Nonlinear Localized Strain Waves in a 2D Medium with Microstructure

Vladimir I. Erofeev, Vladimir V. Kazhaev and Igor S. Pavlov

Abstract A two-dimensional model of the crystalline (granular) medium is considered that represents a square lattice consisting of elastically interacting particles, which possess translational and rotational degrees of freedom. In the long-wavelength approximation the partial derivatives equations have been derived that describe propagation of longitudinal, transverse and rotational waves in such a medium. In the field of low frequencies, when the rotational degree of freedom of particles can be neglected, the obtained nonlinear three-mode system degenerates into a two-mode system. Analytical dependencies of the velocities of elastic waves and the nonlinearity coefficients on the sizes of particles and the parameters of interactions between them have been found for both nonlinear models. Due to these dependencies, numerical estimations of the nonlinearity coefficients are performed. The two-mode system is shown to be reduced by the multi-scale method to Kadomtsev–Petviashvili evolutionary equation for transverse deformation, which has a soliton solution. For some crystals with a cubic symmetry it is found out, whether soliton is steady and what kind of polarity it has.

1 Introduction

As a rule, adequate description of wave processes in a structurally-heterogeneous material necessitates consideration of some scale levels, which interact with each other on account of internal connections [1]. The following scales are usually

V. I. Erofeev $(\boxtimes) \cdot V$. V. Kazhaev $\cdot I$. S. Pavlov

Nizhny Novgorod Mechanical Engineering Research Institute of Russian Academy of Sciences, IMASH RAN 85, Belinskogo st., Nizhny Novgorod, Russia 603024 e-mail: erf04@sinn.ru

I. S. Pavlov e-mail: ispavl@mts-nn.ru

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distinguished: atomic or *microlevel* (characteristic sizes are angstroms and nanometers), *mesolevel* (from 10^{-8} – 10^{-6} m), and *macrolevel* (larger than 10^{-6} m).

Mental breaking of a material into parts is restricted by some limit consisting in a qualitative change of physical properties on a given scale level, i.e. in this case a size effect [2, 3] arises. There are materials, where qualitative changes occur gradually, but in crystal solids this limit is expressed rather accurately and takes place in the field of nanometers. During studying of wave processes in materials, the size effects start to be shown, when the characteristic spatial scale of effect (for example, length of an elastic or electromagnetic wave) becomes comparable with the characteristic spatial scale of a material—the size of grain, the lattice period, etc. In process of accumulation of knowledge about microstructure of a material there arises a transition to new level of knowledge—a theory is created that enables one to explain mechanical behavior of a material from new positions. It is necessary to emphasize that in this case real values of "microscales" of a medium can lie in the field of both microns and nanometers or angstroms. However, with the viewpoint of methodology of theoretical research, smallness of some scales in comparison with other ones is more important than their absolute values.

In the mathematical simulation of microstructured media, two approaches can be distinguished. The first approach consists in the passage from atomic-level models to mesoscale models and is based on the laws of quantum theory. In this case, the medium is considered as a discrete system of particles coupled by the interaction forces determined from the first principles [4]. This approach allows one to understand the nature of physical laws and to explain the origin of some properties having no substantiation in the classical theory.

The second approach means passing from description of a medium on a macrolevel to mesoscale models. The continuum-phenomenological method of modeling of microstructured media is related to this approach. This method lies at the boundary of mechanics and physics of solid-state. It consists in improvement of the classical models of media by including qualitatively new characteristics inherent in actual discrete structures [1, 5, 6]. At present, structurally-heterogeneous materials are frequently simulated by the generalized micropolar theories of the Cosserat continuum type [7-9]. These theories involve a large number of material constants, which have to be determined experimentally. The relationships between these quantities and the material structure are not always clear. Besides, there is an alternative-the method of structural modeling, according to which a certain minimum volume is separated in the bulk material-a representative structural element that is capable of reflecting the main features of the macroscopic behavior of the given material [1, 10-12]. In this method, a 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. The role of these bodies can be played by domains, grains, fullerenes, nanotubes, or clusters consisting of nanoparticles. Advantages of the structural modeling consist in a clear relationship between the structure of a medium and its macroparameters, as well as in possibility of purposeful design of materials with the given properties, and shortcomings are absence of universality of modeling procedure and complexity of the accounting of nonlinear and nonlocal effects of interparticle interactions.

Construction of mechanical and mathematical models is a base of research of the dynamic (wave) phenomena [13] in both natural and artificial materials possessing unique properties. It should be noted that an adequate description of this or that wave process in the certain structured material necessitates a corresponding mathematical model. For example, in [14] it was shown that in the field of high frequencies the accounting of rotation motions of particles is necessary, in a low-frequency range it is enough to use the equations of the classical theory of elasticity, which considers particles as material points and does not take into account rotation of particles, and, at last, in the intermediate area, the equations of the second-order gradient theory of elasticity should be used, which do not contain rotations of particles in an explicit form, but the sizes of particles influence on factors of these equations.

In this work, the nonlinear differential equations describing propagation of longitudinal, transverse and rotational waves in the two-dimensional crystal (granular) medium are derived by the method of structural modeling. After that, in the field of low frequencies, when the rotational wave does not propagate, the received three-mode set of equations degenerates into the two-mode model corresponding to the continuum "with the restricted rotation of particles" [5]. Due to application of the method of structural modeling, analytical dependencies of the linear and nonlinear macroparameters of the medium on sizes of the particles and on parameters of interactions between them have been established, and numerical estimates of the nonlinearity parameters have been performed both for the complete (three-mode) system and for the reduced (two-mode) model. Using the multi-scale method, the two-mode system is reduced to Kadomtsev-Petviashvili evolutionary equation with respect to transverse deformation. This equation has a soliton-type solution. Different variants of behavior of a plane solitary wave are analyzed, depending on initial conditions of Kadomtsev-Petviashvili equation and its factors that depend on the microstructure parameters of the considered medium.

2 Discrete Model

We consider a square lattice (Fig. 1), the sites of which are occupied by homogeneous round particles (granules) having mass *M* and diameter *d*. In the initial state, the centers of mass of the particles are located in lattice sites, and the distance between them is *a*. The lattice sites *N* are enumerated using the subscripts (*i*, *j*). Each particle has three degrees of freedom: displacements $u_{ij}(t)$ and $w_{ij}(t)$ of the center of mass along axes *x* and *y*, respectively, and the angle of rotation $\varphi_{ij}(t)$ with respect to an axis passing through the center of mass of a particle (Fig. 2). The kinetic energy of the cell is as follows:

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

Fig. 1 A square lattice consisting of round particles



where $J = Md^2/8 = MR^2$ is the moment of inertia about the axis passing through its mass center and $R = d/\sqrt{8}$ is the radius of gyration of the particle. The dots denote derivatives with respect to time.

