

Acoustic Identification of the Anisotropic Nanocrystalline Medium with Non-Dense Packing of Particles

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Abstract—A two-dimensional model of the anisotropic nanocrystalline (granular) medium being a rectangular lattice of elastically interacting elliptical particles with translational and rotational degrees of freedom was considered. In the long-wave approximation a system of linear equations in partial derivatives describing the propagation of the longitudinal, transverse, and rotational waves in such a system was obtained. The dependences of the wave velocities on the grain size and form were analyzed. It was shown how to determine the moduli of elasticity of the granular material from the change of the velocities of the acoustic waves propagating along different crystallographic directions.

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INTRODUCTION

At present there is a gap between the level of the development of technologies for the fabrication of materials with micro- and nanostructures and the possibility of their theoretical description and forecasting their properties. In general, a “microstructure” of a medium means that a medium has several scales (structural levels), their self-consistent interaction and the possibility of the energy transfer from one level to the other. The real values of the medium “microscales” can vary in the region of both micrometers and nanometers or angstroms. From the point of view of the methodology of a theoretical investigation, of importance are not their absolute values, but rather the smallness of one scale with respect to the other. It is another story that, when studying real physical, chemical, or biological systems, the effects of the “microstructure” are manifested most vividly at the region of nanometers and below. At the nanoscale level the classical ideas starts to contradict the actual nature of the physical properties of matter and it is necessary to take into account their quantum-mechanical essence. However, the theoretical estimates show that one can use the classical ideas and analogies in order to study acoustic vibrations of the crystalline structures at the nanoscale level [1, 2].

Media with a complicated structure are studied insufficiently (in particular, this refers to the elaboration of the dependences between the parameters of the medium microstructure and its macroproperties). This hampers the development of diagnostics of promising materials the properties of which are determined by their micro- and nanoscale structure. It is appropriate to perform such studies with the help of acoustic waves which, in contrast to the electromagnetic waves

and X-ray radiation, can propagate in the medium bulk, which the latter do not penetrate. Acoustic waves are internal vibrations of the material, and they yield information about its geometric structure and physical properties, but in encoded form. One has to be able to decode this information.

The first experiments on acoustics of the solid state with a microstructure were performed in 1970 by G.N. Savin et al. [3, 4]. The authors established the correlation between the grain size in different metals and aluminum alloys and the dispersion of the acoustic wave. Dispersion of the ultrasound waves was also observed in an artificial composite—ferrite pellets in epoxy resin [5].

It should be noted that, in media with a microstructure, there are several types of waves—the so-called acoustic and optical phonons and pumping of energy from one type of waves to the other is possible [6]. It is necessary to take this into account when performing both theoretical and experimental studies. In [7] it was shown that the presence of microrotations in crystals leads to the appearance of the spatial dispersion and new wave modes. Chapter 4 in [8] deals with the analysis of spin and acoustic waves in ferromagnets. Elastic waves are considered in the classical theory without taking into account microrotations, but it is shown that, due to the relatedness of the elastic deformations with the magnetic field of spins, the stress tensor is no longer symmetric, i.e., in an elastic ferromagnet there appear couple stresses at the excitation of the spin waves. Analysis of the dispersion properties showed that the acoustic wave with the “left-hand” circular polarization interacts with the spin wave much more strongly than the acoustic wave with the “right-hand” polarization.

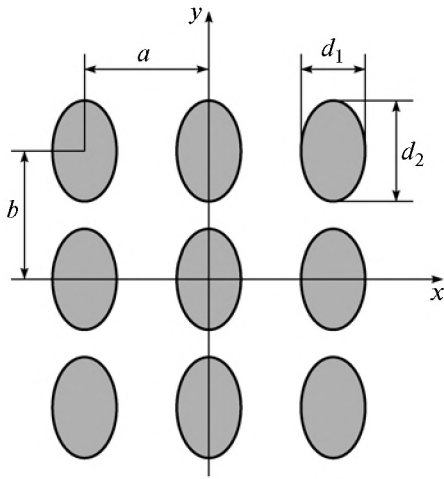


Fig. 1. Rectangular lattice of elliptical particles.

In the last twenty years, the processes of propagation and interaction of acoustic waves in media with microstructure have been extensively studied theoretically and experimentally (see, e.g., [9–13]). However, the main attention is paid to the analysis of the propagation of the longitudinal and shift waves, and the propagation of rotational waves (waves of microrotations) is studied less. Note [14, 15] on studying the nonlinear interactions of the longitudinal waves and waves of microrotations as applied to the problems of seismic acoustics and [16–20] in which the processes of the propagation and interaction of the longitudinal, transverse and rotational waves in crystalline media were studied.

In this work it is proposed to use the acoustic method for the determination of the elastic properties of the anisotropic nanocrystalline (granular) material with the nondense packing of particles based on measuring the velocities of elastic waves propagating along different crystallographic directions [21]. Such material is simulated by a rectangular lattice of rigid ellipsoid particles (an idealization is used in which material grains are considered ellipsoids [22]). Each particle of this lattice has two translational and one rotational degree of freedom. Such a model is a synthesis of a chain of rectangular particles and a square lattice of round particles considered in [18] and [23]. The space between particles is a non-mass medium that transfers the force and momentum impacts. The work is mainly aimed at obtaining equations of motion and elaboration of the interrelations between the physical-mechanical properties of the granular material and parameters of its microstructure. To achieve these aims we use the method of structural simulation [24]. The structural models contain parameters characterizing the geometry of the material (lattice period, particle size and form) and therefore they are the most appropriate ones for studying the influence of

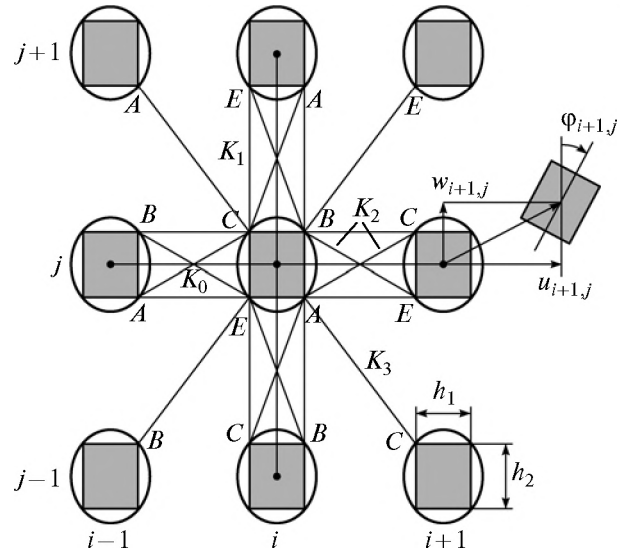


Fig. 2. Scheme of force interactions between anisotropic particles and kinematics.

the dimension effects on the macroproperties of the material.

