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ScienceDirect
Journal of Sound and Vibration 322 (2009) 564–580
JOURNAL OF SOUND AND VIBRATION
www.elsevier.com/locate/jsvi

Acoustic identification of nanocrystalline media

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Accepted 17 September 2008
The peer review of this article was organised by the Guest Editor
Available online 21 December 2008

Abstract

Two-dimensional (2D) models of nanocrystalline media with close proximity (a hexagonal lattice) and with non-dense packing (a square lattice) are considered in this paper. It is supposed that particles have a round shape and possess two translational and one rotational degrees of freedom. The differential equations describing the propagation of acoustic and rotational waves in such media have been derived. Analytical relationships between the macroelasticity constants of the medium and microstructure parameters have been found. These relationships appear to be different for nanocrystalline media with hexagonal and square lattices. It has been shown that identification of macroparameters of a nanocrystalline medium can be obtained by measurement of wave velocities and the form of dispersion dependences of acoustic and rotational waves.

0. Introduction

Actual materials have a hierarchically organised inner structure. An adequate description of the dynamic processes in a material with structural hierarchy necessitates the consideration of micro-, meso- and macrostructural levels, which interact with each other. From the physical viewpoint, the transition of a material to the nanostate is provided by the occurrence of size effects in its physical–mechanical properties [1–4]. Size effects mean the entire complex of phenomena associated with the modification of material properties due to variation in particle size and the increasing role of the boundaries in the system properties, and also due to the commensurability of the length of an elastic wave with the size of the particles. A signal that can collect data about the properties of a material is necessary for the identification and the detection of size effects. It is convenient to employ acoustic waves as a source of information because they are natural oscillations of a medium and their characteristics depend on its structure. For example, the basic physical and mechanical characteristics of a material can be found by comparing the experimentally retrieved dispersion dependencies of the acoustic waves with calculated data [5,6]. However, the identification of a material using acoustic waves is impossible without a mathematical model to establish a correlation between the structural parameters of a material and the characteristics of the elastic waves [6–8].

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0022-460X/$ - see front matter © 2008 Published by Elsevier Ltd.
doi:10.1016/j.jsv.2008.09.031

There are two approaches to the mathematical modelling of media with nanostructure. The first approach is in the transition from models at an atomic level to mesoscale models. It is based on the laws of quantum theory. In this case, the model of a medium represents a discrete system of particles connected by forces of interaction that are found from basic principles [9]. The informative analysis of such models is impossible by means of analytical methods for real systems consisting of large numbers of particles, and numerical modelling is rather laborious. The main advantage of this approach consists of explaining the origins of physical properties that are not justified by classical theory.

On the other hand, the purpose of any theory is not only to develop general principal problems but also to obtain particular results, interpret the experimental data, and rationally understand the nature of phenomena, which has great applied significance. This task—in our case a task of revealing the mechanical and acoustic properties of crystalline nanostructures—can be successfully solved on the basis of simplified semi-empirical methods. In this respect, it is rational to obtain from the theory only the relations between quantities characterizing the physical–mechanical properties of a material, while numerical values of parameters contained in the theoretical formula should be found experimentally. The second direction of investigations lying on the junction of a solid mechanics and a solid-state physics is provided by development of similar theories. It is devoted to improvement of classical models of media on account of including the new qualitative characteristics that are typical for real discrete structures [5,6,10,11].

At present, general micropolar theories such as Cosserat continuum and some others derived from general reasoning are frequently used for the modelling of structural materials. These phenomenological theories contain a large number of material constants that have to be found experimentally, and their connection with the material structure is not always clear. The method of structural modelling is a good alternative here. This method involves selection in a material of some minimal volume (i.e. a structural cell), which is capable of characterising the basic features of the macroscopic behaviour of a material [1,6,12]. The cell is considered as a construction whose operation is provided by its intrinsic structure and by the interaction with its environment. For structural modelling, the nanocrystalline material is represented by a regular or quasi-regular lattice, with small-size bodies possessing internal degrees of freedom (rather than material points) occupying the lattice sites. Domains, granules, fullerenes, nanotubes, or clusters of nanoparticles can play the role of such bodies. Media constructed in such a way are called *metamaterials*. Distinct from phenomenological models, structural models in explicit form contain parameters describing the geometrical arrangement of a material (lattice period, and shape and size of particles) and consequently they are the most appropriate models for the study of the influence of size effects on the macroproperties of a material. The clear coupling between a structure and a phenomenology discloses major opportunities for the purposeful design of materials with given physical–mechanical properties. Structural models enable one not only to reveal the qualitative influence of local structure on the effective moduli of elasticity but also to perform numerical estimations of their quantities, these being generally unavailable from phenomenological theories [6–8].

In this paper, dynamic models are presented for two-dimensional (2D) nanocrystalline media with hexagonal and square lattices, the sites of which are occupied by rigid particles possessing rotational degrees of freedom. The dependence of the dispersion properties of normal waves on the lattice parameters is analyzed. The paper is organised as follows.

The geometry of lattices with dense (hexagonal) and non-dense (square) packaging consisting of round particles that make small rotations with respect to their mass centres is considered in Section 1. The kinematic and force characteristics of such structures are introduced. The continuum approximation of the structural model for a nanocrystalline medium with a rotation degree of freedom is given in Section 2. The relationships between the ultrasonic characteristics of a material and the parameters of its structure are obtained in Section 3. The comparative analysis of the dispersion properties of normal waves propagating along different crystallographic directions is executed in Section 4. The variant of the gradient model for low-frequency acoustic waves is discussed in Section 5. The influence of the medium structure on the effective elastic moduli in the low-frequency range, where the rotational degree of freedom of the particles is negligible, is investigated in Section 6. In Section 7, the governing equations of the continuum approximation are compared with the Cosserat theory, and quantitative estimations of the material constants are performed for some types of metamaterials with the parameters of actual nanocrystalline structures.

1. Kinematic and dynamic characteristics of a structural model

The geometrical description of a structure is the first step in the modelling process. The periodic cell of the structure to be explored is defined, and its characteristic sizes and kinematic variables featuring the current state are introduced at this stage. Hexagonal (Fig. 1a) and square (Fig. 1b) lattices, the sites of which are occupied by the homogeneous round particles with diameter d and mass M, will be considered below. The hexagonal lattice corresponds to a close-packed arrangement of nanostructural particles, while the square one corresponds to a non-compact packing. In the initial state, the mass centres of the particles are located in the lattice sites, and the distance between the neighbouring particles equals a. The lattice sites N are enumerated using a couple of indices: the index i determines the site location along the horizontal x-axis, and j defines the site position along the vertical y-axis. Each particle has three degrees of freedom: the mass centre displacements $u_{ij}(t)$ and $w_{ij}(t)$, respectively, along the x- and y-axis and the rotation $\varphi_{ij}(t)$ with respect to the axis passing through the mass centre of the particle (Fig. 2). The current-state location of the mass centre of the particle of interest is determined by the coordinates $x_{ij}(t) = x^0_{ij} + u_{ij}(t)$, $y_{ij}(t) = y^0_{ij} + w_{ij}(t)$, where x^0_{ij} and y^0_{ij} are the equilibrium state coordinates. The kinetic energy of a unit cell can be calculated after the introduction of the kinematic variables. Both lattices are simple and each of them contains only one particle in a unit cell; therefore, the kinetic energy of a cell is considered to be equal to the kinetic energy of a particle:

$$T_{i,j} = \frac{M}{2}\left(\dot{u}^2_{i,j} + \dot{w}^2_{i,j}\right) + \frac{J}{2}\dot{\varphi}^2_{i,j}, \tag{1}$$

where $J = Md^2/8$ is the moment of inertia of the particle about the axis passing through its mass centre. The upper dots denote derivatives with respect to time.

The following step in the modelling process is the description of force interactions between the particles when they deviate from the equilibrium states. We shall consider small oscillations of the particles near the lattice nodes, when displacements of the particles are small in comparison with the size of a unit cell, and particle rotations are also small. Under these requirements, force and moment interactions of the particles can be described by a potential representing a polynomial of low degree. In the harmonic approximation, the interaction potential is the quadratic form of the system state variables, and the anharmonic effects are featured by terms of the third (quadratic nonlinearity) and fourth (cubic nonlinearity) orders.

