Nonlinear theory of deformation of crystal media with complex structure of lattice: plane deformation

E. L. Aero A. N. Bulygin Yu. V. Pavlov N. A. Reinberg
bulygin_an@mail.ru

Abstract

Nonlinear theory of crystal media with the complex lattice consisting of two sublattices is developed in last years [1], [2]. The model describes formation of defects, phase transformations, fragmentation of a lattice and other physical processes which are realized, in particular, near coast of a crack and which aren't described by the classical elasticity theory. Owing to this fact development of numerical and analytical methods of the solution of the nonlinear theory in relation to problems of fracture mechanics is perspective.

The equations describing plane deformation of complex crystal lattice are received. The equations of acoustic mode are solved by introduction of Airy function. In the nonlinear theory it satisfies to the nonhomogeneous equation. The role of a source is played by plastic deformations of a lattice. The equations describing the structure of lattice, have a form of system of two connected double sine-Gordon equations with variable amplitude. Communication between structure and potential of interaction of sublattices is studied on the example of one-dimensional deformation.

1 Introduction

In the classical theory of deformation of solid bodies including crystal, the preservation condition of local topology in the process of structure change is accepted as a postulate — the nearest neighbors (within a small vicinity of a material particle) remain invariable, and power communications between particles don't switch over. Only changes of distances between small, but macroscopic, volumes are considered. Actually there are changes both distant and the neighboring translational orders in a crystal. For their account it is necessary to introduce structural factors. Somewhat it was made by M.Born and K.Huang [3] at creation of the linear dynamic theory of complex crystal lattices.

Nonlinear model of deformations of crystal media with a complex lattice is offered in Refs. [1], [2]. As in the classical theory [3] the shift of the center of inertia atoms of an elementary cell is described by a vector $\mathbf{U}(x, y, z, t)$ (acoustic fashion), and relative shift of atoms in a cell — by vector $\mathbf{u}(x, y, z, t)$ (optical fashion). Unlike the theory [3] the shift of sublattices $\mathbf{u}$ can be arbitrary large. The principle of translation symmetry is entered into the theory — rigid shift one sublattice concerning another for one period (or their integer) again reproduces structure of the complex lattice. It means that its energy has to be periodic function relative to rigid shift of sublattices, invariant to this translation. Certainly the classical principle of translation symmetry remains also: energy of a lattices is invariant to translation of both sublattices on one (or a integer) the periods of a complex lattice.

Transition to significantly nonlinear equations [1], [2], [4]–[7] allows to predict deep structure reorganization: fall of the potential barriers, switching of interatomic communications, phase transformations [7], lattice fragmentation [6], emergence of singular defects and other fracture of a lattice [4]. Development of nonlinear models of mechanics of the continuous media answers to modern problems which arose in connection with deep penetration into area of the small (nano-) scales. One of the main problems is the problem of receiving, deformation and destruction of materials with nanostructure.. The solution of this problem demands introduction significantly nonlinear models and direct account of deep changes of structure of a solid body.

2 General equations

The equations of motion determining $\mathbf{U}(t,x,y,z)$, $\mathbf{u}(t,x,y,z)$ are received from Lagrange's variation principle. They have the form

$$\rho\ddot{U}_i = \lambda_{ikmn}e_{mn,k} - s_{ik}[\Phi(u_R)]_{,k}, \tag{1}$$

$$\mu\ddot{u}_i = k_{ikmn}\varepsilon_{mn,k} - (p - s_{ik}e_{ik})\frac{\partial\Phi(u_R)}{\partial u_i}. \tag{2}$$

Here (ρ,μ) are average and reduced density of couples of atoms respectively, tensors $(\lambda_{ikmn}, k_{ikmn})$ are elasticity and microelasticity coefficients, s_{ik} is tensor of nonlinear mechanostriction, $(e_{ik}, \varepsilon_{ik})$ are deformation and microdeformation tensors

$$e_{ik} = \frac{1}{2}\left(U_{i,k} + U_{k,i}\right), \qquad \varepsilon_{ik} = \frac{1}{2}\left(u_{i,k} + u_{k,i}\right). \tag{3}$$