DISCRETE MODEL

We consider a two-dimensional rectangular lattice consisting of homogeneous particles (grains or granules) with mass M having the form of an ellipse with axes lengths d_1 and d_2 as a model of medium with nondense packing of particles. In the initial state, they are concentrated in the lattice sites and the distance between the centers of gravity of the neighboring granules along the x axis is a and along the axis y is b (Fig. 1). When moving in the plane, each particle has three degrees of freedom: the displacement of the center of gravity of the particle with the number $N = N(i, j)$ along the axes x and y (translational degrees of freedom $u_{i,j}$ and $w_{i,j}$) and the rotation with respect to the center of gravity (rotational degree of freedom $\phi_{i,j}$) (Fig. 2). The kinetic energy of the particle $N_{i,j}$ is described by the formula

$$T_{i,j} = \frac{M}{2}(\dot{u}_{i,j}^2 + \dot{w}_{i,j}^2) + \frac{J}{2}\dot{\phi}_{i,j}^2,$$

where $J = M(d_1^2 + d_2^2)/16$ is the inertia of the particle with respect to the axis passing through the center of gravity.

It is considered that the particle N interacts only with the eight nearest neighbors in the lattice. The centers of gravity of the four of them are located at the distance a along the axis x and b along the axis y from the particle N (these are particles of the first coordination sphere). The centers of gravity of the other four are in the diagonals of the rectangular lattice (these are particles of the second coordination sphere) (Fig. 2).

The central and non-central interactions of the neighboring granules are simulated by elastic springs of four types [23]: central (with rigidity K_0), noncentral (with rigidity K_1), “diagonal” (K_2), and also springs connecting the central particle with the grains of the second coordination sphere (K_3). The interactions at tension-compression of the material are simulated by the central and noncentral springs. The momenta at the rotations of particles are transferred through springs of the K_1 type. Springs with the rigidity K_2 characterize the force interactions of particles at the shift deformations in the material. The points of junctions of the springs with particles are in the apexes of the rectangle of the maximum area inscribed in the ellipse (Fig. 2).

Each rectangle has the size $h_1 \times h_2$, where $h_1 = d_1/\sqrt{2}$, $h_2 = d_2/\sqrt{2}$.

It is assumed that the displacements of the grains are small in comparison with the dimensions of the elementary cell of the considered lattice. The interaction of particles at the displacements from the equilibrium is determined by the relative elongations of the springs (Fig. 2). The potential energy due to the interaction of the particle N with eight nearest neighbors in the lattice is described by the formula

$$U_N = \frac{1}{2} \left(\sum_{n=1}^4 \frac{K_0}{2} D_{0n}^2 + \sum_{n=1}^8 \frac{K_1}{2} D_{1n}^2 + \sum_{n=1}^8 \frac{K_2}{2} D_{2n}^2 + \sum_{n=1}^4 \frac{K_3}{2} D_{3n}^2 \right), \quad (1)$$

where D_{ln} ($l = 0, 1, 2, 3$) are the elongations of the springs of the four types numbered in the arbitrary order connecting the particle with its neighbors. The elongations of the central springs are determined by the changes of the distances between the geometrical centers of the rectangles $ABCE$ inscribed in the ellipses (Fig. 2), and the tensions of other springs are characterized by the variations of the distances between the apexes of these rectangles. Expression (1) contains an additional factor $1/2$, since the potential energy of each spring is equally divided between two particles connected by this spring.

We denote $\Delta u_i = u_{i,j} - u_{i-1,j}$ and $\Delta u_j = u_{i,j} - u_{i,j-1}$, then $\Delta u_{i+1} = u_{i+1,j} - u_{i,j}$ and $\Delta u_{j+1} = u_{i,j+1} - u_{i,j}$. The expressions for the elongations of the springs calculated in the approximation of smallness of the quantities $\Delta u_i \sim \Delta w_i \sim a\varepsilon$, $\Delta u_j \sim \Delta w_j \sim b\varepsilon$ and $\Phi_i = (\varphi_{i-1,j} + \varphi_{i,j})/2 \ll \pi/2$ have the form

$$\begin{aligned} D_{0(i-1,j)} &= \Delta u_i \sim D_{0(i+1,j)}, \\ D_{0(i,j-1)} &= \Delta w_j \sim D_{0(i,j+1)}, \\ D_{1(i-1,j)}^{CB,EA} &= \Delta u_i \pm \frac{h_2}{2} \Delta \varphi_i \sim D_{1(i+1,j)}^{BC,AE}, \end{aligned}$$

$$D_{1(i,j-1)}^{EC,AB} = \Delta w_j \pm \frac{h_1}{2} \Delta \varphi_j \sim D_{1(i,j+1)}^{CE,BA},$$

$$D_{2(i-1,j)}^{CA,EB} = \frac{1}{r_1} ((a-h_1)\Delta u_i \pm h_2\Delta w_i \pm ah_2\Phi_i) \sim D_{2(i+1,j)}^{AC,BE},$$

$$D_{2(i,j-1)}^{AC,EB} = \frac{1}{r_2} ((b-h_2)\Delta w_j \pm h_1\Delta u_j \mp bh_1\Phi_j) \sim D_{2(i,j+1)}^{CA,BE},$$

$$D_{3(i-1,j-1)}^{EB} = \frac{1}{r_3} ((a-h_1)(u_{i-1,j-1} + u_{i,j}) \quad (2)$$

$$+ (b-h_2)(\Delta w_i + \Delta w_j) + (bh_1 - ah_2)(\varphi_{i-1,j-1} + \varphi_{i,j})),$$

$$D_{3(i+1,j+1)}^{BE} \sim D_{3(i-1,j-1)}^{EB},$$

$$D_{3(i+1,j-1)}^{AC} = \frac{1}{r_3} ((a-h_1)(\Delta u_i - \Delta u_j)$$

$$+ (b-h_2)(\Delta w_j - \Delta w_i) + (ah_2 - bh_1)(\varphi_{i+1,j-1} + \varphi_{i,j})),$$

$$D_{3(i-1,j+1)}^{CA} = \frac{1}{r_3} ((a-h_1)(\Delta u_j - \Delta u_i)$$

$$+ (b-h_2)(\Delta w_i - \Delta w_j) + (ah_2 - bh_1)(\varphi_{i-1,j+1} + \varphi_{i,j})).$$