The potential energy per cell of a periodic structure is equal to the potential energy of a particle located at site N, with coordinates (i, j), and interacting with its neighbours. In a hexagonal lattice, the interaction of a particle with six nearest neighbours is taken into account, for which the mass centres lie on vertices of an exact

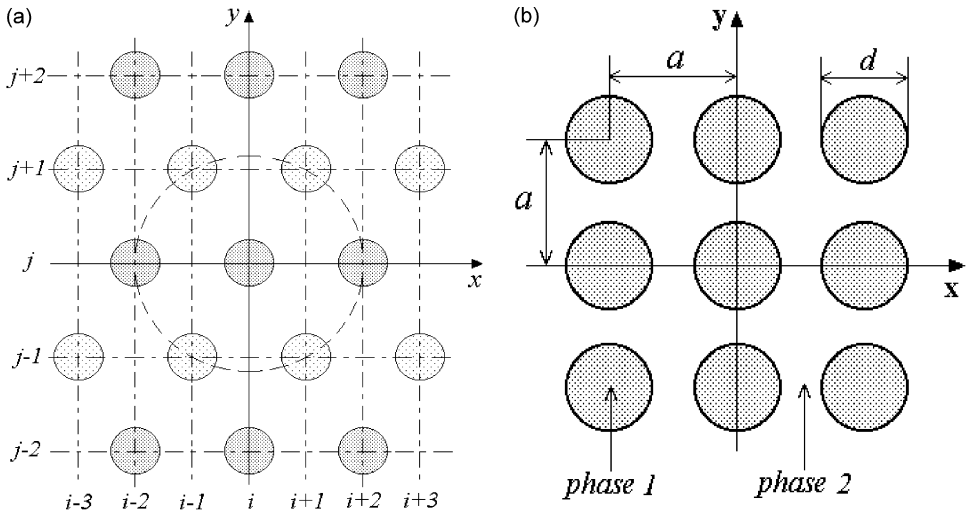

Fig. 1. A hexagonal (a) and a square (b) lattice consisting of round particles.

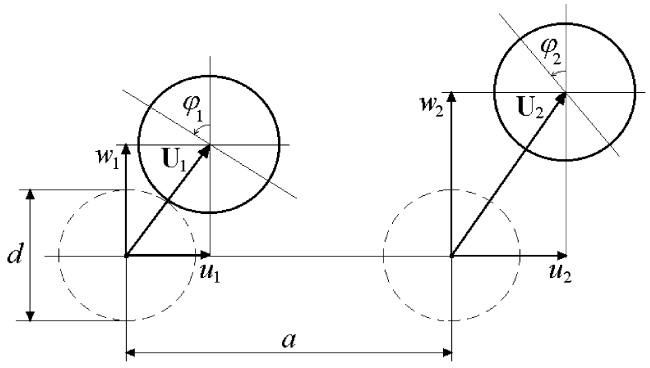

Fig. 2. Schematic of the kinematic system.

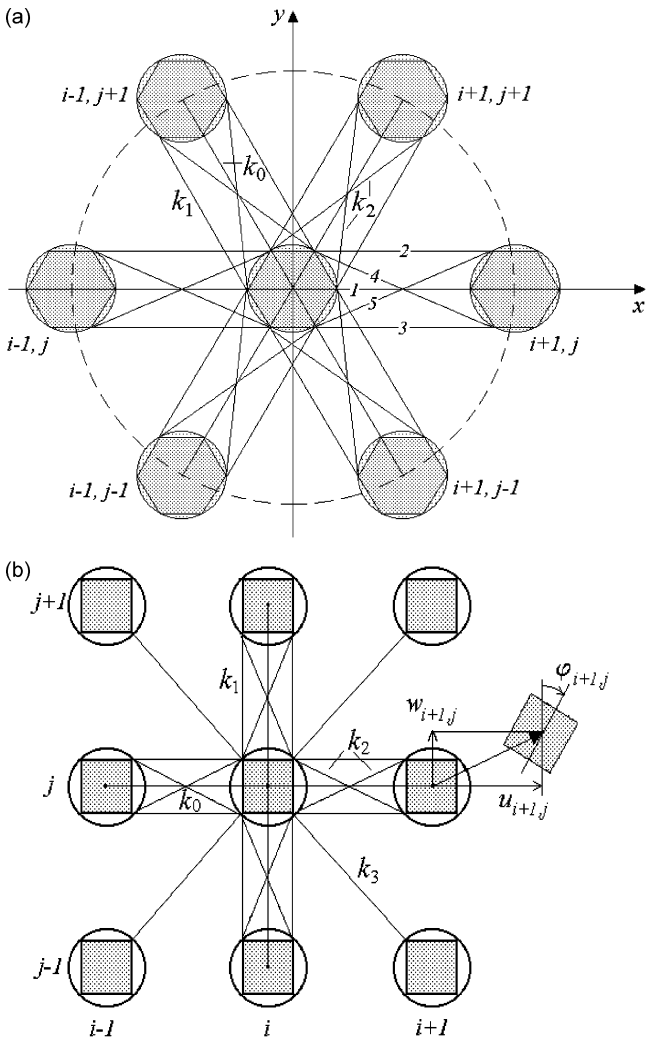

Fig. 3. Schematics for force interactions for a hexagonal (a) and a square (b) lattice.

hexagon lying on a circle of radius a (*the first coordination sphere*) (Fig. 1a and 3a). For the square lattice, each particle is supposed to interact directly with eight nearest neighbours in the lattice. The mass centres of four of them are on the horizontal and vertical lines (particles of the first coordination sphere of radius a), while the

mass centres of the other four neighbouring particles lie along the diagonals (particles of *the second coordination sphere* of radius $a\sqrt{2}$) (Fig. 3b). As the particles are of finite size, the interaction between them has force and moment components depending on the location and orientation of the particles. In the harmonic approximation, the potential energy of a lattice can be represented by the following expression:

$$U_N(\Delta_{nr}q^k, \varphi, \Delta_{nr}\varphi) = \sum_{k,s=1}^{2}\sum_{n,r,l,m}\frac{\partial^2 U}{\partial(\Delta_{nr}q^k)\partial(\Delta_{nr}q^s)}\Delta_{nr}q^k\Delta_{lm}q^s + \sum_{n,r,l,m}\frac{\partial^2 U}{(\partial\Delta_{lm}\varphi)^2}\Delta_{lm}\varphi\Delta_{nr}\varphi + \sum_{k=1}^{2}\sum_{n,r,l,m}\frac{\partial^2 U}{\partial(\Delta_{nr}q^k)\partial(\Delta_{lm}\varphi)}\Delta_{nr}q^k\Delta_{lm}\varphi + \sum_{k=1}^{2}\sum_{n,r}\frac{\partial^2 U}{\partial(\Delta_{nr}q^k)\partial\varphi}(\Delta_{nr}q^k)\varphi + \frac{\partial^2 U}{(\partial\varphi)^2}\varphi^2. \tag{2}$$

Here, $\{q_{ij}^k\} = \{q_{ij}^1, q_{ij}^2\} = \{u_{ij}, w_{ij}\}$ are the components of the vector of the mass centre displacements of a particle located at a site with indices (i, j), $\Delta_{nr}q^k = (q_{i+n\,j+r}^k - q_{ij}^k)/a$ are quantities for the relative variation of the distances between the interacting particles, $\Delta_{nr}\varphi = (\varphi_{i+n\,j+r} - \varphi_{ij})/a$ are quantities for the relative variation of the orientation angles of the interacting particles, and coefficients $n = \pm 1$, $r = \pm 1$ determine the spatial positions of neighbouring particles. As a rule (including this paper), quantities $\Delta_{nr}q^k$ and $\Delta_{nr}\varphi$ are supposed to be small (see details after Eq. (2b)).

The second-order derivatives of the potential energy are the constants of quasi-elastic interactions of the particles and represent elements of force matrices of the crystalline structure. In the phenomenological theories, the force constants should be found experimentally. Their connection with the geometrical structure and with the scheme of force interactions in a concrete crystalline lattice is not clear. From general energy reasoning and the requirements of symmetry of the lattice, it is possible to receive only some restrictions on the values of the force constants. Usage of the structural approach enables one to find an explicit dependence between the elements of the force matrices and the parameters characterising the inner structure of the lattice, i.e. its period, sizes, and shape of its particles.