Since we consider only small deviations of particles from equilibrium positions, their force and moment interactions can be described by a power potential. In the harmonic approximation, the interaction potential is a quadratic form of the variables of the system state. The potential energy per cell is equal to the potential energy of a particle located at site N and interacting with its neighbors and can be described by the following expression:

$$\begin{split} \mathrm{U}_{N}\left(\Delta_{nr}\mathsf{q}^{k},\phi,\Delta_{nr}\phi\right) &= \sum_{k,s=1}^{2} \sum_{n,r,l,m} \frac{\partial^{2}\mathrm{U}}{\partial\left(\Delta_{nr}\mathsf{q}^{k}\right)\partial\left(\Delta_{lm}\mathsf{q}^{s}\right)} \Delta_{nr}\mathsf{q}^{k}\Delta_{lm}\mathsf{q}^{s} \\ &+ \sum_{n,r,l,m} \frac{\partial^{2}\mathrm{U}}{\partial\left(\Delta_{nr}\phi\right)\partial\left(\Delta_{lm}\phi\right)} \Delta_{nr}\phi\Delta_{lm}\phi \\ &+ \sum_{k=1}^{2} \sum_{n,r,l,m} \frac{\partial^{2}\mathrm{U}}{\partial\left(\Delta_{nr}\mathsf{q}^{k}\right)\partial\left(\Delta_{lm}\phi\right)} \Delta_{nr}\mathsf{q}^{k}\Delta_{lm}\phi \\ &+ \sum_{k=1}^{2} \sum_{n,r,l,m} \frac{\partial^{2}\mathrm{U}}{\partial\left(\Delta_{nr}\mathsf{q}^{k}\right)\partial\phi} \Delta_{nr}\mathsf{q}^{k}\phi + \frac{\partial^{2}\mathrm{U}}{\left(\partial\phi\right)^{2}}\phi^{2}. \end{split}$$

Here $\left\{q_{ij}^k\right\} = \left\{q_{ij}^1, q_{ij}^2\right\} = \{u_{ij}, w_{ij}\}$ are the components of the displacement vector of the center of mass for a particle located at the site with subscripts (i, j), $\Delta_{nr}q^k = \left(q_{i+n\,j+r}^k - q_{ij}^k\right) / \alpha$ is the relative variation of interparticle distances, $\Delta_{nr}\varphi = \left(\varphi_{i+n\,j+r} - \varphi_{ij}\right) / \alpha$ is the relative variation of the particle orientation angles, and $n = \pm 1$, $r = \pm 1$ are the subscripts determining the spatial positions of the neighboring particles. The second-order derivatives of the potential energy are



Fig. 2 Schematic for force interactions between the particles and kinematics

the constants of quasi-elastic interactions of the particles and represent the elements of force matrices of the crystalline structure [15]. In phenomenological theories, the material constants are assumed to be known from experiments. Their relation to the geometric structure and interaction parameters in the crystal lattice is generally unclear. From the general energy considerations and the symmetry conditions, only certain restrictions on their values [5] can be derived. The proposed structural approach makes it possible to find explicit relationships between the force matrix elements and lattice parameters.

For structural modeling 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 [10-12] instead of a field description of the interaction of the particles. For convenience, the round particles are replaced by inscribed polygons, the shape of which repeats that of the cell. The springs simulating the interactions between particles are considered anchored at the vertices of polygons.

In the present paper, a spring model is used for modeling. Displacements of the granules are assumed to be small compared to the size of the elementary cell of the lattice. The particle *N* is supposed to interact directly with eight nearest neighbors in the lattice. The mass centers of four of them are on horizontal and vertical lines (these particles are called *particles of the first coordination sphere*), while the mass centers of the other four neighboring particles lie along diagonals (*particles of the second coordination sphere*). The potential energy per cell of the square lattice produced by its interaction with eight neighbors is described by

$$U_{N} = \frac{1}{2} \left(\sum_{n=1}^{4} \frac{K_{0}}{2} D_{0n}^{2} + \sum_{n=1}^{8} \frac{K_{1}}{2} D_{1n}^{2} + \sum_{n=1}^{8} \frac{K_{2}}{2} D_{2n}^{2} + \sum_{n=1}^{4} \frac{K_{3}}{2} D_{3n}^{2} \right), \quad (2)$$

where D_{1n} (l = 0, 1, 2, 3) are extensions of arbitrary enumerated springs of four types, which connect a particle with its neighbors. The central springs having rigidity K₀, together with the non-central springs with rigidity K₁ define interaction forces of extension/compression of the material, whereas the springs with K₁ transmit also moments to particle rotation. The diagonal springs with rigidity K₂ characterize force interactions of the granules of shear deformations in the material. The springs possessing rigidity K₃ model interactions with the particles of the second coordination sphere. For convenience of further calculations, we shall assume that points of connection of springs K₀ are located in the centers of the particles, whereas ones of the springs K₁, K₂ and K₃ lie in the vertices of a square that is entered in a circumference and has a side $h = d/\sqrt{2}$ (Fig. 2). Equation (2) contains additional factor 0.5 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.

We shall calculate expressions for extensions of the springs, D_{ln} , supposing that quantities $\Delta u_i \sim \Delta w_i \sim \Delta u_j \sim \Delta w_j \sim \alpha \varepsilon$, $\Delta \phi_i \sim \Delta \phi_j \sim \varepsilon^{3/2}$, and $\Phi_i \sim \sqrt{\varepsilon}$ are small, where $\Delta u_i = u_{i,j} - u_{i-1,j}$, $\Delta u_j = u_{i,j} - u_{i,j-1}$, $\Phi_i = (\phi_{i-1,j} + \phi_{i,j})/2 \ll \pi/2$, and $\varepsilon \ll 1$ is a measure of cell deformation. After substitution of these expressions into (2) we shall make up Lagrange function $L = T_{i,j} - U_{i,j}$ for the particle with number (*i*, *j*) to an accuracy of terms of order $\varepsilon^{5/2}$. Thus, only geometrical nonlinearity is taken into account in this model. Then, using Lagrange equations of the second kind it is possible to obtain differential-different equations describing dynamics of the considered lattice. However, the continuum approximation of the proposed model will be considered in this chapter.

3 Continuum Approximation

For a comparison of the structural model of the medium with the well-known models of a deformable solid, it is expedient to pass from the discrete description to a continuous description. In the case of the long wavelength perturbations, for which $\alpha / \Lambda \ll 1$ (Λ is the characteristic spatial deformation scale), the discrete variables *i* and *j* can be replaced by the continuous variables x = ia and y = ja, and the functions $u_{ij}(t), w_{ij}(t), \phi_{ij}(t)$ can be interpolated by the fields of displacements u(x, y, t), w(x, y, t) and microrotations $\varphi(x,y,t)$, respectively.