Here $r_1 = \sqrt{(a-h_1)^2 + h_2^2}$, $r_2 = \sqrt{(b-h_2)^2 + h_1^2}$, $r_3 = \sqrt{(a-h_1)^2 + (b-h_2)^2}$ are the distances at the initial time moment between the neighboring particles, respectively, along the x -axis, y -axis, and along the diagonal (Fig. 2). In (2), the notations of the elongations of all springs except for the central ones consist of three components. The first subscript corresponds to the rigidity of this spring (0, 1, 2 or 3). The second subscript is in parentheses and indicates the number of the particle, which the given spring connects with the central particle $N_{i,j}$. The third (super)script stands for the apexes of the rectangles connected by the given spring. The apex of the central rectangle is given first. In formulas (2) there are \pm and \mp signs; therefore, the third index consists of two parts: first, the apexes of the rectangles connected by the first spring (the upper signs of the \pm and \mp symbols are taken for the elongations of such springs) are indicated and after the comma those of the second spring (in this case the bottom signs of such symbols are taken). Tensions of springs denoted by the equivalence signs are obtained by the substitution of indices i by $i+1$ and j by $j+1$. The notations of the tensions of the central springs consist of only the two mentioned above subscripts. It should be also noted that tensions of the springs of the second coordination sphere in this approximation depend on the rotations of particles, but this dependence disappears when the condition of the similarity between the form of the particles and the lattice form holds, when $b/a = h_2/h_1$. This condition will be discussed in detail below.

With the help of relationships (2), in which only linear terms for the elongations of springs are taken into account, the following expression for the potential energy per particle with the number $N = N_{i,j}$ is deduced with accuracy to the terms on the order of ε^2 inclusive (the analogous expression with the accuracy to the terms on the order of ε^3 inclusive was obtained in [25]):

$$\begin{aligned} U_{i,j} = & (B_1(\Delta u_i)^2 + B'_1(\Delta w_j)^2) \\ & + (B_2(\Delta u_j)^2 + B'_2(\Delta w_i)^2) \\ & + R^2(B_3(\Delta \varphi_i)^2 + B'_3(\Delta \varphi_j)^2) \\ & + (B_4\Delta u_i\Delta w_j + B'_4\Delta u_j\Delta w_i) \\ & + (B_5\Delta w_i\Phi_i - B'_5\Delta u_j\Phi_j) + B_6\varphi_{ij}^2. \end{aligned} \quad (3)$$

In (3) terms with the coefficients B_1 , B'_1 and B_2 , B'_2 describe the energy of the longitudinal and shift deformations, terms with the coefficients B_3 , B'_3 , and B_6 describe the energy related to the noncentral (moment) interactions of the particles, and the terms in the two last parentheses describe the coupling energy of the transverse displacements with the longitudinal displacements and rotations of the particles, respectively. Here, $R = \sqrt{J/M} = \sqrt{d_1^2 + d_2^2}/4$ is the radius of inertia of the microparticles of the medium with respect to the center of gravity (obviously, $R = d/\sqrt{8}$ for the round particles with the diameter $d = d_1 = d_2$). The coefficients of expression (3) are explicitly expressed through the parameters of the micromodel and constants of the force interaction between particles:

$$\begin{aligned} B_1 = & \frac{a^2}{2} \left(K_0 + 2K_1 + \frac{2(a-h_1)^2}{r_1^2} K_2 + \frac{2(a-h_1)^2}{r_3^2} K_3 \right), \\ B'_1 = & \frac{b^2}{2} \left(K_0 + 2K_1 + \frac{2(b-h_2)^2}{r_2^2} K_2 + \frac{2(b-h_2)^2}{r_3^2} K_3 \right), \\ B_2 = & a^2 \left(\frac{h_2^2}{r_1^2} K_2 + \frac{(b-h_2)^2}{r_3^2} K_3 \right), \\ B'_2 = & b^2 \left(\frac{h_1^2}{r_2^2} K_2 + \frac{(a-h_1)^2}{r_3^2} K_3 \right), \\ B_3 = & \frac{a^2}{4R^2} \left(h_2^2 K_1 + \frac{a^2 h_2^2}{r_1^2} K_2 + \frac{(ah_2 - bh_1)}{r_3^2} K_3 \right), \end{aligned}$$

$$B'_3 = \frac{b^2}{4R^2} \left(h_1^2 K_1 + \frac{b^2 h_1^2}{r_2^2} K_2 + \frac{(ah_2 - bh_1)}{r_3^2} K_3 \right), \quad (4)$$

$$B_4 = 2a^2 \frac{(a-h_1)(b-h_2)}{r_3^2} K_3,$$

$$B'_4 = 2b^2 \frac{(a-h_1)(b-h_2)}{r_3^2} K_3,$$

$$B_5 = 2a \left(\frac{ah_2^2}{r_1^2} K_2 + \frac{(b-h_2)(ah_2 - bh_1)}{r_3^2} K_3 \right),$$

$$B'_5 = 2b \left(\frac{ah_1^2}{r_2^2} K_2 + \frac{(a-h_1)(ah_2 - bh_1)}{r_3^2} K_3 \right),$$

$$B_6 = \left(\frac{a^2 h_2^2}{r_1^2} + \frac{b^2 h_1^2}{r_2^2} \right) K_2 + \frac{(ah_2 - bh_1)^2}{r_3^2} K_3.$$

From the Lagrange equations of the second kind, one can obtain differential-difference equations describing the dynamics of the rectangular lattice of anisotropic particles. However, for the correlation of this model with the known solid-state theories, it is appropriate to consider the continuum approximation.

CONTINUUM APPROXIMATION

In the case of the long-wave perturbations, when $\lambda \gg a$, where λ is the characteristic spatial deformation scale, one can transfer from the discrete variables i and j to the continuous spatial variables $x = ia$ and $y = ja$. The functions given in the discrete points are interpolated by the continuous functions and their partial derivatives:

$$\begin{aligned} u_{i+l_1, j+l_2}(t) &= u(x+l_1a, y+l_2a, t) \\ &= u(x, y, t) + a \left(l_1 \frac{\partial u}{\partial x} + l_2 \frac{\partial u}{\partial y} \right) \\ &+ \frac{a^2}{2} \left(l_1^2 \frac{\partial^2 u}{\partial x^2} + 2l_1 l_2 \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} + l_2^2 \frac{\partial^2 u}{\partial y^2} \right) \\ &+ \frac{a^3}{6} \left(l_1^3 \frac{\partial^3 u}{\partial x^3} + 3l_1^2 l_2 \frac{\partial^2 u}{\partial x^2} \frac{\partial u}{\partial y} \right. \\ &\left. + 3l_1 l_2^2 \frac{\partial^2 u}{\partial x} \frac{\partial^2 u}{\partial y^2} + l_2^3 \frac{\partial^3 u}{\partial y^3} \right) + \dots, \end{aligned} \quad (5)$$