For structural modelling of crystalline media, an equivalent force scheme is introduced as a system of rods or springs that incorporates the transmission of forces and moments between the structural elements instead of a field description of the interaction of the particles [1,13]. The mechanical characteristics of the connecting rods and springs should be generally determined from the requirement of equality of the strain energy in the investigated object and in its model. However, another way is used in practice. A one-to-one correspondence between the microstructure parameters and the effective elastic moduli or acoustic wave characteristics that can be measured experimentally, is found using the model. Then, the characteristics of the rods and springs are calculated. Using these relations, it is possible also to solve the inverse problem, i.e. to estimate the effective elastic moduli due to the known values of the mechanical characteristics of the connection elements. In the present paper, spring models are used for modelling nanocrystalline structures [5,6,14,15].

In order to describe the structural models and to determine the force interaction scheme, it is convenient to change the round particles to polygons, whose shape coincides with a periodic cell. The springs that transmit force interactions between the particles are attached to the vertices of a polygon.

In the case when a lattice possesses hexagonal symmetry, Eq. (2) for the potential energy of the particle with label $N = N(i, j)$ takes on the form[1]:

$$U_N = \frac{1}{4}\sum_{(n,r)}\Big(k_0 D_{1(n,r)}^2 + k_1(D_{2(n,r)}^2 + D_{3(n,r)}^2) + k_2(D_{4(n,r)}^2 + D_{5(n,r)}^2)\Big). \tag{2a}$$

Here, $D_{l(n,r)}$ $(l = 1, 2, 3, 4, 5)$ are variations in the distances between the corresponding points of a particle $N(i, j)$ and its neighbours with labels $(i+n, j+r)$, where $n = \pm 1$ is a shift of the number along the horizontal axis, $r = 0, \pm 1$ is a shift of the number along the vertical axis, and coefficients k_0, k_1, and k_2 are the parameters

[1]Hereinafter, we shall mark by character *a* those formulas that are valid for the hexagonal lattice, and by character *b* for the square lattice.

of the force interactions: k_0 characterizes central interactions at extension/compression of the material, k_1 describes non-central interactions at extension/compression of the material and moments of rotations of the particles, whereas k_2 characterizes force interactions of the particles of shear deformation in the material. In the model representation, parameters k_0, k_1, and k_2 can be interpreted as representing the rigidity of the corresponding springs: central (in Fig. 3a such a spring is marked by number 1), non-central (2 and 3), and diagonal (4 and 5) [6,8], and the connection points of the springs k_1 and k_2 coincide with the vertices of the exact hexagon entered in a particle. Expressions for $D_{l(n,r)}$ are given in Appendix A.

In the square lattice, the potential energy of the particle of number $N = N(i, j)$ also depends on the parameter of interaction with granules of the second coordination sphere, k_3:

$$U_N = \frac{1}{2}\left(\frac{k_0}{2}\sum_{m=1}^{4} D_{0m}^2 + \frac{k_1}{2}\sum_{m=1}^{8} D_{1m}^2 + \frac{k_2}{2}\sum_{m=1}^{8} D_{2m}^2 + \frac{k_3}{2}\sum_{m=1}^{4} D_{3m}^2\right). \tag{2b}$$

Here, D_{lm} ($l = 0, 1, 2, 3$) are variations in the distances between the corresponding points of a particle $N(i, j)$ and its neighbours. Expressions for D_{lm} are given in Appendix B. Both Eqs. (2a) and (2b) contain additional factor $\frac{1}{2}$ because the potential energy of the spring is equal to the sum of the potential energies of two particles, which are connected by this spring.

After substitution of relations for $D_{l(n,r)}$ into Eq. (2a) and expressions for D_{lm} into Eq. (2b), all finite differences in formulas (2a) and (2b) should be transformed to the form $\Delta g_i = (g_{i,j} - g_{i-1,j})/a$, $\Delta g_j = (g_{i,j} - g_{i,j-1})/a$, where $g = u,w,\varphi$, and half-sums $\Phi_i = (\varphi_{i,j} + \varphi_{i-1,j})/2$ should be selected. Then, we shall assume that the calculated quantities $\Delta u_i \sim \Delta w_i \sim \varphi_{ij} \sim \varepsilon$ (here $\varepsilon \ll 1$ is a measure of cell deformation) and $\Phi_i = \varphi_{ij} - 0{,}5a\Delta\varphi_i \ll \pi/2$ are small. As a result, the expression for the potential energy per particle (cell) is obtained, which, to an accuracy of terms of order ε^2, has the same form for both the lattices considered:

$$\begin{aligned} U_{ij} = {} & B_1((\Delta u_i)^2 + (\Delta w_j)^2) + B_2((\Delta u_j)^2 + (\Delta w_i)^2) + \frac{d^2}{8} B_3((\Delta\varphi_i)^2 + (\Delta\varphi_j)^2) \\ & + B_4(\Delta u_i \Delta w_j + \Delta u_j \Delta w_i) + B_5(\Delta w_i \Phi_i - \Delta u_j \Phi_j) + B_5\varphi_{ij}^2. \end{aligned} \tag{3}$$

Here, the first two terms with coefficients B_1 and B_2 describe the energy of longitudinal and shear deformations, the third and sixth contributions characterize the energy provided by non-central (moment) interactions of the particles, and the fourth and fifth terms stand for the energy of coupling of the translational motion and rotations of the particles. Coefficients $B_1, \ldots, B_5$ are expressed in terms of the micromodel parameters, but differently for the hexagonal and square lattices:

$$\begin{aligned} & B_1 = \frac{9a^2}{16}\left(k_0 + 2k_1 + \frac{2(a^2 - ad) + d^2}{l_{20}^2}k_2\right), \quad B_2 = \frac{3a^2}{16}\left(k_0 + 2k_1 + \frac{2(a^2 - ad) + 5d^2}{l_{20}^2}k_2\right), \\ & B_3 = \frac{9a^2}{16}\left(2k_1 + \frac{a^2}{l_{20}^2}k_2\right), \quad B_4 = \frac{3a^2}{8}\left(k_0 + 2k_1 + \frac{2(a^2 - ad) - d^2}{l_{20}^2}k_2\right), \; B_5 = \frac{9a^2d^2}{4l_{20}^2}k_2, \end{aligned} \tag{4a}$$

$$\begin{aligned} & B_1 = \frac{a^2}{2}\left(k_0 + 2k_1 + \frac{2h^2}{r^2}k_2 + k_3\right), \quad B_2 = \frac{a^2}{2}\left(\frac{d^2}{r^2}k_2 + k_3\right), \\ & B_3 = a^2\left(k_1 + \frac{a^2}{r^2}k_2\right), \; B_4 = a^2k_3, \; B_5 = \frac{a^2d^2}{r^2}k_2, \end{aligned} \tag{4b}$$

where $l_{20} = a^2 - ad + d^2$ is the initial length of spring k_2, $h = a - d/\sqrt{2}$ and $r = \sqrt{0,5d^2 + h^2}$ are, respectively, the lengths of the horizontal and diagonal springs in the initial state.

The equations describing the lattice dynamics can be obtained from the Lagrange equations of the second kind

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{g}_{ij}^{(l)}}\right) - \frac{\partial L}{\partial g_{ij}^{(l)}} = 0.$$

In the last formula, $L=\sum_{i,j}(T_{i,j}-U_{i,j})$ is the Lagrange function compiled from expressions (1) and (4), $g_{ij}^{(l)}$ and $\dot{g}_{ij}^{(l)}$ are the generalized coordinates ($g_{ij}^{(1)}=u_{ij}$, $g_{ij}^{(2)}=w_{ij}$, $g_{ij}^{(3)}=\varphi_{ij}$) and the generalized velocities. Obtaining differential-difference equations is useful for numerical simulation of the system response to external dynamic forcing in the wide frequency range, up to threshold values. However, for a comparison of the proposed mathematical model of a nanocrystalline medium with the known theories of solids, it is convenient to pass over from the discrete to the continuous description.

2. Continuum approximation of the structural model

For long-wavelength perturbations, when $\lambda \gg a$ (where λ is a characteristic spatial scale of deformation), discrete labels i and j can be changed by means of continuous spatial variables $x=ia$ and $y=ja$. In this case, the functions specified at discrete points are interpolated by the continuous functions and their partial derivatives in accordance with the standard Taylor formula:

$$u_{i+p,j+q}(t)=u(x+pa,y+qa,t)=u(x,y,t)+a\left(p\frac{\partial u}{\partial x}+q\frac{\partial u}{\partial y}\right)+\cdots. \tag{5}$$

Similar expansions are also used for functions $w_{i\pm1,j\pm1}(t)$ and $\varphi_{i\pm1,j\pm1}(t)$. Here, $p=\cos(\pi n/3)$, $q=\sin(\pi n/3)$ ($n=0, 1, 2, 3, 4, 5$) for the hexagonal lattice and $p=0, \pm1$, $q=0, \pm1$ for the square lattice. Depending on the number of terms kept in Eq. (5), one can consider various approximations of the discrete model for a nanocrystalline medium [6,15].