Depending on the order of approximation, it is possible to consider various continuous models. In the first approximation the following Lagrangian of the considered medium with microstructure yields:

$$\begin{split} L &= \frac{M}{2} \left(u_t^2 + w_t^2 + R^2 \varphi_t^2 \right) - \frac{M}{2} [c_1^2 (u_x^2 + w_y^2) + c_2^2 (w_x^2 + u_y^2) \\ &+ R^2 c_3^2 (\varphi_x^2 + \varphi_y^2) + s^2 (u_x w_y + u_y w_x) + 2\beta^2 (w_x - u_y) \varphi + 2\beta^2 \varphi^2 \end{split}$$

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$$\begin{split} &+ \alpha_{1}(u_{x}^{3} + w_{y}^{3}) + \alpha_{2}(u_{y}^{3} + w_{x}^{3} + u_{x}^{2}u_{y} + u_{x}u_{y}^{2} + w_{x}^{2}w_{y} + w_{x}w_{y}^{2} \\ &- u_{x}^{2}w_{x} - u_{y}^{2}w_{x} - u_{x}^{2}w_{y} - u_{y}w_{y}^{2} - u_{y}w_{x}^{2} - u_{x}w_{y}^{2}) \\ &- 2\alpha_{2}(u_{x}u_{y}(w_{x} + w_{y}) + w_{x}w_{y}(u_{x} + u_{y})) + \alpha_{3}(u_{x}w_{x}^{2} + u_{y}^{2}w_{y}) \\ &+ \alpha_{4}(w_{x}w_{y}\phi - u_{x}u_{y}\phi + \frac{1}{2}(w_{x}^{2} - u_{x}^{2} + w_{y}^{2} - u_{y}^{2})\phi) \qquad (3) \\ &+ \alpha_{5}(u_{y}\phi^{2} + w_{x}\phi^{2}) + \alpha_{6}(u_{x}\phi^{2} + w_{y}\phi^{2}) + \alpha_{7}(u_{x}w_{x}\phi + u_{y}w_{y}\phi)]. \end{split}$$

Using Lagrangian (3), a set of nonlinear differential equations describing the dynamic processes in a 2D crystalline medium with non-dense packing of the particles is derived in agreement with Hamilton's variational principle:

$$u_{tt} = c_1^2 u_{xx} + c_2^2 u_{yy} + s^2 w_{xy} - \beta^2 \varphi_y + \frac{1}{2} \frac{\partial F_1}{\partial x} + \frac{1}{2} \frac{\partial F_2}{\partial y},$$

$$w_{tt} = c_2^2 w_{xx} + c_1^2 w_{yy} + s^2 u_{xy} + \beta^2 \varphi_x + \frac{1}{2} \frac{\partial F_3}{\partial x} + \frac{1}{2} \frac{\partial F_4}{\partial y},$$

$$R^2 \varphi_{tt} = R^2 c_3^2 (\varphi_{xx} + \varphi_{yy}) + \beta^2 (u_y - w_x) - 2\beta^2 \varphi - F_5.$$
 (4)

Here, the following notation has been introduced: c_i (i = 1, 2, 3) are the velocities of propagation of longitudinal, transverse, and rotational waves, respectively, *s* is the coefficient of linear coupling between the longitudinal and transverse deformations in a material, β is the dispersion parameter. Dependencies of the coefficients of equations (4) on the force constants K₀, K₁, K₂, and K₃, the lattice period *a* and grain size $h = d/\sqrt{2}$ (*d* is a diameter of the particle) have the following form [14]:

$$c_{1}^{2} = \frac{a^{2}}{M} \left(K_{0} + 2K_{1} + \frac{2(a-h)^{2}}{(a-h)^{2} + h^{2}} K_{2} + K_{3} \right),$$

$$c_{2}^{2} = \frac{a^{2}}{M} \left(\frac{2h^{2}}{(a-h)^{2} + h^{2}} K_{2} + K_{3} \right),$$

$$c_{3}^{2} = \frac{a^{2}h^{2}}{2MR^{2}} \left(K_{1} + \frac{a^{2}}{(a-h)^{2} + h^{2}} K_{2} \right),$$

$$s^{2} = \frac{2a^{2}}{M} K_{3}, \quad \beta^{2} = \frac{2a^{2}}{M} \left(\frac{h^{2}}{(a-h)^{2} + h^{2}} K_{2} \right).$$
(5)

Moreover, the nonlinearity functions contain in the right-hand sides of Eqs. (4):

$$\begin{split} F_1 &= 3\alpha_1 u_x^2 + \alpha_2 (2u_x u_y + u_y^2 - 2u_x w_x - u_x w_y - w_y^2) + \alpha_3 w_x^2 \\ &- 2\alpha_2 (u_y w_x + u_y w_y + w_x w_y) - \alpha_4 (u_y \phi + u_x \phi) + \alpha_6 \phi^2 + \alpha_7 w_x \phi, \\ F_2 &= \alpha_2 (3u_y^2 + u_x^2 + 2u_x u_y - 2u_y w_x - w_y^2 - w_x^2) + 2\alpha_3 u_y w_y \end{split}$$

$$\begin{split} &-2\alpha_2(u_xw_x+u_xw_y+w_xw_y)-\alpha_4(u_x\phi+u_y\phi)+\alpha_5\phi^2+\alpha_7w_y\phi,\\ F_3&=\alpha_2(3w_x^2+2w_xw_y+w_y^2-u_x^2-u_y^2-2u_yw_x\\ &-2u_xu_y+u_xw_y)+2\alpha_3u_xw_x+\alpha_4(w_y\phi+w_x\phi)+\alpha_5\phi^2+\alpha_7u_x\phi,\\ F_4&=3\alpha_1w_y^2+\alpha_2(w_x^2+2w_xw_y-u_x^2-2u_yw_y-2u_xw_y)+\alpha_3u_y^2 \qquad (6)\\ &-2\alpha_2(u_xu_y+u_xw_x+u_yw_x)+\alpha_4(w_x\phi+w_y\phi)+\alpha_6\phi^2+\alpha_7u_y\phi,\\ F_5&=\alpha_4\left(w_xw_y-u_xu_y+\frac{1}{2}(w_x^2-u_x^2+w_y^2-u_y^2)\right)\\ &+2\alpha_5(u_y\phi+w_x\phi)+2\alpha_6(u_x\phi+w_y\phi)+\alpha_7(u_xw_x+u_yw_y), \end{split}$$

where α_i (i = 1,...,7) are the nonlinearity coefficients depending on the microstructure parameters:

$$\begin{split} &\mathcal{M}\alpha_{1}=\frac{K_{2}}{r^{4}}a^{3}(a-h)h^{2}+\frac{K_{3}}{4(a-h)}a^{3}, \quad \mathcal{M}\alpha_{2}=\frac{K_{3}}{4(a-h)}a^{3}, \\ &\mathcal{M}\alpha_{3}=K_{0}a^{2}+K_{1}\frac{a^{3}}{a-h}+\frac{K_{2}}{r^{4}}a^{3}(a-h)(a^{2}-2ah-h^{2})-\frac{K_{3}a^{3}}{4(a-h)}, \\ &\mathcal{M}\alpha_{4}=\frac{2a^{2}hK_{3}}{a-h}, \quad \mathcal{M}\alpha_{5}=\frac{K_{3}}{(a-h)^{2}}a^{2}h^{2}, \end{split}$$
(7)
$$&\mathcal{M}\alpha_{6}=K_{1}\frac{ah^{2}}{a-h}+K_{2}\frac{ah^{2}}{r^{4}}(2h-a)(5ah-2h^{2}-a^{2})+\frac{K_{3}}{(a-h)^{2}}a^{2}h^{2}, \\ &\mathcal{M}\alpha_{7}=K_{1}\frac{2a^{2}h}{a-h}+\frac{2a^{3}h}{r^{4}}K_{2}\left(5h^{2}-5ah+a^{2}\right). \end{split}$$

Here $r = \sqrt{(a - h)^2 + h^2}$ is the initial length of the springs with rigidity K₂ (Fig. 2). Equations (4) describe the dynamics of a crystalline (granular) medium

Equations (4) describe the dynamics of a crystalline (granular) medium accounting for local interactions of the grain, and coincide with the dynamic equations of the 2D anisotropic Cosserat continuum consisting of centrally-symmetric particles [5]. Such equations differ 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.

4 Approximation of the Second-Order Gradient Theory of Elasticity

Theoretical estimates [14] and experimental data [16] show that rotational waves in solids exist in the high-frequency range ($>10^9-10^{11}$ Hz), where it is quite difficult, with a technical point of view, to carry out acoustic experiments. Nevertheless,

information about microstructure of the medium can be received even by means of acoustic measurements on rather low frequencies (10^6-10^7 Hz) , when the rotational waves do not propagate in a medium. Therefore we will consider low-frequency approximation of Eqs. (4), in which the microrotations of the particles of the medium are not independent and are determined by a displacement field. The inter-relationship between the microrotations φ_j and displacements *u* and *w* can be found from the third Eq. (4) by the method of stepwise approximations. In the first approximation

$$\varphi(\mathbf{x}, \mathbf{t}) \approx \frac{1}{2} \left(\mathbf{u}_{y} - \mathbf{w}_{x} \right).$$
(8)

This relationship between the rotations of the particles of the medium and a vorticity of a displacement field, is a characteristic feature of the *Cosserat pseudo-continuum* model (continuum with the restricted rotation of the particles) [5]. Taking account of Eq. (8) leads to the "freezing" of the rotational degree of freedom. Thus, excitations, which are caused by the microrotations, do not propagate in the medium, but they influence on propagation of the longitudinal and transverse waves. In this case, the Lagrange function *L* takes on the simpler form:

$$\begin{split} \mathsf{L} &= \frac{\mathsf{M}}{2} \Biggl(\mathsf{u}_{t}^{2} + \mathsf{w}_{t}^{2} + \frac{\mathsf{R}^{2}}{4} (\mathsf{u}_{yt} - \mathsf{w}_{xt})^{2} \Biggr) \\ &- \frac{\mathsf{M}}{2} \Biggl[\mathsf{c}_{1}^{2} (\mathsf{u}_{x}^{2} + \mathsf{w}_{y}^{2}) + \mathsf{c}_{2}^{2} (\mathsf{w}_{x}^{2} + \mathsf{u}_{y}^{2}) + \frac{\mathsf{R}^{2}}{4} \mathsf{c}_{3}^{2} ((\mathsf{u}_{xy} - \mathsf{w}_{xx})^{2} \\ &+ (\mathsf{u}_{yy} - \mathsf{w}_{xy})^{2}) + \mathsf{s}^{2} (\mathsf{u}_{x} \mathsf{w}_{y} + \mathsf{u}_{y} \mathsf{w}_{x}) - \frac{\beta^{2}}{2} (\mathsf{w}_{x} - \mathsf{u}_{y})^{2} \qquad (9) \\ &+ \alpha_{1} (\mathsf{u}_{x}^{3} + \mathsf{w}_{y}^{3}) - \alpha_{2} (\mathsf{u}_{x}^{2} \mathsf{w}_{y} + \mathsf{u}_{x} \mathsf{w}_{y}^{2} + 2\mathsf{u}_{x} \mathsf{u}_{y} \mathsf{w}_{y} + 2\mathsf{u}_{x} \mathsf{w}_{x} \mathsf{w}_{y}) \\ &+ \gamma_{1} (\mathsf{u}_{y}^{3} + \mathsf{w}_{x}^{3} - \mathsf{u}_{y} \mathsf{w}_{x}^{2} - \mathsf{u}_{y}^{2} \mathsf{w}_{x}) + \gamma_{2} (\mathsf{u}_{x} \mathsf{u}_{y}^{2} + \mathsf{w}_{x}^{2} \mathsf{w}_{y}) \\ &+ \gamma_{3} \mathsf{u}_{x} \mathsf{w}_{x}^{2} + \gamma_{4} \mathsf{u}_{y}^{2} \mathsf{w}_{y} + \gamma_{5} (\mathsf{u}_{x}^{2} \mathsf{u}_{y} + \mathsf{w}_{x} \mathsf{w}_{y}^{2} - \mathsf{u}_{x}^{2} \mathsf{w}_{x} - \mathsf{u}_{y} \mathsf{w}_{y}^{2}) \\ &- (2\gamma_{5} + \gamma_{6}) \mathsf{u}_{x} \mathsf{u}_{y} \mathsf{w}_{x} - (2\gamma_{5} + \gamma_{7}) \mathsf{u}_{y} \mathsf{w}_{x} \mathsf{w}_{y} \Biggr]. \end{split}$$

Here

$$\gamma_1 = \alpha_2 + \frac{\alpha_5 - \alpha_4}{4}, \quad \gamma_2 = \alpha_2 + \frac{\alpha_6}{4} - \frac{\alpha_4}{2}, \quad \gamma_3 = \alpha_3 + \frac{\alpha_6}{4} - \frac{\alpha_7}{2},$$
 (10)

$$\gamma_4 = \alpha_3 + \frac{\alpha_6}{4} + \frac{\alpha_7}{2}, \quad \gamma_5 = \alpha_2 - \frac{\alpha_4}{4}, \quad \gamma_6 = \frac{1}{2} \left(\alpha_6 - \alpha_7 \right), \quad \gamma_7 = \frac{1}{2} \left(\alpha_6 + \alpha_7 \right).$$