where $l_1 = 0, \pm 1$ and $l_2 = 0, \pm 1$ are the shifts of the numbers along the axes x and y of eight particles interacting with the central one. Then, if in expansions (5) we limit ourselves to taking into account only the terms on the order of $O(a)$, then the two-dimensional den-

sity of the Lagrange function L of the medium composed of the anisotropic particles has the form

$$L = \frac{\rho}{2}(u_t^2 + w_t^2 + R^2\varphi_t^2) - \frac{\rho}{2}[c_1^2(u_x^2 + \delta_1 w_y^2) + c_2^2(w_x^2 + \delta_2 u_y^2) + R^2 c_3^2(\varphi_x^2 + \delta_3 \varphi_y^2) + s^2(u_x w_y + \delta_4 u_y w_x) + 2\beta_1(w_x - \delta_5 u_y)\varphi + 2\beta_2\varphi^2]. \quad (6)$$

With the help of the Hamilton–Ostrogradsky variational principle, a system of the first-approximation differential equations describing the dynamic processes in the anisotropic crystalline medium is deduced from Lagrangian (6):

$$\begin{aligned} u_{tt} &= c_1^2 u_{xx} + \delta_2 c_2^2 u_{yy} + \frac{1 + \delta_4}{2} s^2 w_{xy} - \delta_1 \beta_1 \varphi_y, \\ w_{tt} &= c_2^2 w_{xx} + \delta_1 c_1^2 w_{yy} + \frac{1 + \delta_4}{2} s^2 u_{xy} - \beta_1 \varphi_x, \\ \varphi_{tt} &= c_3^2(\varphi_{xx} + \delta_3 \varphi_{yy}) + \frac{\beta_1}{R^2}(\delta_5 u_y - w_x) - \frac{2\beta_2}{R^2} \varphi. \end{aligned} \quad (7)$$

Here, the following notations are introduced: $c_i = \sqrt{2B_i/\rho ab}$ ($i = 1, 2, 3$) are the propagation velocities, respectively, of the longitudinal, shift waves and waves of microrotations, $s = \sqrt{2B_4/\rho ab}$ is the coefficient of the linear coupling between the longitudinal and shift deformations in the material, $\beta_1 = B_5/\rho ab$ and $\beta_2 = B_6/\rho ab$ are the dispersion parameters, $\rho = M/ab$ is the average value of the density of the studied two-dimensional medium, δ_i ($i = 1-5$) are the correction coefficients appearing due to the anisotropy of the studied medium:

$$\begin{aligned} \delta_1 &= \frac{b^2 r_1^2 r_2^2 r_3^2 (K_0 + 2K_1) + 2(b - h_2)^2 (r_3^2 K_2 + r_2^2 K_3)}{a^2 r_2^2 r_1^2 r_3^2 (K_0 + 2K_1) + 2(a - h_1)^2 (r_3^2 K_2 + r_1^2 K_3)}, \\ \delta_2 &= \frac{b^2 r_1^2 h_1^2 r_3^2 K_2 + (a - h_1)^2 r_2^2 K_3}{a^2 r_2^2 h_2^2 r_3^2 K_2 + (b - h_2)^2 r_1^2 K_3}, \\ \delta_3 &= \frac{b^2 r_1^2 h_1^2 r_2^2 r_3^2 K_1 + b^2 h_1^2 r_3^2 K_2 + (ah_2 - bh_1)^2 r_2^2 K_3}{a^2 r_2^2 h_2^2 r_1^2 r_3^2 K_1 + a^2 h_2^2 r_3^2 K_2 + (ah_2 - bh_1)^2 r_1^2 K_3}, \\ \delta_4 &= \frac{b^2}{a^2}, \\ \delta_5 &= \frac{br_1^2 bh_1^2 r_3^2 K_2 + (a - h_1)(ah_2 - bh_1)r_2^2 K_3}{ar_2^2 ah_2^2 r_3^2 K_2 + (b - h_2)(ah_2 - bh_1)r_1^2 K_3}. \end{aligned} \quad (8)$$

In the case when $\delta_i \neq 1$ at least at one i , Eqs. (7) become noninvariant with respect to the rotation of

the crystalline lattice by 90° and, therefore, they are a mathematical model of a strongly anisotropic medium [26]. If all anisotropy parameters δ_i are unity, then system (7) with accuracy to coefficients coincides with the equations for the hexagonal lattice of round particles deduced earlier [19, 27].

DEPENDENCE OF THE ANISOTROPY ON THE MICROSTRUCTURE

The structural simulation used in the work allows one to establish the interrelation between the microstructure and the macroproperties of the medium. In mechanics, this refers, first of all, to the dependence of the anisotropy and moduli of macroelasticity of the medium on its geometrical structure. These problems remain open in the phenomenological theories.

It is seen from expressions (8) that the dependences of the anisotropy parameters δ_i on the microstructure parameters are rather complicated, since they contain four force constants (K_0, K_1, K_2, K_3) and four geometrical parameters (a, b, h_1 and h_2). To simplify these expressions, we decrease the number of the geometrical parameters twice by assuming that the condition of similarity of the form of the particles to the lattice form holds

$$\frac{d_2}{d_1} = \frac{b}{a} \quad (9)$$

and introducing two new dimensionless quantities: $f = b/a = h_2/h_1$ is the *similarity coefficient* (or *form parameter*) and $p = d_1/a = h_1\sqrt{2}/a = h_2\sqrt{2}/b = d_2/b$ is the *relative particle size*. Then we consider the analysis of the dependence δ_i on these two quantities in more detail. With these assumptions equalities (8) take the form

$$\begin{aligned} \delta_1 &= \frac{f^2 r_1^2}{r_2^2} \times \frac{r_2^2 (K_0 + 2K_1) + f^2 (\sqrt{2} - p)^2 a^2 (K_2 + (r_2^2/r_3^2) K_3)}{r_1^2 (K_0 + 2K_1) + (\sqrt{2} - p)^2 a^2 (K_2 + (r_1^2/r_3^2) K_3)}, \\ \delta_2 &= \frac{p^2 (r_3^2/r_2^2) K_2 + (\sqrt{2} - p)^2 K_3}{p^2 (r_3^2/r_1^2) K_2 + (\sqrt{2} - p)^2 K_3}, \\ \delta_3 &= \frac{K_1 + (f^2 a^2/r_2^2) K_2}{K_1 + (a^2/r_1^2) K_2}, \\ \delta_4 &= f^2, \quad \delta_5 = \frac{r_1^2}{r_2^2} = \frac{(\sqrt{2} - p)^2 + f^2 p^2}{f^2 (\sqrt{2} - p)^2 + p^2}. \end{aligned}$$