If only quantities of order $O(a)$ are taken into consideration in expansions (5), then the 2D Lagrange function L (Lagrangian) takes on the form

$$\begin{aligned}L=\frac{M}{2}(u_t^2+w_t^2+R^2\varphi_t^2)-\frac{M}{2}\Big[&c_1^2(u_x^2+w_y^2)+c_2^2(w_x^2+u_y^2)+R^2c_3^2(\varphi_x^2+\varphi_y^2)\\&+s^2(u_xw_y+u_yw_x)+2\beta(w_x-u_y)\varphi+R^2\omega_0^2\varphi^2\Big].\end{aligned} \tag{6}$$

Using the Lagrange function (7), a set of differential equations of the first approximation describing the dynamic processes in a nanocrystalline medium is derived in agreement with Hamilton's variational principle:

$$\begin{aligned}&u_{tt}=c_1^2u_{xx}+c_2^2u_{yy}+s^2w_{xy}-\beta\varphi_y,\quad w_{tt}=c_2^2w_{xx}+c_1^2w_{yy}+s^2u_{xy}+\beta\varphi_x,\\&\varphi_{tt}=c_3^2(\varphi_{xx}+\varphi_{yy})-\omega_0^2\varphi+\frac{\beta}{R^2}(u_y-w_x).\end{aligned} \tag{7}$$

Here, the following notation has been introduced: $c_i=\sqrt{2B_i/M}$ ($i=1$ to 3) are the velocities of propagation of longitudinal, transverse, and rotational[2] waves, respectively, $s=\sqrt{2B_4/M}$ is the coefficient of coupling between the longitudinal and transverse deformations, $\beta=B_5/M$ is the parameter of coupling of microrotations with the transverse and longitudinal waves, $\omega_0=\sqrt{2|B_5|/MR^2}$ is the minimal frequency of the microrotation wave, below which it does not propagate, and $R=\sqrt{J/M}=d/\sqrt{8}$ is the radius of the mass moment of inertia of the medium microparticles relative to the mass centre.

Eqs. (7) describe the dynamics of a nanocrystalline medium accounting for local interactions of the grain, and differs from the equations of the classical theory of elasticity by the additional equation for the microrotation wave. In the continuous approach, this equation follows from the conservation law of moment of momentum (or angular momentum), if the internal moments of the particles of the medium are introduced into the consideration [16]. It should be noted that the third Eq. (7) describing the microrotations of the particles differs from the first two, as it has a solution that is homogeneous in space and oscillating in time with frequency ω_0.

[2]The rotational wave has a dispersion of waveguide (Klein–Gordon) type and therefore c_3 represents the asymptotic value of the phase and group velocities of the waves in the high-frequency range.

3. Dependence of acoustic characteristics of a material on its structure

The quadratic forms of the wave velocities in Eq. (7) are expressed in terms of the force constants of the micromodel, k_0, k_1, k_2, k_3, the distance between the particles a, and their diameter d:

$$c_1^2=\frac{3\sqrt{3}}{4\rho}\left(k_0+2k_1+\left(2-\frac{d^2}{a^2-ad+d^2}\right)k_2\right),\quad c_2^2=\frac{\sqrt{3}}{4\rho}\left(k_0+2k_1+\left(2+\frac{3d^2}{a^2-ad+d^2}\right)k_2\right),$$
$$c_3^2=\frac{3\sqrt{3}}{4\rho}\left(2k_1+\frac{a^2}{a^2-ad+d^2}k_2\right),\quad \beta=\frac{3d^2\sqrt{3}}{2\rho(a^2-ad+d^2)}k_2,\ s^2=c_1^2-c_2^2, \tag{8a}$$

$$c_1^2\frac{1}{\rho}\left(k_0+2k_1+\frac{2(a\sqrt{2}-d)^2}{d^2+(a\sqrt{2}-d)^2}k_2+k_3\right),\quad c_2^2=\frac{1}{\rho}\left(\frac{2d^2}{d^2+(a\sqrt{2}-d)^2}k_2+k_3\right),$$
$$c_3^2=\frac{2}{\rho}\left(k_1+\frac{a^2}{d^2+(a\sqrt{2}-d)^2}k_2\right),\quad \beta=\frac{2d^2}{\rho(d^2+(a\sqrt{2}-d)^2)}k_2,\quad s^2=\frac{2k_3}{\rho}. \tag{8b}$$

Here, ρ is the density of the 2D medium ($\rho=M/a^2$ for the square lattice [6], and $\rho=2M/a^2\sqrt{3}$ for the hexagonal lattice [8]; hence, the hexagonal lattice represents more compact packing in comparison with the square lattice).

It is necessary to note that in both models the critical (minimal) frequency, ω_0, depends on parameter β, and, by virtue of its dimensionality, on the radius of gyration of particles, $R=d/\sqrt{8}$:

$$\omega_0=\sqrt{2|\beta|/R^2}=4\sqrt{|\beta|/d^2} \tag{9}$$

and parameters c_2, β, and s are inter-related by the following relationship:

$$\beta=c_2^2-s^2/2 \tag{10}$$

and in the hexagonal lattice due to the last equality (8a)

$$\beta=\tfrac{1}{2}(3c_2^2-c_1^2). \tag{10a}$$

The analysis of relations (8a) and (8b) shows that the wave velocities depend on the size of the particles in the nanocrystalline (granular) media. So, the dependencies of the velocities of the longitudinal (c_1), transverse (c_2) and rotational (c_3) waves on the relative size of particles d/a are given in Fig. 4 (for the hexagonal lattice) and Fig. 5a and b (for the square lattice). In all cases, $k_1/k_0=0.1$ and curves 1 correspond to the value

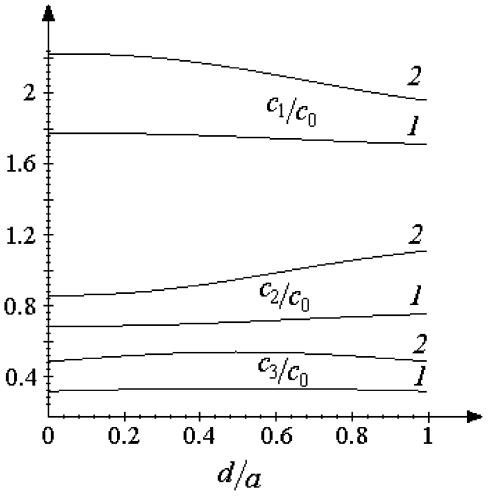

Fig. 4. Dependencies of elastic wave velocities on the size of particles in a hexagonal lattice. $k_1/k_0=0.1$, $k_2/k_0=0.1$ (curves 1), $k_2/k_0=0.5$ (curves 2).

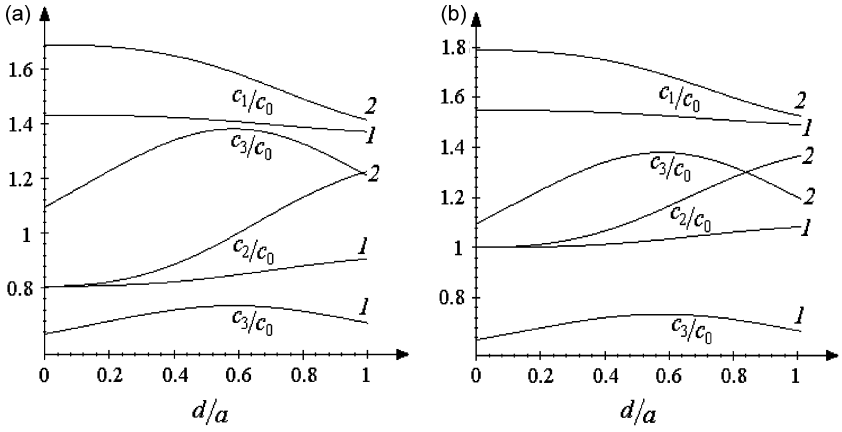

Fig. 5. Dependencies of elastic wave velocities on the size of particles in a square lattice. $k_1/k_0 = 0.1$, $k_2/k_0 = 0.1$ (curves 1), $k_2/k_0 = 0.5$ (curves 2), $k_3/k_0 = 0.65$ (a), $k_3/k_0 = 1$ (b).