In contrast to the classical case, in Lagrangian (9), there are terms containing second-order derivatives from the field of displacements. 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 nonlinear 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:

$$\begin{aligned} u_{tt} - c_1^2 u_{xx} - \left(c_2^2 - \frac{\beta^2}{2}\right) u_{yy} - \left(s^2 + \frac{\beta^2}{2}\right) w_{xy} \\ &= \frac{R^2}{4} \frac{\partial}{\partial y} \left[\frac{\partial^2}{\partial t^2} \left(u_y - w_x\right) - c_3^2 \Delta \left(u_y - w_x\right)\right] + \frac{1}{2} \frac{\partial H_1}{\partial x} + \frac{1}{2} \frac{\partial H_2}{\partial y}, \quad (11) \\ w_{tt} - \left(c_2^2 - \frac{\beta^2}{2}\right) w_{xx} - c_1^2 w_{yy} - \left(s^2 + \frac{\beta^2}{2}\right) u_{xy} \\ &= -\frac{R^2}{4} \frac{\partial}{\partial x} \left[\frac{\partial^2}{\partial t^2} \left(u_y - w_x\right) - c_3^2 \Delta \left(u_y - w_x\right)\right] + \frac{1}{2} \frac{\partial H_3}{\partial x} + \frac{1}{2} \frac{\partial H_4}{\partial y}. \end{aligned}$$

Here, the symbol Δ means the 2D Laplacian $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $H_{1,2,3,4}$ are the nonlinearity functions:

$$\begin{split} \mathsf{H}_{1} &= 3\alpha_{1}u_{x}^{2} - 2\alpha_{2}\left(u_{x}w_{y} + \frac{1}{2}w_{y}^{2} + u_{y}w_{y} + w_{x}w_{y}\right) \\ &+ \gamma_{2}u_{y}^{2} + \gamma_{3}w_{x}^{2} + 2\gamma_{5}(u_{x}u_{y} - u_{x}w_{x}) - (2\gamma_{5} + \gamma_{6})u_{y}w_{x}, \\ \mathsf{H}_{2} &= -2\alpha_{2}u_{x}w_{y} + \gamma_{1}(3u_{y}^{2} - w_{x}^{2} - 2u_{y}w_{x}) + 2\gamma_{2}u_{x}u_{y} + 2\gamma_{4}u_{y}w_{y} \\ &+ \gamma_{5}(u_{x}^{2} - w_{y}^{2}) - (2\gamma_{5} + \gamma_{6})u_{x}w_{x} - (2\gamma_{5} + \gamma_{7})w_{x}w_{y}, \\ \mathsf{H}_{3} &= -2\alpha_{2}u_{x}w_{y} + \gamma_{1}(3w_{x}^{2} - u_{y}^{2} - 2u_{y}w_{x}) + 2\gamma_{2}w_{x}w_{y} + 2\gamma_{3}u_{x}w_{x} \\ &+ \gamma_{5}(w_{y}^{2} - u_{x}^{2}) - (2\gamma_{5} + \gamma_{6})u_{x}u_{y} - (2\gamma_{5} + \gamma_{7})u_{y}w_{y}, \\ \mathsf{H}_{4} &= 3\alpha_{1}w_{y}^{2} - 2\alpha_{2}\left(u_{x}w_{y} + \frac{1}{2}u_{x}^{2} + u_{x}u_{y} + u_{x}w_{x}\right) \\ &+ \gamma_{2}w_{x}^{2} + \gamma_{4}u_{y}^{2} + 2\gamma_{5}(w_{x}w_{y} - u_{y}w_{y}) - (2\gamma_{5} + \gamma_{7})u_{y}w_{x}. \end{split}$$

Equations such as Eqs. (11) are usually called *equations of the second-order* gradient theory of elasticity [17], as the terms with spatial fourth-order derivatives take into account the coupled stresses arising at the translational displacements of the particles. It should be noted that, in spite of absence of microrotations in Eqs. (11), the coefficients of these equations changed because of influence of microstructure—in the considered low-frequency approximation, the transverse wave velocity is diminished by quantity $\beta^2/2$, and the parameter s² increases by the same quantity.

5 The Problem of Parametric Identification

The real-world problem of identification of the Cosserat continuum (see Eqs. (4)) is still actual for a lot of heterogeneous materials that are suitable for application of this model [18]. However, even in the simplest case of the elastic isotropic Cosserat continuum, there are rather few reliable results, confirmed by different researchers, concerning determination of model parameters. The further proposed procedure of estimating of macroparameters of the medium, which is based on the method of structural modeling, is intended for solving this problem.

Among velocities of propagation of translational waves in a square lattice consisting of round particles there are three independent quantities—in accordance with number of elasticity constants of the second order (C_{11} , C_{12} and C_{44}) in Lame equations of the classical theory of elasticity for media with cubic symmetry [19]:

$$\rho u_{tt} = C_{11} u_{xx} + C_{44} u_{yy} + (C_{12} + C_{44}) w_{xy},$$

$$\rho w_{tt} = C_{44} w_{xx} + C_{11} w_{yy} + (C_{12} + C_{44}) u_{xy}.$$

From comparison of these equations with Eqs. (11), which factors depend on the sizes of the particles, it is possible to receive the following relationships:

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

It should be noted that the equality $c_2^2 = \beta^2 + s^2/2$ follows both from (12) and from (5). Taking into account that $C_{11} - C_{12} = 2\rho v^2$ [19], where ρ is the density of the medium, v is the transverse wave velocity in the crystallographic direction (110)

$$v^2 = (2c_1^2 - s^2)/4, \tag{13}$$

Equations (12) will be rewritten in the form [20]:

$$C_{11} = \rho c_1^2, \quad C_{12} = \rho (c_1^2 - 2\nu^2), \quad C_{44} = \rho (c_1^2 + c_2^2 - 2\nu^2)/2.$$
 (14)

Formulas (14) show, how to determine effective moduli of elasticity of the nanocrystalline medium using acoustic measurements. Due to equations (12)–(14), it is possible to use freely any set of basis quantities: (c_1, c_2, s) , (c_1, c_2, v) or (C_{11}, C_{12}, C_{44}) . In particular, starting from known constants of elasticity of the second order, we come to the following expressions of parameters of interparticle interactions:

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$$\frac{K_1}{a} = \frac{1}{2+K} \left[C_{11} - C_{12} - 2(C_{44} - C_{12}) \left(\frac{1}{p} - 1 \right)^2 \right], \quad (15)$$

$$\frac{K_2}{a} = (C_{44} - C_{12}) \left(1 + \left(\frac{1}{p} - 1 \right)^2 \right), \quad \frac{K_3}{a} = C_{12},$$

where $K = K_0/K_1$ is the relation between the central and noncentral interactions, $p = h/a = d/a\sqrt{2}$ is the relative size of the particle.