Here,

$$\begin{aligned} r_1/a &= \sqrt{1 - p\sqrt{2} + p^2(f^2 + 1)/2}, \\ r_2/a &= \sqrt{f^2(1 - p\sqrt{2}) + p^2(f^2 + 1)/2}, \\ r_3/a &= \sqrt{(f^2 + 1)(\sqrt{2} - p)^2/2}. \end{aligned}$$

Note that at $f = 1$ $r_1/a = r_2/a = \sqrt{1 - p\sqrt{2} + p^2}$, $r_3/a = \sqrt{2} - p$ and, consequently, all $\delta_i = 1$ and, in addition, $\beta_1 = \beta_2$ (see. (11)). In other words, Eqs. (7) degenerate into the analogous equations for the medium with dense packing of particles [27], which, in turn, coincide with the equations of the Cosser two-dimensional continuum consisting of the central-symmetric particles [28]. A more detailed analysis of the dependence of the anisotropy parameters δ_i on the relative size of articles p and the form parameter f is given in [29].

EFFECT OF THE MICROSTRUCTURE ON THE ACOUSTIC CHARACTERISTICS OF THE MEDIUM

In two previous sections, the interrelation between the microstructure of the anisotropic medium with nondense packing and its macroparameters was established on the basis of structural simulation. Now we analyze the dependence of the acoustic characteristics of medium on the particle form and also on the particle size and parameters of the interparticle interaction with the help of this interrelation.

It follows from (4) that the coefficients of Eqs. (7) are expressed via the force constants K_0, K_1, K_2, K_3 , lattice parameters a and b and particle sizes h_1 and h_2 as follows:

$$\begin{aligned} c_1^2 &= \frac{a^2}{M} \left(K_0 + 2K_1 + \frac{2(a - h_1)^2}{(a - h_1)^2 + h_2^2} K_2 + \frac{2(a - h_1)^2}{(a - h_1)^2 + (b - h_2)^2} K_3 \right), \\ c_2^2 &= \frac{2a^2}{M} \left(\frac{h_2^2}{(a - h_1)^2 + h_2^2} K_2 + \frac{(b - h_2)^2}{(a - h_1)^2 + (b - h_2)^2} K_3 \right), \\ c_3^2 &= \frac{a^2}{2MR^2} \left(h_2^2 K_1 + \frac{a^2 h_2^2}{(a - h_1)^2 + h_2^2} K_2 + \frac{(ah_2 - bh_1)^2}{(a - h_1)^2 + (b - h_2)^2} K_3 \right), \\ s^2 &= \frac{4a^2}{M} \frac{(a - h_1)(b - h_2)}{(a - h_1)^2 + (b - h_2)^2} K_3, \end{aligned} \quad (10)$$

$$\begin{aligned} \beta_1 &= \frac{2a^2}{M} \left(\frac{h_2^2}{(a - h_1)^2 + h_2^2} K_2 + \frac{(b - h_2)(ah_2 - bh_1)}{a((a - h_1)^2 + (b - h_2)^2)} K_3 \right), \\ \beta_2 &= \frac{1}{M} \left(\left(\frac{a^2 h_2^2}{(a - h_1)^2 + h_2^2} + \frac{b^2 h_1^2}{(b - h_2)^2 + h_1^2} \right) K_2 + \frac{(ah_2 - bh_1)^2}{(a - h_1)^2 + (b - h_2)^2} K_3 \right). \end{aligned}$$

It is seen from relations (10) that, in the nanocrystalline (granular) media, the velocity of the wave propagation depends on four force constants K_0, K_1, K_2, K_3 and four geometric parameters: a, b, h_1 and h_2 . To simplify the analysis of such dependence, we assume as above that the condition of similarity of the form of the particles to lattice form (9) holds and substitute four geometric parameters by two dimensionless quantities: form parameter f and relative particle size p . In this case expressions (10) take the form

$$\begin{aligned} c_1^2 &= \frac{a^2}{M} \left(K_0 + 2K_1 + \frac{2(\sqrt{2} - p)^2}{(\sqrt{2} - p)^2 + f^2 p^2} K_2 + \frac{2}{1 + f^2} K_3 \right), \\ c_2^2 &= \frac{2a^2}{M} \left(\frac{f^2 p^2}{(\sqrt{2} - p)^2 + f^2 p^2} K_2 + \frac{f^2}{1 + f^2} K_3 \right), \\ c_3^2 &= \frac{4a^2 f^2}{M(1 + f^2)} \left(K_1 + \frac{2}{(\sqrt{2} - p)^2 + f^2 p^2} K_2 \right), \\ s^2 &= \frac{4a^2}{M} \frac{f}{1 + f^2} K_3, \\ \beta_1 &= \frac{2a^2}{M} \left(\frac{f^2 p^2}{(\sqrt{2} - p)^2 + f^2 p^2} K_2 \right), \\ \beta_2 &= \frac{a^2}{M} \left(\left(\frac{f^2 p^2}{(\sqrt{2} - p)^2 + f^2 p^2} + \frac{f^2 p^2}{f^2 (\sqrt{2} - p)^2 + p^2} \right) K_2 \right). \end{aligned} \quad (11)$$

It follows from (11) that $c_2^2 = \beta_1 + fs^2/2$. This means that $c_2^2 \geq \beta_1$ and the equality is achieved only in two cases: when $f = 0$ (particles are rods elongated along the x -axis) or $K_3 = 0$ (one-dimensional model). If the particles are round, then $\beta_1 = \beta_2 = \beta$ and, independent of the lattice type, $c_2^2 = \beta + s^2/2$ [19].