$k_2/k_0 = 0.1$, while curves 2 stand for the value $k_2/k_0 = 0.5$. In the case of a medium with cubic symmetry, k_3/k_0 is assumed to be equal to 0.65 (Fig. 5a) or 1 (Fig. 5b). All velocities are normalised by the longitudinal wave velocity c_0 ($c_0^2 = 3k_0\sqrt{3}/4\rho$ in a hexagonal lattice and $c_0^2 = k_0/\rho$ in a square lattice), taking account only of the central interactions (i.e. for $k_1 = k_2 = 0$). From these figures, it is clear that the longitudinal wave velocity decreases monotonically as the grains grow in size, while the transverse wave velocity, c_2, on the contrary, increases monotonously. The rotational wave velocity has a maximum for some value of d/a. In the range of small moment interactions ($k_2 \ll k_0$), the grain size does not essentially affect the quantities of the wave velocities (see curve 1).

In turn, the parameters k_0, k_1, k_2, k_3, and grain size d can be expressed in terms of the acoustic characteristics of the medium due to formulas (8)–(10):

$$k_2 = \frac{\rho(a^2 - ad + d^2)}{3d^2\sqrt{3}}(3c_2^2 - c_1^2), \quad k_1 = \frac{\rho}{3\sqrt{3}}\left(2c_3^2 - \frac{\beta a^2}{d^2}\right),$$
$$k_0 = \frac{4\rho}{3\sqrt{3}}\left(c_1^2 - c_3^2 - \frac{(a-d)^2}{2d^2}\beta\right), \quad d = \sqrt{8|3c_2^2 - c_1^2|}/\omega_0, \tag{11a}$$

$$k_3 = \rho s^2/2, \;\; k_2 = \frac{\rho(d^2 + (a\sqrt{2} - d)^2)}{4d^2}(2c_2^2 - s^2),$$
$$k_1 = \frac{\rho}{2}\left(c_3^2 - \frac{a^2}{d^2}(2c_2^2 - s^2)\right), \quad k_0 = \rho(c_1^2 - c_2^2 - c_3^2) + \frac{\rho a\sqrt{2}}{d}(2c_2^2 - s^2). \tag{11b}$$

Thus, Eqs. (8)–(11) establish one-to-one correspondences between the micromodel parameters and the macrocharacteristics of a medium. This inter-relation can be used, in particular, for diagnostics of nanomaterials due to data of wave (acoustic) experiments.

4. Dispersion properties of normal waves

We shall search for the solutions of Eq. (7) as plane harmonic waves in the form $u(r,t),\ w(r,t), \varphi(r,t) \propto \exp[\mathrm{i}(\omega t - kr)]$, where ω is an oscillation frequency, $kr = k_x x + k_y y$ is a variation of a wave phase along the direction of propagation. Then, from the equation of motion, one can obtain the dispersion equation

$$\omega^6 - A_1\omega^4 + A_2\omega^2 + A_3 = 0 \tag{12}$$

with coefficients

$$
\begin{aligned}
A_1 &= (c_1^2 + c_2^2 + c_3^2)k^2 + \omega_0^2,\\
A_2 &= (c_1^2c_2^2 + c_1^2c_3^2 + c_2^2c_3^2)k^4 + ((c_1^2 - c_2^2)^2 - s^4)k_x^2k_y^2 + \omega_0^2(c_1^2 + c_2^2 - \beta/2)k^2,\\
A_3 &= \omega_0^2c_1^2(\beta/2 - c_2^2)k^4 + \omega_0^2[\beta(c_2^2 - c_1^2 + s^2) - (c_1^2 - c_2^2)^2 + s^4]k_x^2k_y^2 - c_1^2c_2^2c_3^2k^6\\
&\quad + c_3^2(s^4 - (c_1^2 - c_2^2)^2)k^2k_x^2k_y^2,
\end{aligned}
\tag{13}
$$

where $k = \sqrt{k_x^2 + k_y^2}$. Transformation into the polar coordinate frame $k_x = k\cos\theta$ and $k_y = k\sin\theta$ yields $k_x^2k_y^2 = \frac{1}{4}\sin^2 2\theta$. It is necessary to note that equality $c_1^2 - c_2^2 = s^2$ is valid for the hexagonal lattice, and coefficients of the $k_x^2k_y^2$ term are equal to zero in this case. This fact indicates isotropy of the medium with hexagonal symmetry. For an isotropic medium, the dispersion equation (12) can be written in a much more simple form

$$
(\omega^2 - c_1^2k^2)\left[\omega^4 - ((c_2^2 + c_3^2)k^2 + \omega_0^2)\omega^2 + c_2^2c_3^2k^4 + \omega_0^2c_2^2k^2 - \frac{\beta}{2}\omega_0^2k^2\right] = 0. \tag{14}
$$

It is also possible to derive the same equation by considering of the wave propagating only along the axis of symmetry, when $\theta = 0$ (i.e. $k = k_x$). The dispersion curves determined by Eqs. (14) and (12) are represented in the normalised form (in $(k/k_0, \omega/\omega_0)$ coordinates, where $k_0 = \omega_0/c_2$) in Fig. 6a and b, respectively. In both figures, the following designations are introduced: L is the longitudinal mode, T the transverse mode, and R the rotational mode. The graphics have been plotted for numerical data corresponding to NaF crystals: $c_1/c_2 = 1.79$, $c_3/c_2 = 0.69$, $\beta/c_2^2 = 0.158$ (see Table 1). In Fig. 6b, the dispersion dependencies for the waves propagating along the x-axis ($\theta = 0$) are plotted in the left-hand half-plane, while the dispersion curves for the waves travelling angularly $\theta = \pi/6$ along the x-axis are displayed in the right-hand half-plane. From this

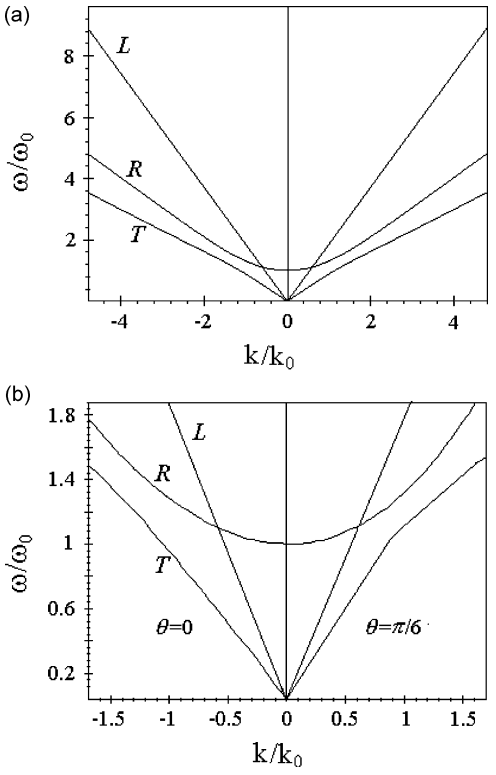

Fig. 6. Dispersion curves for a medium with hexagonal (a) and square (b) lattices.

Table 1
Structural parameters for crystals with hexagonal and cubic symmetry.

Structural parameters	Crystals					
	Hexagonal			Cubic		
	Be	Cd	Zn	LiF	NaF	NaBr
Experimental data						
Density (kg/m^3)						
ρ_V	1816	8642	7140	2600	2800	3200
Elasticity constants ($10^9\,N/m^2$)						
C_{11}	292.3	114.5	161.1	113.00	97.00	32.55
C_{12}	26.7	39.5	34.2	48.00	25.60	13.14
C_{44}	–	–	–	63.00	28.00	13.26
Calculated characteristics						
Wave velocities (m/s)						
c_1	12,687	3640	4750	6593	5890	3190
c_2	11,470	2027	3603	5477	3295	2045
c_3	9317	1404	2823	3164	2262	1024
Normalised threshold frequency of rotational waves $\omega_0 d$ (m/s)						
$\omega_0 d$	10,810	2721	11450	13587	5237	1095
Elasticity coefficients in the Cosserat theory ($10^9\,N/m^2$)						
λ	26.7	39.5	34.2	48.00	25.60	13.14
μ	132.8	37.5	63.5	63.00	28.00	13.26
γ/R^2	157.7	17.0	56.9	26.04	14.33	3.36
κ	212.2	−4.0	58.5	30.00	4.8	0.24
Normalised parameters of force interactions between the particles ($10^9\,N/m^2$)						
k_0/a	83.81	61.28	65.28	46.01	58.19	16.11
k_1/a	8.381	6.128	6.528	4.601	5.819	1.611
k_2/a	74.921	−1.412	20.654	19.897	3.183	0.159
k_3/a	–	–	–	48.00	25.60	13.14

figure, it is seen that the dispersion of a transverse mode is more indicative for the waves propagating angularly $\theta = \pi/6$.