Relations (5) depending on the values of microstructure parameters were analyzed in details in [14] and chap. 3 of monograph [1]. As a result of the analysis, using known experimental data ρ , C₁₁, C₁₂ and C₄₄ (at normal temperature) [21], the wave velocities c₁,c₂,c₃, parameters β and *s*, and also modeling parameters of power interactions between particles are calculated for some cubic crystals. The calculations were carried out for K = 10 (the central interactions dominate) and d/a = 0.9. In this work by means of equalities (15) we will estimate factors of nonlinearities (7) (see Table 1) which dependencies on microstructure parameters K and *p*, and the elasticity constants of the second order have the following appearance:

$$\begin{split} \rho \alpha_{1} &= \frac{1-p}{(1-p)^{2}+p^{2}} \left(C_{44} - C_{12} \right), \quad \rho \alpha_{2} = \frac{C_{12}}{4(1-p)}, \\ \rho \alpha_{3} &= \frac{K(1-p)+1}{(2+K)(1-p)} \left[C_{11} - C_{12} - 2 \left(C_{44} - C_{12} \right) \frac{(1-p)^{2}}{p^{2}} \right] \\ &\quad + \left(C_{44} - C_{12} \right) \frac{(1-p)(1-2p-p^{2})}{((1-p)^{2}+p^{2})p^{2}}, \\ \rho \alpha_{4} &= \frac{2pC_{12}}{1-p}, \quad \rho \alpha_{5} = \frac{p^{2}C_{12}}{(1-p)^{2}}, \\ \rho \alpha_{6} &= \frac{1}{2+K} \left[\left(C_{11} - C_{12} \right) \frac{p^{2}}{1-p} - 2 \left(C_{44} - C_{12} \right) \left(1-p \right) \right] \\ &\quad + \left(C_{44} - C_{12} \right) \frac{(2p-1)(5p-2p^{2}-1)}{(1-p)^{2}+p^{2}}, \\ \rho \alpha_{7} &= \frac{2}{2+K} \left[\left(C_{11} - C_{12} \right) \frac{p}{1-p} - 2 \left(C_{44} - C_{12} \right) \frac{1-p}{p} \right] \\ &\quad + 2 \left(C_{44} - C_{12} \right) \frac{(5p^{2} - 5p + 1)}{p((1-p)^{2}+p^{2})} \end{split}$$

From (16) it follows that, if $p \to 0$, as shown in work [11], the Cauchy relation $C_{12} = C_{44}$ is valid and, as a result

$$\alpha_2 \to rac{C_{12}}{4
ho}, \quad \alpha_3 \to rac{K+1}{(2+K)
ho} (C_{11} - C_{12}),$$

Structural parameters		Crystals		
		LiF	NaF	NaBr
Density (kg/m ³)	ρ	2600	2800	3200
Elasticity constants (10 ⁹ N/m ²)	C ₁₁ C ₁₂ C ₄₄	113.00 48.00 63.00	97.00 25.60 28.00	32.55 13.14 13.26
Wave velocities (m/s)	c ₁ c ₂ v c ₃	6593 5477 3536 5659	5890 3295 3571 2896	3190 2045 1741 1092
Coefficient of linear coupling between the longitudinal and transverse deformations (m/s)	S	6076	4276	2866
Dispersion parameter (m/s)	β	3396	1309	274
Parameters of force interactions between the particles (10^9 N/m^2)	K ₀ /a K ₁ /a K ₂ /a K ₃ /a	46.01 4.601 19.897 48.00	58.19 5.819 3.183 25.60	16.11 1.611 0.159 13.14
Nonlinearity coefficients in the original model $(10^6 \text{ m}^2/\text{s}^2)$	$\begin{array}{c} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \\ \alpha_6 \\ \alpha_7 \end{array}$	$ \begin{array}{r} 16.60\\ 12.69\\ -34.75\\ 64.63\\ 56.65\\ 62.55\\ 0.90\\ \end{array} $	6.87 6.29 0.38 32.00 28.01 30.92 6.49	2.85 2.82 -4.91 14.37 12.58 13.17 1.73
Nonlinearity coefficients in the two-mode model $(10^6 \text{ m}^2/\text{s}^2)$	Υ1 Υ2 Υ3 Υ4 Υ5 Υ6 Υ7	$10.68 \\ -3.98 \\ -19.56 \\ -18.66 \\ -3.46 \\ 30.83 \\ 31.72$	5.29 -1.99 4.87 11.36 -1.71 12.22 18.70	$2.37 \\ -1.07 \\ -2.49 \\ -0.76 \\ -0.77 \\ 5.72 \\ 7.45$

 Table 1
 Structural parameters for crystals with cubic symmetry

and all the other nonlinearity factors tend to zero. For p=1/2 the Cauchy relation is not valid and

$$\begin{split} &\alpha_1 = (C_{44} - C_{12})/\rho, \quad \alpha_2 = C_{12}/2\rho, \quad \alpha_3 = (C_{11} + 2C_{12} - 3C_{44})/\rho, \\ &\alpha_4 = 2C_{12}/\rho, \quad \alpha_5 = C_{12}/\rho, \\ &\alpha_6 = \frac{C_{11} + C_{12} - 2C_{44}}{2(2+K)\rho}, \quad \alpha_7 = \frac{C_{11} + 3C_{12} - 4C_{44}}{2(2+K)\rho}. \end{split}$$

Here α_3 does not depend on the parameter of interparticle interactions $K = K_0/K_1$, and any of nonlinearity coefficients does not tend to zero.

Numerical estimates of the nonlinearity factors presented in Table 1 show that only parameters γ_2 and γ_5 are negative for all considered crystals, whereas factors α_3 , γ_3 and γ_4 can be both positive and negative. In the three-mode model, parameter α_4 is the greatest for all considered materials, and parameter γ_7 has maximal values in the two-mode one. For the certain material γ_7 exceeds the smallest absolute value of a factor γ_i up to 11 times, and for parameters α_i this ratio is greater—up to 72 times. Besides, some α_i can even surpass a square of the longitudinal wave velocity, c_1^2 , that proves importance of the accounting of the nonlinear terms.

