressed by (20).

Using these dates it was defined: the moment of inertia of cross section of the beam
\(I = 5.8 \cdot 10^3 \text{m}^4\); the flexural stiffness \(E I = E \cdot I = 1.17 \cdot 10^9 \text{Nm}^2\); the shearing rigidity of the
beam cross section \(GF = G \cdot F = 7.7 \cdot 10^8 \text{N}\) (the area of the cross-section for shearing rigidity is
equal to cross-section of the wall \(F = 10^{-2} \text{m}^2\)); the per unit length mass \(m = 234 \text{kg/m}\); the
moment of inertia of gyration of masses \(L = \rho \cdot I = 45.5 \text{Nm}\).

Given below the results of numerical calculations of free vibration of the considered beam are
obtained by usage of the dependences of the Timoshenko beam theory (TBT) (section 3) and by
usage of the dependences of the finite element method (FEM) (section 4). At usage of FEM the
beam is divided into 100 equal finite elements.

The first five frequencies for the first and second spectra were calculated by TBT and FEM
and given in table 1. The ordinal number of the second spectrum frequency is given in the last but
one column of the table 1. From this table one can conclude that numerical values for the
frequencies obtained by TBT and FEM practically coincide. It is one of the proofs of actual
existence of the second spectrum of TBT.

All results given below are concerned with the modes of free vibration with the third
frequencies of the first and the second spectra of Timoshenko beam theory.
Table 1. Comparison of natural frequencies obtained by TBT and FEM solutions

<table>
<thead>
<tr>
<th>No</th>
<th>First spectrum</th>
<th>Second spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TBT</td>
<td>FEM</td>
</tr>
<tr>
<td>1</td>
<td>9,09</td>
<td>9,09</td>
</tr>
<tr>
<td>2</td>
<td>24,22</td>
<td>24,22</td>
</tr>
<tr>
<td>3</td>
<td>41,93</td>
<td>41,94</td>
</tr>
<tr>
<td>4</td>
<td>60,66</td>
<td>60,67</td>
</tr>
<tr>
<td>5</td>
<td>98,70</td>
<td>98,71</td>
</tr>
</tbody>
</table>

The following notations are used:

\( \eta^{(i)}(\xi) \) is the whole transversal deflection for \( i-th \) spectrum (\( i=1 \) - the first and \( i=2 \) - the second spectrum), calculated by TBT;

\( \eta_b^{(i)}(\xi) \) is the bending component of \( \eta^{(i)}(\xi) \);

\( \eta_s^{(i)}(\xi) \) is the shearing component of \( \eta^{(i)}(\xi) \);

\( \phi_{\text{lim}}^{(i)}(\xi) \) is the angle of rotation of cross-section of a beam, calculated by TBT.

\( \nu^{(i)}(\xi), \nu_b^{(i)}(\xi), \nu_s^{(i)}(\xi), \phi_{\text{fem}}^{(i)}(\xi) \) are analogical values but calculated by FEM.

Figure 1 shows the mode shapes of free vibrations with the frequency of the first spectrum calculated by TBT and FEM respectively. The mode shapes of free vibrations with the frequency of the second spectrum calculated by TBT and FEM are presented in figure 2. One can see that mode shapes in figures 1 and 2 obtained with TBT are completely conformed to the analogical mode shapes obtained by FEM. This result can be considered as one additional proof for the existence of the second spectrum in the Timoshenko beam theory.

![Figure 1](image-url)

**Figure 1.** The mode shapes of the first spectrum:

\( \eta^{(1)}(\xi) \) (–) and \( \nu^{(1)}(\xi) \) (…)
The whole mode shapes for the free vibrations with the frequencies of the first and second spectra respectively are presented in figure 3. It is evident that their shapes are essentially differed. However, their average amplitudes are enough similar.

The whole mode shape with it’s bending and shearing components for the third frequency of the first spectrum are shown in figure 4. Here the well known fact that for frequencies of the first spectrum the bending and shearing components have the same phase with the whole mode shape.

Figure 2. The mode shapes of the second spectrum:
\( \eta^{(2)}(\xi) \) (−) and \( v^{(2)}(\xi) \) (…).

Figure 3. The whole mode shapes of free vibrations for the fist spectrum
\( \eta^{(1)}(\xi) \) (−) and for the second spectrum \( \eta^{(2)}(\xi) \) (…).
Figure 4. The mode shape \( \eta^{(1)}(\xi) \) (—) with it’s the bending \( \eta^{(1)}_b(\xi) \) (····) and shearing \( \eta^{(1)}_s(\xi) \) (−−−) components of the first spectrum.