5. Approximation of the second-order gradient theory of elasticity

If the frequencies of the acoustic waves are smaller than ω_0, the spin wave does not propagate and the microrotations of the particles of the medium are determined by a displacement field. The inter-relationship between the microrotations φ and displacements u and w can be found from the third Eq. (7) by the method of stepwise approximations. In the first approximation,

$$\varphi(x,t) \approx \tfrac{1}{2}(u_y - w_x). \tag{15}$$

Taking account of Eq. (15) in the Lagrangian of Eq. (6) leads to the "freezing" of the rotational degree of freedom. Thus, in the medium, as in the classical theory, there are only two translational degrees of freedom, and the 2D density of the Lagrange function L takes on the form

$$L = \frac{\rho}{2}\left(u_t^2 + w_t^2 + \frac{R^2}{2}(u_{yt} - w_{xt})^2\right) - \frac{\rho}{2}\left[c_1^2(u_x^2 + w_y^2) + c_2^2(w_x^2 + u_y^2) + \frac{R^2}{4}c_3^2((u_{xy} - w_{xx})^2 + (u_{yy} - w_{xy})^2) + s^2(u_x w_y + u_y w_x) - \frac{\beta}{2}(w_x - u_y)^2\right]. \tag{16}$$

In contrast to the classical case, in Lagrangian (16), there are terms containing second-order derivatives from the displacements u and w. The terms u_{yt} and w_{xt} take into account the contribution of the rotational motions to the kinetic energy, and the terms with spatial derivatives u_{xy}, w_{xx}, etc. describe the contribution to the potential energy of the stresses provided by bending of the lattice. The differential equations describing the propagation and interaction of the longitudinal and transverse waves in the nanocrystalline medium in the low-frequency approximation have the form

$$u_{tt} - c_1^2 u_{xx} - \left(c_2^2 - \frac{\beta}{2}\right) u_{yy} - \left(s^2 + \frac{\beta}{2}\right) w_{xy} = -\frac{R^2}{2}\frac{\partial}{\partial y}\left[\frac{\partial^2}{\partial t^2}(u_y - w_x) - c_3^2 \Delta(u_y - w_x)\right],$$
$$w_{tt} - \left(c_2^2 - \frac{\beta}{2}\right) w_{xx} - c_1^2 w_{yy} - \left(s^2 + \frac{\beta}{2}\right) u_{xy} = \frac{R^2}{2}\frac{\partial}{\partial x}\left[\frac{\partial^2}{\partial t^2}(u_y - w_x) - c_3^2 \Delta(u_y - w_x)\right]. \quad (17)$$

Here, the symbol Δ means the Laplacian $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

Equations such as Eq. (17) are usually called equations *of the second-order gradient theory of elasticity*, as the terms with spatial fourth-order derivatives take into account the coupled stresses arising at the translational displacements of the particles. From Eq. (17), it follows that in the considered low-frequency approximation, the transverse wave velocity is diminished by quantity $\beta/2$, and the parameter s^2 increases by the same quantity.

6. Determination of effective modules of macroelasticity

We investigate the influence of the structure of a medium on the effective moduli of macroelasticity, which are determined experimentally in three-dimensional (3D) media. The role of a "bridge" between the 2D and 3D models can be represented by the 2D degeneration of the well-known Lamé equations for media with hexagonal symmetry [17]

$$\rho_V u_{tt} = C_{11} u_{xx} + C_{66} u_{yy} + \tfrac{1}{2}(C_{11} + C_{12}) w_{xy},$$
$$\rho_V w_{tt} = C_{66} w_{xx} + C_{11} w_{yy} + \tfrac{1}{2}(C_{11} + C_{12}) u_{xy} \quad (18a)$$

and with cubic symmetry

$$\rho_V u_{tt} = C_{11} u_{xx} + C_{44} u_{yy} + (C_{12} + C_{44}) w_{xy},$$
$$\rho_V w_{tt} = C_{44} w_{xx} + C_{11} w_{yy} + (C_{12} + C_{44}) u_{xy}. \quad (18b)$$

Here, ρ_V is the volume density of the medium ($\rho_V = \rho/a$ for the square lattice, and $\rho_V = \rho\sqrt{6}/2a$ for the hexagonal lattice, since in the latter case the volume of a 2D elementary cell is equal to $V_2 = 0.5a^2\sqrt{3}$ and the volume of a 3D elementary cell equals $V_3 = 0.5a^3\sqrt{2}$ [18]).

In the previous section, it has been shown that the basic Eq. (7) degenerate into Eq. (17) in the low-frequency range. Eq. (17) will coincide with Eqs. (18a) and (18b), if we desire to neglect the fourth-order derivatives. By comparing the coefficients in Eqs. (18a) and (18b) and in the right-hand sides of Eq. (17), one can find the relationship between the velocities of propagation of the longitudinal and shear waves and the parameter s and β, on the one hand, and the second-order elastic constants C_{11}, C_{12}, C_{44}, and C_{66}, on the other hand:

$$c_1^2 = \frac{C_{11}}{\rho_V}, \quad c_2^2 - \frac{\beta}{2} = \frac{C_{66}}{\rho_V} = \frac{C_{11} - C_{12}}{2\rho_V}, \quad (19a)$$

$$c_1^2 = \frac{C_{11}}{\rho_V}, \quad c_2^2 - \frac{\beta}{2} = \frac{C_{44}}{\rho_V}, \quad s^2 + \frac{\beta}{2} = \frac{C_{12} + C_{44}}{\rho_V}. \quad (19b)$$

Such inter-relationships enable one to express the elasticity constants in terms of the parameters of the material microstructure:

$$C_{11} = \frac{9\sqrt{2}}{8}\left(\frac{k_0 + 2k_1}{a} + \frac{2(a^2 - ad) + d^2}{a^2 - ad + d^2}\frac{k_2}{a}\right), \quad C_{12} = \frac{3\sqrt{2}}{8}\left(\frac{k_0 + 2k_1}{a} + \frac{2(a^2 - ad) - d^2}{a^2 - ad + d^2}\frac{k_2}{a}\right), \quad (20a)$$

$$C_{11}=\frac{k_0+2k_1+k_3}{a}+\frac{2(a\sqrt{2}-d)^2}{d^2+(a\sqrt{2}-d)^2}\frac{k_2}{a},\quad C_{12}=\frac{k_3}{a},\quad C_{44}=\frac{d^2}{d^2+(a\sqrt{2}-d)^2}\frac{k_2}{a}+\frac{k_3}{a}. \tag{20b}$$

From Eqs. (20a) and (20b), it follows that the relationships $C_{11}^0=9(k_0+2k_1+2k_2)\sqrt{2}/8=3C_{12}^0$ and $C_{12}^0=C_{44}^0$ take place for media consisting of material points and possessing, accordingly, hexagonal and cubic symmetry. Generally, equalities

$$C_{11}-3C_{12}=\frac{9d^2\sqrt{2}}{4(a^2-ad+d^2)}\frac{k_2}{a}, \tag{21a}$$

$$C_{44}-C_{12}=\frac{d^2}{d^2+(a\sqrt{2}-d)^2}\frac{k_2}{a} \tag{21b}$$

are valid for non-zero particle sizes. However, relationships $C_{11}<3C_{12}$ and $C_{44}<C_{12}$ are accordingly valid for many crystals with hexagonal and cubic symmetry. In such cases, as follows from Eqs. (21a) and (21b), the force constant k_2 is negative (see Table 1). Hence, in the expression for the potential energy (3) coefficient B_5 of terms with the rotational degree of freedom is also negative (see Eqs. (4a) and (4b)). Such a situation takes place, for example, for some molecular crystals [19].