6 Kadomtsev–Petviashvili Evolutionary Equation for the Two-Mode Model

We shall consider propagation of localized strain waves in a medium, depending on parameters of its microstructure. For this purpose, we introduce new coordinates and time $\xi = x - vt$, $\eta = \sqrt{\varepsilon}y$, $\tau = \varepsilon t$; $u = \sqrt{\varepsilon}u$, w = w in Eqs.(11). So, these equations take on the form:

$$\begin{split} \sqrt{\varepsilon}v^{2}\frac{\partial^{2}u}{\partial\xi^{2}} - 2\varepsilon\sqrt{\varepsilon}v\frac{\partial^{2}u}{\partial\xi\partial\tau} - \sqrt{\varepsilon}c_{1}^{2}\frac{\partial^{2}u}{\partial\xi^{2}} - (c_{2}^{2} - \frac{\beta^{2}}{2})\varepsilon\sqrt{\varepsilon}\frac{\partial^{2}u}{\partial\eta^{2}} - (s^{2} + \frac{\beta^{2}}{2})\frac{\partial^{2}w}{\partial\xi\partial\eta}\sqrt{\varepsilon} \\ &= \frac{R^{2}}{4}\sqrt{\varepsilon}\frac{\partial}{\partial\eta}\left[v^{2}\frac{\partial^{2}}{\partial\xi^{2}}\left(\varepsilon\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right) - 2\varepsilon v\frac{\partial^{2}}{\partial\xi\partial\tau}\left(\varepsilon\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right) \\ &- c_{3}^{2}\left(\frac{\partial^{2}}{\partial\xi^{2}} + \varepsilon\frac{\partial^{2}}{\partial\eta^{2}}\right)\left(\sqrt{\varepsilon}\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right)\right] + \frac{1}{2}\frac{\partial H_{1}}{\partial\xi} + \frac{1}{2}\frac{\partial H_{2}}{\partial\eta}, \end{split}$$
(17)
$$v^{2}\frac{\partial^{2}w}{\partial\xi^{2}} - 2\varepsilon v\frac{\partial^{2}w}{\partial\xi\partial\tau} - \left(c_{2}^{2} - \frac{\beta^{2}}{2}\right)\frac{\partial^{2}w}{\partial\xi^{2}} - \varepsilon c_{1}^{2}\frac{\partial^{2}w}{\partial\eta^{2}} - \left(s^{2} + \frac{\beta^{2}}{2}\right)\varepsilon\frac{\partial^{2}u}{\partial\xi\partial\eta} \\ &= -\frac{R^{2}}{4}\frac{\partial}{\partial\xi}\left[v^{2}\frac{\partial^{2}}{\partial\xi^{2}}\left(\varepsilon\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right) - 2\varepsilon v\left(\varepsilon\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right) \\ &- c_{3}^{2}\left(\frac{\partial^{2}}{\partial\xi^{2}} + \varepsilon\frac{\partial^{2}}{\partial\eta^{2}}\right)\left(\sqrt{\varepsilon}\frac{\partial u}{\partial\eta} - \frac{\partial w}{\partial\xi}\right)\right] + \frac{1}{2}\frac{\partial H_{3}}{\partial\xi} + \frac{1}{2}\frac{\partial H_{4}}{\partial\eta}. \end{split}$$

As various terms of Eqs. (17) have different orders of smallness, we shall consider some approximations step-by-step.

Approximation of
$$\varepsilon^0$$
-order has the form: $\left(v^2 - \left(c_2^2 - \frac{\beta^2}{2}\right)\right)\frac{\partial^2 w}{\partial \xi^2} = 0$, hence,

$$v^2 = c_2^2 - \frac{\beta^2}{2}.$$
 (18)

Nonlinear Localized Strain Waves in a 2D Medium with Microstructure

Approximation of
$$\sqrt{\varepsilon}$$
-order: $(v^2 - c_1^2) \frac{\partial^2 u}{\partial \xi^2} - \left(s^2 + \frac{\beta^2}{2}\right) \frac{\partial^2 w}{\partial \xi \partial \eta} = 0$, therefore,

$$\frac{\partial u}{\partial \xi} = \frac{s^2 + \beta^2/2}{\nu^2 - c_1^2} \frac{\partial w}{\partial \eta}.$$
(19)

Approximation of ε -order:

$$-2\varepsilon v \frac{\partial^2 w}{\partial \xi \partial \tau} - \varepsilon c_1^2 \frac{\partial^2 w}{\partial \eta^2} - \left(s^2 + \frac{\beta^2}{2}\right) \varepsilon \frac{\partial^2 u}{\partial \xi \partial \eta}$$
$$= -\frac{R^2}{4} \frac{\partial}{\partial \xi} \left[v^2 \frac{\partial^2}{\partial \xi^2} \left(\varepsilon \frac{\partial u}{\partial \eta} \right) - 2\varepsilon v \left(-\frac{\partial w}{\partial \xi} \right) \right]$$
$$- c_3^2 \left(\varepsilon \frac{\partial^2}{\partial \eta^2} \right) \left(-\frac{\partial w}{\partial \xi} \right) \right] + 3\gamma_1 \frac{\partial w}{\partial \xi} \frac{\partial^2 w}{\partial \xi^2}. \tag{20}$$

After entering the designation $\frac{\partial w}{\partial \xi} = U$ in Eq. (20) and taking into account expressions (18) and (19), Eq. (20) is reduced to the following equation:

$$2\nu U_{\xi\tau} + q_1(U^2)_{\xi\xi} + \frac{R^2}{4}q_2 U_{\xi\xi\xi\xi} + q_3 U_{\eta\eta} = 0, \qquad (21)$$

where

$$\frac{3\gamma_1}{2\varepsilon} = q_1, \ \frac{2c_2^2 - 2c_3^2 - \beta^2}{2\varepsilon} = q_2, \ c_1^2 + \frac{(2s^2 + \beta^2)^2}{4(c_2^2 - c_1^2) - 2\beta^2} = q_3.$$
(22)

We will introduce designations: $U/U_0 = W$, $\xi/\xi_0 = X$, $\tau/\tau_0 = T$, $\eta/\eta_0 = Y$. If to put $U_0 = 1$ and $\eta_0 = \xi_0$, then W = U and, in terms of new variables, Eq. (22) yields:

$$2\frac{\partial^2 U}{\partial X \,\partial T} + \frac{q_1}{\nu} \frac{\tau_0}{\xi_0} \frac{\partial^2 (U^2)}{\partial X^2} + \frac{R^2}{4\nu} q_2 \frac{\tau_0}{\xi_0^3} \frac{\partial^4 U}{\partial X^4} + q_3 \frac{\tau_0}{\nu \xi_0} \frac{\partial^2 U}{\partial Y^2} = 0.$$
(23)

We choose scales ξ_0 and τ_0 so, that the last coefficient in Eq. (23) would be equal to 1: $\tau_0 = v$

$$\frac{\tau_0}{\xi_0} = \frac{\nu}{q_3}.$$

If to take in this relation $\xi_0 = R/2$, then Eq.(23) is transformed into well-known Kadomtsev–Petviashvili equation



$$2\frac{\partial^2 U}{\partial X \,\partial T} + \frac{q_1}{q_3}\frac{\partial^2 (U^2)}{\partial X^2} + \frac{q_2}{q_3}\frac{\partial^4 U}{\partial X^4} + \frac{\partial^2 U}{\partial Y^2} = 0.$$
(24)

This equation has a solution in the form of a plane solitary strain wave (soliton) (Fig. 3):

$$U(\theta) = A_{s} ch^{-2}(\theta/\Delta), \qquad (25)$$

where $\theta = X - kY - VT$ is the wave phase. The amplitude of soliton, A_s, and its width Δ are determined by relations:

$$A_{s} = \left| \frac{3q_{3}(k^{2} - 2V)}{2q_{1}} \right|, \qquad (26)$$
$$\Delta = 2\sqrt{\left| \frac{q_{2}}{q_{3}(k^{2} - 2V)} \right|}.$$

It should be noted that product

$$A_s \Delta^2 = \left| \frac{6q_2}{q_1} \right| = \left| \frac{2c_2^2 - 2c_3^2 - \beta^2}{\gamma_1} \right|$$

is the constant for each material.