The third frequency mode shape, but for the second spectrum, with it’s bending and shearing components are shown in figure 5. One can see that in this case the bending and shearing components are in anti-phase and the mode shape amplitude is significant less than amplitudes of its components.
The curves of the angles of rotation of gross-section of the beam for the third mode shapes of both spectra are given in figure 6. The forms of the two curves in this figure is enough identical. But one, the deserved special attention fact: the both curves have the same number of nodal points and this number coincides with the ordinal number of the corresponding frequencies in each distinct spectrum.

Two fragments of graphical definition of frequencies are given in figures 7 and 8. Here additional notations for the left and right parts of the frequency equation (23) are used:

\[ F_1(\omega) = \frac{d_2(\phi(\omega))}{d_1(\phi(\omega))} \tan p(\phi(\omega)), \quad F_2(\omega) = -\tanh(\phi(\omega)). \]

The frequency region \((\omega 1)\) in figure 7 is located from the left with respect to cut-off frequency \(\omega^*\). In this region the intersections of the curves \(F_1(\omega)\) and \(F_2(\omega)\) determine only the frequency of the first spectrum. The frequency region shown in fig.8 is arranged to right from \(\omega^*\). In this region the hyperbolic tangent in \(F_2(\omega)\) transforms in the trigonometric tangent and each branch of the last tangent has two points of intersection with the function \(F_1(\omega)\). The
cross point located on the right corresponds to the frequency of the first spectrum, and the second point of intersection determines the frequency of the second spectrum.

**Figure 7.** The fragment of graphical definition of the frequencies in the region $\omega < \omega^*$. $F_1(\omega l)$ (→), $F_2(\omega l)$ (⋯)

From the executed numerical calculations it can be concluded that the conditions of orthogonality (24) and (25) for the Timoshenko beam and the condition of orthogonality (26) for its discrete model are completely fulfilled, both, inside of each spectrum, and between modes belonging to different spectra.

**Figure 8.** The fragment of graphical definition of the frequencies in the region $\omega > \omega^*$. $F_1(\omega l)$ (→), $F_2(\omega l)$ (⋯)

**Conclusion**

All specific features of the Timoshenko beam bounded with the frequencies of the second spectrum were in detail conformed by the comparison with the behavior of its discrete multi mass modal. The final statement – the second spectrum in the Timoshenko beam theory is the physical reality.
References


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V.A.. Postnov, St. Petersburg State Marine Technical University, Lozmanskay str., 3, St. Petersburg, 190008.
Figure 1. The mode shapes of the first spectrum:
\( \eta^{(1)}(\xi) \) (—) and \( \nu^{(1)}(\xi) \) (····)

Figure 2. The mode shapes of the second spectrum:
\( \eta^{(2)}(\xi) \) (—) and \( \nu^{(2)}(\xi) \) (····)
Figure 3. The whole mode shapes of free vibrations for the first spectrum \( \eta^{(1)}(\xi) \) (—) and for the second spectrum \( \eta^{(2)}(\xi) \) (····).

Figure 4. The mode shape \( \eta^{(1)}(\xi) \) (—) with its bending \( \eta_b^{(1)}(\xi) \) (····) and shearing \( \eta_s^{(1)}(\xi) \) (····) components of the first spectrum.
Figure 5. The mode shape $\eta^{(2)}(\xi)$ (→) with it’s the bending $\eta^{(2)}_{b}(\xi)$ (····) and shearing $\eta^{(2)}_{s}(\xi)$ (·--·) components of the second spectrum.

Figure 6. The curves of the angles of rotation of cross-section of the beam: $\varphi^{(1)}(\xi)$ for the first spectrum (→) and $\varphi^{(2)}(\xi)$ for the second spectrum (····). $\eta^{(1)}(\xi)$ (→) and for the second spectrum $\eta^{(2)}(\xi)$ (····).
Figure 7. The fragment of graphical definition of the frequencies in the region $\omega < \omega^*$. $F_1(\omega l)$ (―), $F_2(\omega l)$ (· · ·)

Figure 8. The fragment of graphical definition of the frequencies in the region $\omega > \omega^*$. $F_1(\omega l)$ (―), $F_2(\omega l)$ (· · ·)