The inverse dependences can be obtained from Eqs. (21a), (21b), (20a) and (20b):

$$\begin{aligned}&k_2=\frac{2a(1-h+h^2)\sqrt{2}}{9h^2}(C_{11}-3C_{12}),\\&k_0+2k_1=\frac{2a\sqrt{2}}{9}\left[C_{11}+3C_{12}+\frac{2(h-1)}{h^2}(C_{11}-3C_{12})\right],\end{aligned} \tag{22a}$$

$$\begin{aligned}&k_3=aC_{12},\quad k_2=a(C_{44}-C_{12})\left(1+\left(\frac{\sqrt{2}}{h}-1\right)^2\right),\\&k_0+2k_1=a(C_{11}-C_{12})-2a(C_{44}-C_{12})\left(\frac{\sqrt{2}}{h}-1\right)^2,\end{aligned} \tag{22b}$$

where $h=d/a$ is the relative size of the particles. Normalised parameters of force interactions are determined due to formulas following from Eqs. (22a) and (22b):

$$\begin{aligned}&\frac{k_2}{a}=\frac{2(1-h+h^2)\sqrt{2}}{9h^2}(C_{11}-3C_{12}),\\&\frac{k_1}{a}=\frac{2\sqrt{2}}{9(K+2)}\left[C_{11}+3C_{12}+\frac{2(h-1)}{h^2}(C_{11}-3C_{12})\right],\end{aligned} \tag{23a}$$

$$\frac{k_3}{a}=C_{12},\quad \frac{k_2}{a}=(C_{44}-C_{12})\left(1+\left(\frac{\sqrt{2}}{h}-1\right)^2\right),\quad \frac{k_1}{a}=\frac{1}{K+2}\left[C_{11}-C_{12}-2(C_{44}-C_{12})\left(\frac{\sqrt{2}}{h}-1\right)^2\right]. \tag{23b}$$

Here, $K=k_0/k_1$ is the relation between the central and non-central forces of interaction. Relationships (23a) and (23b) can be useful for the estimation of quantities of the force constants contained in the discrete models of nanocrystalline media, if the macroelasticity moduli and typical particle sizes are known.

Spin waves in ferromagnetics [20] are close analogues of microrotation waves in solids with a granular structure. At present, there is no direct experimental proof of the existence of rotational waves in solids, so an estimate of the values of the velocity and critical frequency of such a wave in a granular medium would be of great interest. From Eqs. (8a), (8b), (23a) and (23b), it is possible to obtain an expression for the velocity of a

microrotation wave:

$$c_3 = \sqrt{\frac{1}{\rho_V(K+2)}\left(C_{11} + 3C_{12} + \frac{4h-2+K}{2h^2}(C_{11} - 3C_{12})\right)}, \tag{24a}$$

$$c_3 = \sqrt{\frac{2}{\rho_V(K+2)}\left[C_{11} + C_{12} - 2C_{44} + \frac{K + 4h\sqrt{2} - 2}{h^2}(C_{44} - C_{12})\right]}. \tag{24b}$$

Theoretical estimates of the value of the velocity of a rotational wave and its critical frequencies

$$\omega_0 d = 4\sqrt{|C_{11} - 3C_{12}|/\rho_V}, \tag{25a}$$

$$\omega_0 d = 4\sqrt{2|C_{44} - C_{12}|/\rho_V} \tag{25b}$$

are listed as an example in Table 1 for some crystals with hexagonal (beryllium (Be), cadmium (Cd), zinc (Zn)), and cubic symmetry (LiF, NaF, NaBr). In this table, values for the elasticity constants C_{11}, C_{12}, and C_{44}, as well as the density ρ_V, were taken from known experimental data at normal temperature (see Ref. [21]). Values of the longitudinal, c_1, and transverse, c_2, wave velocities have been calculated from Eqs. (19a), (19b), (9), (25a), and (25b):

$$c_1 = \sqrt{\frac{C_{11}}{\rho_V}}, \quad c_2 = \sqrt{\frac{C_{11} - 2C_{12}}{\rho_V}}, \tag{26a}$$

$$c_1 = \sqrt{\frac{C_{11}}{\rho_V}}, \quad c_2 = \sqrt{\frac{2C_{44} - C_{12}}{\rho_V}}. \tag{26b}$$

The rest of the quantities listed in the table have been calculated from formulas derived in this paper: the rotational wave velocity—due to formulas (24a) and (24b), the normalised threshold frequency of this wave—due to Eqs. (25a) and (25b), and the parameters of force interactions—due to formulas (23a) and (23b). The calculations were carried out for $h = 0.9$ and $K = 10$ (for which the central interactions dominate). Analysis showed that for $0.9 < h < 0.99$, quantities c_3, k_0, k_1, and k_2 varied by less than 10%.

It is clear from this table (see also Figs. 4 and 5a, b) that the rotational wave velocity is minimal for all the considered materials, and the threshold frequencies lie in the hypersonic range. Therefore, if it is to be supposed that the size of a crystal grain $d = 10\,\text{nm} = 10^{-8}\,\text{m}$, then for hypothetical nanocrystalline material with elasticity constants and density, as for cadmium, $\omega_0 \approx 2.721 \times 10^{11}\,\text{s}^{-1}$, and for nanomaterial with parameters of LiF $\omega_0 \approx 1.359 \times 10^{12}\,\text{s}^{-1}$. Therefore, in the sonic and ultrasonic ranges, the microrotation waves can be neglected. However, their presence can be of principal importance for high-frequency processes.

7. Calculation of material constants in the continuum Cosserat theory

It is interesting to compare Eq. (7) with equations for the dynamics of a 2D Cosserat continuum obtained by other authors [16,22,23] consisting of centrally symmetric particles. The Lagrangian of this continuum has the form

$$L = \frac{\rho_V}{2}(u_t^2 + w_t^2 + R^2\varphi_t^2) - \frac{1}{2}\left[B(u_x^2 + w_y^2) + \left(\mu + \frac{\kappa}{2}\right)(w_x^2 + u_y^2) + \gamma(\varphi_x^2 + \varphi_y^2) + \left(\lambda + \mu - \frac{\kappa}{2}\right)(u_x w_y + u_y w_x) + 2\kappa(w_x - u_y)\varphi + 2\kappa\varphi^2\right]. \tag{27}$$

Here, B is a macroelasticity constant of the second order, λ and μ are Lamé constants, and γ and κ are phenomenological constants to be found from experiments. In the case of the isotropic Cosserat continuum,

$$B = \lambda + 2\mu. \tag{28}$$

From a comparison of Lagrangians (27) and (6), it is clear that the acoustic characteristics of a medium can be expressed in terms of the constants of the Cosserat theory:

$$c_1^2=\frac{B}{\rho_V},\quad c_2^2=\frac{2\mu+\kappa}{2\rho_V},\quad s^2=\frac{2\lambda+2\mu-\kappa}{2\rho_V},\quad c_3^2=\frac{\gamma}{\rho_V R^2},\quad \beta=\frac{\kappa}{\rho_V} \tag{29}$$

and for a medium with hexagonal symmetry the first Eq. (29) taking relation (28) into account, takes on the form

$$c_1^2=\frac{\lambda+2\mu}{\rho_V}.$$

The dependence being inverse to Eq. (29), with the allowance for the relation $2c_2^2-s^2=2\beta$ for both models, and the equality $s^2=c_1^2-c_2^2$ for the hexagonal lattice only is written in the form

$$\lambda=\frac{\rho_V(c_1^2-c_2^2)}{2}=C_{12},\ \ \mu=\frac{\rho_V(c_1^2+c_2^2)}{4}=\frac{C_{11}-C_{12}}{2},$$
$$\kappa=\rho_V\beta=\frac{\rho_V}{2}(3c_2^2-c_1^2)=C_{11}-3C_{12},\ \ \gamma=\rho_V R^2c_3^2, \tag{30a}$$

$$B=\rho_V c_1^2=C_{11},\ \ \lambda=\rho_V(c_2^2-\beta)=C_{12},\ \ \mu=\rho_V\left(c_2^2-\frac{\beta}{2}\right)=C_{44},$$
$$\kappa=\rho_V\beta=2(C_{44}-C_{12}),\ \ \gamma=\rho_V R^2c_3^2. \tag{30b}$$

Here the constants of the Cosserat medium are also expressed in terms of the elasticity constants of the second order, due to Eqs. (19a) and (19b). Parameter γ can be expressed in terms of the elasticity constants only in the case of additional assumptions about the values of $K=k_0/k_1$ and $h=d/a$ (see Eqs. (24a) and (24b)). It should be noted that the relation $\mu-\lambda=\kappa/2$ follows from Eqs. (30a) and (30b). The relation shows that in the models considered, the Lamé constants λ and μ are interlinked through the parameter κ, which is responsible for the interaction between the microrotations of the particles and the shift strains. The value of a threshold frequency of a microrotation wave also depends on parameter κ:

$$\omega_0=\sqrt{2|\kappa|/\rho_V R^2}=4\sqrt{|\kappa|/\rho_V d^2}.$$

Relations (30a) and (30b), together with Eqs. (8a) and (8b), enable one to obtain quantitative estimations for the coefficients, which are included in decomposition of the internal energy in the Cosserat theory, for various materials (see, for example, Table 1). Earlier performance of such estimates was impossible. It should be noted that similar relations were obtained in Ref. [22]; however in that work the size of the particles had not been introduced in an explicit form, and therefore the dependence of the material constants on this remained unclear.