The plane solitary wave (25) is known to be stable, if $q_2/q_3 > 0$, and it is unstable with respect to transverse perturbations, when $q_2/q_3 < 0$ [22]. In this case, Kadomtsev–Petviashvili equation has an other precise solution [23]:

$$U(X, Y, T) = \frac{6q_2}{q_1} \frac{\partial^2}{\partial X^2} \ln \left[1 + \exp(2q\theta) + \exp(2p(\theta + \psi) + A\exp((q + p)\theta + p\psi)\cos kY)\right].$$
(27)

Here p and q are integration constants,

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Fig. 4 The plane wave modulated in the transverse direction [22]

$$\theta = X - (1 + \frac{2q_2}{q_3}q^2)T, \quad \psi = -4p\frac{q_2}{q_3}(p^2 - q^2)T,$$
$$A = \frac{4\sqrt{pq}}{p+q}, \quad k = (q^2 - p^2)\sqrt{\frac{-3q_2}{q_3}}.$$

Formula (27) describes a periodic chain of two-dimensional solitary strain waves (Fig. 4). If $q_2/q_3 < 0$, i.e. the condition of soliton instability with respect to transverse perturbations takes place, the plane solitary wave (25) plotted in Fig. 3 will be transformed into Eq. (27). Polarity of solitons (25) and (27) depends on sign of expression q_1/q_2 . The solitons have a positive polarity (this case is represented in Figs. 3 and 4), when $q_1/q_2 > 0$, and their polarity is negative, if $q_1/q_2 < 0$.

Let us analyze obtained from (27) dependencies of coefficients q_1/q_2 and q_2/q_3 on the macroparameters of the medium:

$$\frac{q_1}{q_2} = \frac{3\gamma_1}{2c_2^2 - 2c_3^2 - \beta^2},$$
(28)

$$\frac{\mathbf{q}_2}{\mathbf{q}_3} = \frac{(2\mathbf{c}_2^2 - 2\mathbf{c}_3^2 - \beta^2)(2\mathbf{c}_2^2 - 2\mathbf{c}_1^2 - \beta^2)}{\varepsilon(2\mathbf{c}_1^2(2\mathbf{c}_2^2 - \beta^2) - 4\mathbf{c}_1^4 + (2\mathbf{s}^2 + \beta^2)^2)}.$$
(29)

From (10) and (7) follows that

$$\begin{split} \gamma_1 &= \alpha_2 + \frac{\alpha_5 - \alpha_4}{4} = \frac{K_3}{M} \left(\frac{a^3}{4(a-h)} + \frac{a^2h^2}{4(a-h)^2} - \frac{a^2h}{2(a-h)} \right) \\ &= \frac{K_3 a^2(a^2 - 3ah + 3h^2)}{4M(a-h)^2} > 0. \end{split}$$

Thus, $q_1/q_2 > 0$ for $c_2^2 > c_3^2 + \beta^2/2$, and $q_1/q_2 < 0$ for $c_2^2 < c_3^2 + \beta^2/2$.

Crystal	LiF	NaF	NaBr
Sign of q_2/q_3	+	+	_
Sign of q_1/q_2	_	+	+
Stable solitons of plane deformation and their polarity	\sim	_/_	no

Table 2 Existence of stable plane solitons of deformations and their polarity in some cubic crystals









If to take as an initial condition for Kadomtsev–Petviashvili equation a 2D soliton without plane front (Fig. 5), i.e. perturbation in the form

$$U_0(X,Y) = 12\operatorname{sech}^2\left(\frac{X-32}{4}\right)\operatorname{sech}(Y-8),\tag{30}$$

and to carry out numerical simulation by means of the semi-implicit pseudo-spectral scheme [24] with parameters: 256×64 is dimension of a grid, $\Delta X = 0.25$ is a length of a step along *X*-axis, $\Delta Y = 0.25$ is a length of a step along *Y*-axis, $\Delta T = 0.003$ is a length of a step along *T*-axis, then an other behavior of the solitary wave will

be observed. In fact, the peak of excitations (30) moves forward (along X-axis) and simultaneously spreads along Y-axis. Eventually, the amplitude of excitation grows till a certain value (A = 7.1) near the boundaries, spreading aside and moving forward, that leads to appearance of the crosswise structures (Fig. 6).

7 Conclusions

The nonlinear mathematical model of the two-dimensional crystalline (granular) medium with a non-dense packing of the particles possessing two translational and one rotational degrees of freedom, has been elaborated in this work. In the field of low frequencies the obtained set of equations is reduced to the two-mode set, linear parts of which equations coincide with a two-dimensional analog of the classical Lame equations for media 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.

Analytical dependencies of the elastic and rotational wave velocities and the nonlinearity factors on the sizes of particles and the parameters of interactions between them have been found. The velocities of elastic waves along the various crystallographic directions can be measured experimentally without any difficulties, but it is rather complicated or even, sometimes, impossible to determine from experiments the rotational wave velocity, the threshold frequency of this wave and the factors of nonlinear interactions between the waves of various types. For this reason, the estimates of these quantities can be very useful that are obtained by the following way. First, due to obtained expressions (5) for the experimentally measured velocities of elastic waves depending on the microstructure parameters of the material, inverse relationships (15) are derived, and then they are used for calculation of other macroparameters of the medium. In this work, by such a way the factors of nonlinear interactions of complete three-mode set (7) and two-mode model of the medium with the restricted rotation of particles (10) are calculated. Some of these factors are shown to be negative, whereas the other ones can exceed a square of the longitudinal wave velocity.

In its turn, the two-mode system is reduced by the multi-scale method to Kadomtsev–Petviashvili evolutionary equation with respect to shear deformation, which has a solution in the form of plane soliton. Due to the method of structural modeling used in this work, it is shown that in the crystal medium with parameters as for NaBr, the plane soliton is unstable with respect to two-dimensional perturbations, in NaF-crystal the soliton has a positive polarity, and in LiF-crystal it has a negative polarity.

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