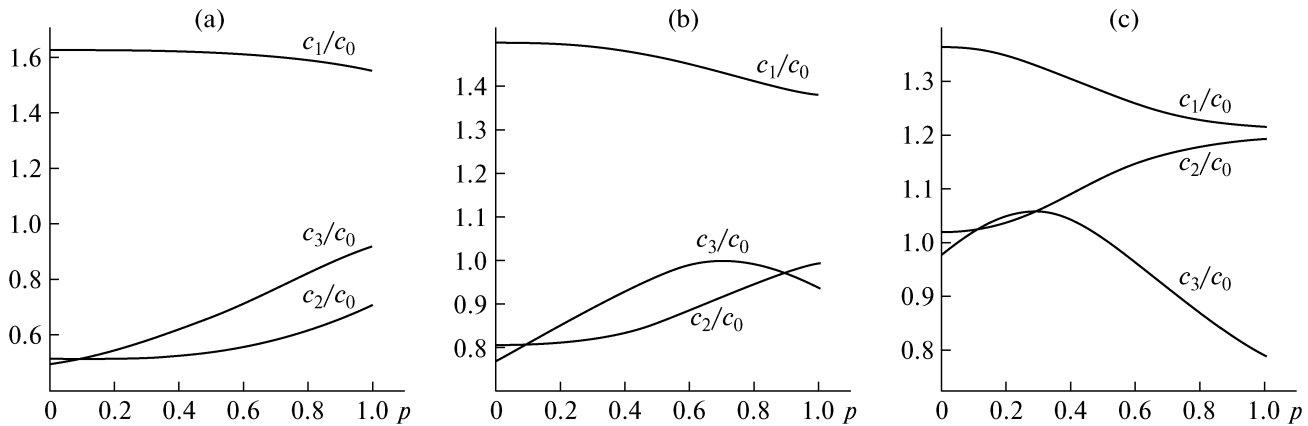


Fig. 3. Dependence of the velocities of the longitudinal (c_1), transverse (c_2), and rotational waves (c_3) on the relative particle size p at $K_1/K_0 = 0.1$, $K_1/K_0 = 0.2$, $K_2/K_0 = 0.65$, and the form parameter $f = 0.5$ (a), 1 (b), and 2 (c).

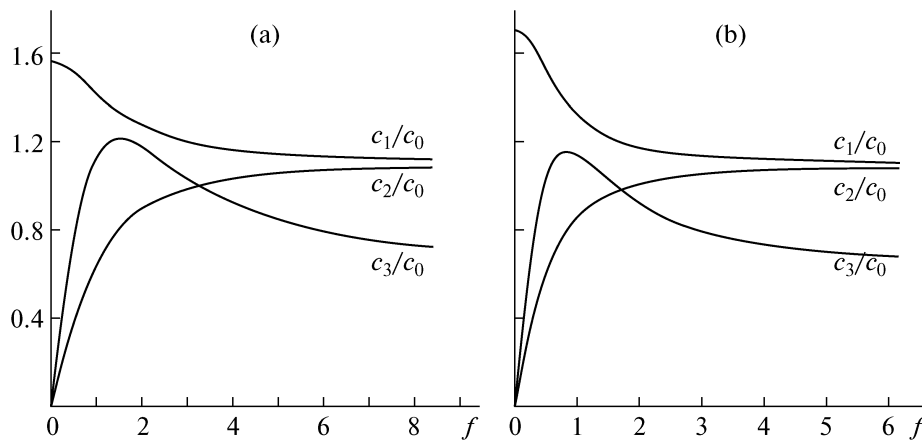


Fig. 4. Dependence of the velocities longitudinal (c_1), transverse (c_2), and rotational waves (c_3) on the form parameter f at $K_1/K_0 = 0.1$, $K_2/K_0 = 0.3$, $K_3/K_0 = 0.3$ and the relative particle size $p = 0.5$ (a) and 0.9 (b).

The analysis of relations (10) and (11) shows that if the square lattice ($a = b$) made of round particles ($f = 1$) the velocity of the rotational wave c_3 and dispersion parameter β does not depend on K_3 , the parameter of the force interaction with the second coordination sphere, then when the condition of similarity of the form of the particles to lattice form (9) does not hold, such a dependence appears for c_3 , β_1 and β_2 . On the other hand, this analysis implies that this dependence is absent not only in the case of the square lattice of round particles, but also for the rectangular lattice of elliptical particles under the similarity condition $b/a = d_2/d_1$, although in this case $\beta_1 \neq \beta_2$ still. Consequently, in the linear equations of dynamics for the rectangular lattice, in addition to the radius of the particle inertia R , “equalizing” the dimensionality of the translational shifts and rotations, there are six independent constants ($c_1, c_2, c_3, s, \beta_1, \beta_2$) even if similarity condition (9) holds; for the square lattice of round particles—there are five (c_1, c_2, c_3, s, β); and for the hexagonal lattice of the same particles which is isotropic in the acoustic

properties in the long-wave approximation, there are four (c_1, c_2, c_3, β) [19].

Figure 3 shows the dependences of the values of the velocities of the longitudinal (c_1), transverse (c_2) and rotational waves (c_3) on the particle size normalized to $c_0 = a\sqrt{K_0/M}$. It is seen that the velocity of the longitudinal wave monotonously decreases with increase in the grain size p , the velocity of the shift wave monotonously grows, and the velocity of the rotational wave, if f is close or larger than unity, has a maximum at a certain p value.

The dependences of the wave velocities of different types on the parameters of the interparticle interaction were given in [19]. In particular, it was shown there that, at low values of the moment interactions ($K_2 \ll K_0$), the grain size does not considerably affect the values of the wave velocities.

Figure 4 shows the dependence of the wave velocities of different types on the form parameter f . If $f < 1$, then the particles are elongated along the x axis, if

$f > 1$ along the axis y , and at $f = 1$ the particles are round. It is seen that, in the rectangular lattice of anisotropic particles the velocity of the longitudinal wave decreases monotonously with increase in the form parameter, and the velocity of the transverse wave grows monotonously. The velocity of the rotational wave has a local maximum at a certain f value depending on the particle size and parameters of the force interactions. The point of the maximum is shifted to the left with increase in the particle size. At low particle sizes, the variations of the wave velocities are smoother than at high p values. Given $f \rightarrow \infty$ all three velocities tend to some limiting values: $c_1/c_0 \rightarrow \sqrt{1 + 2K_1/K_0}$, $c_2/c_0 \rightarrow \sqrt{2(K_2 + K_3)/K_0}$ and $c_3/c_0 \rightarrow 2\sqrt{K_1/K_0}$, and at $f \rightarrow 0$ (i.e., when $h_2/h_1 \rightarrow 0$) $c_2 \rightarrow 0$ and $c_3 \rightarrow 0$.

It also follows from Figs. 3 and 4 that the velocity of the longitudinal wave always exceeds the velocity of the transverse wave, which, in turn, can be either larger or smaller than the velocity of the rotational wave. The first fact is well known in theory. The second fact is favored by experimental data [30] indicating that in artificial granular materials the velocity of the rotational waves can exceed the velocity of the transverse waves.