8. Conclusions

In this paper, 2D dynamic models of nanocrystalline media have been developed. It has been shown that the structure of the equations obtained, Eq. (7), coincides with the equations of the 2D Cosserat continuum. However, in the Cosserat continuum, the coefficients contained in the governing equations are determined empirically, while in the proposed models the coefficients depend explicitly on the sizes of the particles and on the parameters of their force interaction. The dependency of the acoustic wave velocities on the size of the grains has been theoretically analyzed. Estimates performed in the work show that in real crystalline media the rotational wave velocity must be less than the translational wave velocities, and the threshold frequency of the rotational wave lies in the hypersonic range. In the field of low (sonic and ultrasonic) frequencies, the rotational degrees of freedom of particles are negligible, and Eq. (7) reduce to the well-known Lamé equations (18a) and (18b) for a medium with cubic symmetry. But even in this case, the effect of the medium microstructure is still left in the form of the relationship between the macroscopic characteristic parameters of the medium and the micromodel parameters (see Eqs. (8a), (8b), (20a), and (20b)).

The research was carried out under the financial support of the RFBR (project no. 07-02-00172).

Appendix A. Spring extensions for the hexagonal lattice

Spring extensions $D_{l(n,r)}$ calculated for small dimensionless displacement differences $\Delta u_{n,r} = (u_{i+n,j+r} - u_{i,j})/a \sim \Delta w_{n,r} = (w_{i+n,j+r} - w_{i,j})/a \sim \varphi_{i,j} \sim \varepsilon$ (here ε is a measure of cell deformation) and $\Phi_{n,r} = (\varphi_{i,j} + \varphi_{i+n,j+r})/2 = \varphi_{i,j} - 0,5a\Delta\varphi_{n,r} \ll \pi/2$ have the following form:

$$
\begin{aligned}
D_{1(n,r)} &= \frac{a}{2}(n\Delta u_{n,r} + r\sqrt{3}\Delta w_{n,r}),\\
D_{1(n,0)} &= na\Delta u_{n,0},\\
D_{2,3(n,r)} &= \frac{a}{4}(2n\Delta u_{n,r} + 2r\sqrt{3}\Delta w_{n,r} \mp rd\sqrt{3}\Delta\varphi_{n,r}),\\
D_{2,3(n,0)} &= na\left(\Delta u_{n,0} \pm \frac{d\sqrt{3}}{4}\Delta\varphi_{n,0}\right),\\
D_{4(n,n)} &= \frac{na}{2l_{20}}\left((a-2d)\Delta u_{n,n} + a\sqrt{3}\Delta w_{n,n} + ad\sqrt{3}\Phi_{n,n}\right),\\
D_{5(n,n)} &= \frac{na}{2l_{20}}\left((a+d)\Delta u_{n,n} + (a-d)\sqrt{3}\Delta w_{n,n} - ad\sqrt{3}\Phi_{n,n}\right),\\
D_{4,5(n,0)} &= \frac{a}{2l_{20}}\left(n(2a-d)\Delta u_{n,0} \pm d\sqrt{3}\Delta w_{n,0} \pm nad\sqrt{3}\Phi_{n,0}\right),\\
D_{4,5(\mp1,\pm1)} &= \frac{a}{2l_{20}}\left(\mp(a+d)\Delta u_{\mp1,\pm1} \pm (a-d)\sqrt{3}\Delta w_{\mp1,\pm1} + ad\sqrt{3}\Phi_{\mp1,\pm1}\right),\\
D_{4,5(\pm1,\mp1)} &= \frac{a}{2l_{20}}\left(\pm(a-2d)\Delta u_{\pm1,\mp1} \mp (a-d)\sqrt{3}\Delta w_{\pm1,\mp1} - ad\sqrt{3}\Phi_{\pm1,\mp1}\right),
\end{aligned}
\tag{31}
$$

where $l_{20} = a^2 - ad + d^2$ is the initial length of the springs k_2. In Eq. (31), $n = \pm1$, $r = \pm1$. In the expressions for $D_{2,3}$ and $D_{4,5}$ the upper signs of symbols $\pm$ and $\mp$ are taken as extensions of springs 2 and 4, and the lower ones—for springs 3 and 5.

Appendix B. Spring extensions for the square lattice

Before calculating spring extensions let us note that, because of the symmetry of the lattice, if we rotate it by 90° or 180°, some springs transform into other springs. Due to this, we need not write down 24 expressions for deformations of all the springs. One expression can be suitable for extensions of several springs. Spring extensions calculated for small dimensionless displacement differences $\Delta u_i = (u_{i,j} - u_{i-1,j})/a \sim \Delta w_i = (w_{i,j} - w_{i-1,j})/a \sim \varphi_{i,j} \sim \varepsilon \ll 1$ (here ε is a measure of cell deformation) and $\Phi_i = (\varphi_{i,j} + \varphi_{i-1,j})/2 = \varphi_{i,j} - 0,5a\Delta\varphi_i \ll \pi/2$, have the following form[3]:

$$
\begin{aligned}
&D_{0(i-1,j)} = a\Delta u_i \sim D_{0(i+1,j)},\quad D_{0(i,j-1)} = a\Delta w_j \sim D_{0(i,j+1)},\quad D^{l,r}_{1(i-1,j)} = a\Delta u_i \pm \frac{ad}{2\sqrt{2}}\Delta\varphi_i \sim D^{r,l}_{1(i+1,j)},\\
&D^{r,l}_{1(i,j-1)} = a\Delta w_j \pm \frac{ad}{2\sqrt{2}}\Delta\varphi_j \sim D^{l,r}_{1(i,j+1)},\quad D^{+,-}_{2(i-1,j)} = \frac{a}{r}\left(h\Delta u_i \pm \frac{d}{\sqrt{2}}\Delta w_i \pm \frac{d}{\sqrt{2}}\Phi_i\right) \sim D^{-,+}_{2(i+1,j)},\\
&D^{+,-}_{2(i,j-1)} = \frac{a}{r}\left(h\Delta w_j \pm \frac{d}{\sqrt{2}}\Delta u_j \mp \frac{d}{\sqrt{2}}\Phi_j\right) \sim D^{+,-}_{2(i,j+1)},\\
&D_{3(i-1,j-1)} = \frac{a}{\sqrt{2}}(\Delta u_i + \Delta u_j + \Delta w_i + \Delta w_j) \sim D_{3(i+1,j+1)},\\
&D_{3(i+1,j-1)} = \frac{a}{\sqrt{2}}(\Delta u_i - \Delta u_j - \Delta w_i + \Delta w_j) = D_{3(i-1,j+1)},
\end{aligned}
\tag{32}
$$

where $h = a - d/\sqrt{2}$ and $r = \sqrt{0,5d^2 + h^2}$ are, respectively, the lengths of horizontal and diagonal springs in the initial state. Here, the first lower index for D means the type of spring (0, 1, 2, or 3) and the second lower label, in brackets, shows the coordinates of the particle connected by this spring with particle N. In Eq. (32),

[3]Linear terms for the spring extensions are retained in Eq. (32) only.

some formulas are written for the extensions of two or four springs, as mentioned above. First, the spring extensions indicated by the signs of equivalence have been obtained by the substitution of all indices i by $i+1$ and j by $j+1$. Secondly, the special upper labels are introduced in order to distinguish the springs with parameters k_1 and k_2 in pairs. Sign l is used for the left springs, and r—for the right ones, for pairs of horizontal and vertical springs. Here the springs are considered to be left or right taking the viewpoint of an observer located at the centre of particle N and looking at the neighbouring particle. The diagonal spring pairs can point in one direction, with the viewpoint of the same observer, either clockwise (upper label $+$) or counter clockwise (label $-$). In both cases, the upper indices of D are separated by commas ($+$, $-$ or r, l), and in symbols $\pm$ and $\mp$ the upper sign is taken for extensions of the springs with the first label, and the lower one with the second number.

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