CALCULATION OF THE MODULI OF ELASTICITY ON THE BASIS OF MEASURING THE ACOUSTIC WAVE VELOCITIES

Theoretical estimates [19] and experimental data [31] show that the rotational waves in solid state are in the high-frequency region ($> 10^9 - 10^{11}$ Hz), where performing acoustic experiments meets with big technical difficulties. Nevertheless, information about the microstructure of medium can be obtained even from the acoustic measurements at rather low frequencies ($10^6 - 10^7$ Hz) when the rotational waves in the medium do not propagate. To substantiate this statement, we consider the low-frequency approximation of Eqs. (7), in which microrotations of the medium particles are not independent and are determined by the field of displacements. The relation between the microrotations φ and displacements u and w can be found from the third Eq. (7) by the step-by-step approach. In the first approximation,

$$\varphi(x, t) \approx \frac{\beta_1}{2\beta_2} (\delta_5 u_y - w_x). \quad (12)$$

This is a classical relation of the elasticity theory relating the rotations of the medium particles with the turbulence of the field of displacements. Taking into account relation (12) leads to "freezing" of the rotational degree of freedom. In the medium the translational degrees of freedom and two types of waves, lon-

gitudinal and shift (transverse) remain and the Lagrange function L takes the form:

$$\begin{aligned} L = & \frac{M}{2} \left(u_t^2 + w_t^2 + \frac{R^2 \beta_1^2}{4\beta_2^2} (\delta_5 u_{yt} - w_{xt})^2 \right) \\ & - \frac{M}{2} \left[c_1^2 (u_x^2 + \delta_1 w_y^2) + c_2^2 (w_x^2 + \delta_2 u_y^2) \right. \\ & + \frac{R^2 \beta_1^2}{4\beta_2^2} c_3^2 ((\delta_5 u_{xy} - w_{xx})^2 + \delta_3 (\delta_5 u_{yy} - w_{xy})^2) \\ & \left. + s^2 (u_x w_y + \delta_4 u_y w_x) - \frac{\beta_1^2}{2\beta_2} (w_x - \delta_5 u_y)^2 \right]. \end{aligned} \quad (13)$$

Additional terms appear in (13), which contain second derivatives with respect to the field of displacements absent in the classical version of the elasticity theory. Information about the microstructure of the medium is kept in these terms. Terms with mixed derivatives with respect to time and space u_{yt} and w_{xt} take into account the contribution of the rotational motions to the kinetic energy, and terms with the spatial derivatives u_{xy} , w_{xx} , etc. describe the contribution to the potential energy of tensions due to the lattice twist. It is possible to obtain from (13) the so-called *equations of the gradient elasticity theory* containing terms with high-order derivatives (in this case, fourth-order):

$$\begin{aligned} u_{tt} - c_1^2 u_{xx} - \left(\delta_2 c_2^2 - \frac{\delta_5^2 \beta_1^2}{2\beta_2} \right) u_{yy} - \left(\frac{1 + \delta_4 s^2}{2} + \frac{\delta_5 \beta_1^2}{2\beta_2} \right) w_{xy} \\ = \frac{R^2 \beta_1^2}{4\beta_2^2} \frac{\partial}{\partial y} \left[\frac{\partial^2}{\partial t^2} (\delta_5 u_y - w_x) - c_3^2 \Delta (\delta_5 u_y - w_x) \right], \\ w_{tt} - \left(c_2^2 - \frac{\beta_1^2}{2\beta_2} \right) w_{xx} - \delta_1 c_1^2 w_{yy} - \left(\frac{1 + \delta_4 s^2}{2} + \frac{\delta_5 \beta_1^2}{2\beta_2} \right) u_{xy} \\ = - \frac{R^2 \beta_1^2}{4\beta_2^2} \frac{\partial}{\partial x} \left[\frac{\partial^2}{\partial t^2} (\delta_5 u_y - w_x) - c_3^2 \Delta (\delta_5 u_y - w_x) \right]. \end{aligned} \quad (14)$$

Here, the symbol Δ denotes the differential operator $\Delta = \partial^2/\partial x^2 + \delta_3 \partial^2/\partial y^2$, which at $\delta_3 = 1$ transforms into a two-dimensional Laplacian.

It should be emphasized that in spite of the absence of microrotations in Eqs. (14), the medium microstructure affected the coefficients of these equations: in the given low-frequency approximation, if compared with initial Eqs. (7), the coefficients at u_{yy} , w_{xy} , w_{xx} and u_{xy} changed.

Furthermore, we consider how one can determine the effective moduli of elasticity of the nanocrystalline medium from the low-frequency acoustic measurements. Usually, the moduli of elasticity are calculated from the experimental data for three-dimensional media. Equations which are the two-dimensional

degeneracy of the classical Lam equations for media with cubic symmetry can play the role of a kind of a “bridge” from the two-dimensional models to the three-dimensional ones:

$$\begin{aligned}\rho_V u_{tt} &= C_{11} u_{xx} + C_{44} u_{yy} + (C_{12} + C_{44}) w_{xy}, \\ \rho_V w_{tt} &= C_{44} w_{xx} + C_{11} w_{yy} + (C_{12} + C_{44}) u_{xy}.\end{aligned}\quad (15)$$

Here, $\rho_V = \rho/a$ is the “bulk” density of the medium.

To compare Eqs. (15) and (14), we assume $f = 1$ (in this case all $\delta_i = 1$ and $\beta_1 = \beta_2 = \beta$) and ignore fourth-order derivatives in the latter. As a result, the coupling is established between the propagation velocities of the longitudinal and shift waves and parameters s and β , on the one hand, and the second-order elastic constants C_{11} , C_{12} , and C_{44} , on the other hand:

$$c_1^2 = \frac{C_{11}}{\rho_V}, \quad c_2^2 - \frac{\beta}{2} = \frac{C_{44}}{\rho_V}, \quad s^2 + \frac{\beta}{2} = \frac{C_{12} + C_{44}}{\rho_V}. \quad (16)$$

It should be noted that equalities (16) differ from the classic ones by the presence of the dispersion parameter β related to the critical frequency of the rotational waves [19]. For the degeneracy to the classical case, i.e., $\beta = 0$, it is sufficient that one of the conditions: $p = 0$ (point particles), $f = 0$ (particles are rods elongated along the horizontal axis) or $K_2 = 0$ (noncentral interactions between particles are not taken into account) is met.

Taking into account the relation $c_2^2 = \beta + s^2/2$, equalities (16) can be rewritten as follows:

$$\begin{aligned}c_1^2 &= \frac{C_{11}}{\rho_V}, \quad c_2^2 = \frac{2C_{44} - C_{12}}{\rho_V}, \\ s^2 &= \frac{2C_{12}}{\rho_V}, \quad \beta = \frac{2(C_{44} - C_{12})}{\rho_V}.\end{aligned}\quad (17)$$

The dependences inverse to (17) have the form

$$\begin{aligned}C_{11} &= \rho_V c_1^2, \quad C_{12} = \rho_V s^2/2, \\ C_{44} &= \rho_V (2c_2^2 + s^2)/4.\end{aligned}\quad (18)$$

There are three independent quantities by the number of the second-order elastic constants among the propagation velocities of the translational waves in the square lattice of round particles. Taking into account that $C_{11} - C_{12} = 2\rho_V v_{tr}^2$ [21], where v_{tr} is the velocity of the transverse wave in the crystallographic direction $\langle 110 \rangle$,

$$s^2 = 2c_1^2 - 4v_{tr}^2, \quad (19)$$

and, consequently, Eqs. (18) are rewritten as

$$\begin{aligned}C_{11} &= \rho_V c_1^2, \quad C_{12} = \rho_V (c_1^2 - 2v_{tr}^2), \\ C_{44} &= \rho_V (c_1^2 + c_2^2 - 2v_{tr}^2)/2.\end{aligned}\quad (20)$$

Formulas (20) show how one can determine the effective moduli of elasticity of the nanocrystalline medium from the acoustic measurements.

ESTIMATE OF THE VELOCITY OF THE ROTATIONAL WAVE

Spin waves in ferromagnets are close analogs of the waves of microrotations in solid state with the granular structure [8]. Since up to now there have been no direct experimental proofs that the waves of microrotations exist in the solid state, it is of interest to estimate the value of the velocity of such wave in the granular medium.

The dependences of the acoustic characteristics of the medium on microstructure parameters (11) were found and analyzed above. Now we obtain dependences inverse to (11):

$$\begin{aligned}K_3 &= \frac{Ms^2(1+f^2)}{4a^2f} = \frac{M(1+f^2)(c_2^2 - \beta_1)}{2a^2f^2}, \\ K_2 &= \frac{M\beta_1(f^2p^2 + (\sqrt{2} - p)^2)}{2a^2f^2p^2}, \\ K_0 + 2K_1 &= \frac{M}{a^2} \left[c_1^2 - \frac{\beta_1(\sqrt{2} - p)^2}{f^2p^2} - \frac{s^2}{2f} \right] \\ &= \frac{M}{a^2} \left[c_1^2 - \frac{c_2^2(\sqrt{2} - p) + fs^2(p\sqrt{2} - 1)}{f^2p^2} \right].\end{aligned}\quad (21)$$

Expressions (21) and (11) establish the correlation between the parameters of the micromodel and macrocharacteristics of the medium. This interrelation can be used for identification of nanomaterials on the data of acoustic experiments.

By using the third equality (11) and expressions (21), we obtain the formula for the velocity of the wave of microrotations:

$$c_3 = \sqrt{\frac{2}{K+2} \left(c_1^2 - \frac{c_2^2}{f^2} + \frac{(2c_2^2 - fs^2)(2p\sqrt{2} + K)}{2f^2p^2} \right)}, \quad (22)$$

where $K = K_0/K_1$ is the ratio of the central to the non-central force interactions.

For the medium of round particles ($f = 1$) and taking into account (19), expression (22) is transformed as follows:

$$c_3 = \sqrt{\frac{2}{K+2} \left(c_1^2 - c_2^2 + \frac{(c_2^2 - f(c_1^2 - 2v_{tr}^2))(2p\sqrt{2} + K)}{p^2} \right)}. \quad (23)$$

With the help of (23), one can theoretically estimate the velocity of the wave of microrotations in different crystals with the cubic symmetry from the propagation velocities of the acoustic waves along crystallographic directions $\langle 100 \rangle$ and $\langle 110 \rangle$. As an example, the table presents the theoretical estimates of the values of the velocity of the rotational wave and the dispersion parameter for some materials with cubic crystal parameters (lithium fluoride, sodium fluoride, sodium bromide). It contains the values of the elastic constants C_{11} , C_{12} and C_{44} , as well as the density ρ_V taken from the known experimental data at the normal temperature (see [32]). The values of the velocities of the longitudinal (c_1) and transverse (c_2) waves along the axis $\langle 100 \rangle$, as well as the dispersion parameter $\sqrt{\beta}$, were calculated according to formulas (17); the velocity of the rotational wave was calculated from formula (23); the velocity of the transverse waves along the axis $\langle 110 \rangle$ was calculated from formula $v_{tr} = \sqrt{(C_{11} - C_{12})/2\rho_V}$ [21]; the parameters of the force interactions were calculated from formulas (21) at $f = 1$. In the calculations $p = 0.9$ and $K = 10$ (central interactions dominate).

Structure parameters for crystals with cubic symmetry

	Parameters structure		Crystals		
			LiF	NaF	NaBr
Experimental data	Density (kg/m ³)	ρ_V	2600	2800	3200
	Elasticity constants (10 ⁹ N/m ²)	C_{11}	113.00	97.00	32.55
		C_{12}	48.00	25.60	13.14
		C_{44}	63.00	28.00	13.26
Calculated characteristics	Velocities of waves (m/s)	c_1	6593	5890	3190
		c_2	5477	3295	2045
		v_{tr}	3536	3571	1741
		c_3	5659	2896	1092
	Dispersion parameter (m/s)	$\sqrt{\beta}$	3396	1309	274
	Parameters of the force interactions between particles (10 ⁹ N/m ²)	K_0/a	46.01	58.19	16.11
		K_1/a	4.601	5.819	1.611
		K_2/a	19.897	3.183	0.159
		K_3/a	48.00	25.60	13.14

CONCLUSIONS

A two-dimensional model medium with nondense packing of anisotropic particles was constructed. It was shown that the form and sizes of particles, as well as the structure of the crystalline lattice, affect only the coefficients of the equations of dynamics with accuracy to the coefficients coinciding with equations of the Cosser two-dimensional continuum consisting of central-symmetric particles. The interrelation between the macroparameters of such media and parameters of their microstructure was elaborated and analyzed. The transparency of such a correlation opens great possibilities for designing of materials with desired physical-mechanical properties. This model allows both obtaining an idea about the qualitative effect of the local structure on the effective moduli of elasticity and performing quantitative estimates of their values. Formulas are obtained that allow the determination of the moduli of elasticity of the granular material from the measurements of the velocities of the acoustic waves propagating along different crystallographic directions. For some materials, the velocity of the rotational wave was estimated.

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