Function $\Phi(u_R)$ represents triple periodic energy of interactions of sublattices, invariant to translation of Bravais sublattices lengthways directions of vectors $\mathbf{k}, \mathbf{m}, \mathbf{n}$ for the periods a_1, a_2, a_3 respectively. Argument is

$$u_R = \sqrt{u_i a_{ik} u_k}, \qquad a_{ik} = a_1^{-2}k_i k_k + a_2^{-2}m_i m_k + a_3^{-2}n_i n_k. \tag{4}$$

Here a_{ik} is tensor of the inverse periods of a lattice (a_1, a_2, a_3), $(\mathbf{n_1}/a_1, \mathbf{n_2}/a_2, \mathbf{n_3}/a_3)$ are vectors of inverse lattice. On physical sense $\Phi(u_R)$ has to be function even and the periodic. In general case (for Dirichlet conditions) $\Phi(u_R)$ can be expanded in Fourier series

$$\Phi(u_R) = (1 - \cos u_R) + \delta(1 - \cos 2u_R) + \ldots \tag{5}$$

In expansion (5) it is accepted that energy of interaction of sublattices it is equal to zero, if $u_R = 0$. The factor before function $\Phi(u_R)$

$$P = p - s_{ik}e_{ik} \tag{6}$$

represents an effective interatomic barrier—energy of activation of couplings. Here p is half of energy of activation of rigid shift of sublattices, and s_{ik} is tensor of nonlinear mechanostriction. The coefficient P represents energy of activation of couplings. It is very sensitive instrument of management of a microstructure and properties of a lattice with help of macroscopic fields of deformations and tension.

Eq. (1) can be written in a standard form of the equations of mechanics of continuous medium

$$\rho\ddot{U}_i = \sigma_{ik,k}, \tag{7}$$

if to enter a stress tensor

$$\sigma_{ik} = \lambda_{ikmn} e_{mn} - s_{ik}\Phi(u_R). \tag{8}$$

The stress tensor σ_{ik}, unlike classical, is the sum two terms

$$\sigma_{ik} = \sigma_{ik}^U + \sigma_{ik}^p, \tag{9}$$

$$\sigma_{ik}^U = \lambda_{ikmn} e_{mn}, \qquad \sigma_{ik}^p = -s_{ik}\Phi(u_R). \tag{10}$$

Obviously, σ_{ik}^U represents an elastic component of shift stress. The value σ_{ik}^p is an inelastic component, because it is quadratically on shift $\mathbf{u}$ and doesn't depend on its direction. It has the sign opposite to a sign of macroshift $\mathbf{U}$. Force σ_{ik}^p in the corresponding plane can take as friction force. It is small at small microshifts and reaches limit high value $2s_{ik}$, when $u_R = (2n+1)\pi$, i.e. at shift of atoms from potential holes in maxima on tops of interatomic potential barriers. Obviously, the value of a material tensor of s_{ik} is that limit for the inelastic tension which describes losses of stability of a lattice. Further plastic deformations, phase transitions and other bifurcation processes are possible.. They are defined by a field of microshifts which is the solution of Eq. (2).

If the optical mode doesn't excite ($u_R = 0$), then Eqs. (2) are satisfied identically, and (1) pass into the equations of classical mechanics of the continuous medium.

Tensors $(\lambda_{ikmn}, k_{ikmn})$ are symmetric to shift of couples of indexes and couple indexes among themselves. For crystals of cubic symmetry the components of tensor λ_{ikmn}

$$\lambda_{1111}, \quad \lambda_{2222}, \quad \lambda_{3333}, \quad \lambda_{1122}, \lambda_{1133}, \quad \lambda_{2233}, \quad \lambda_{1212}, \quad \lambda_{1313}, \quad \lambda_{2323}$$

aren't equal to zero They are connected by relationships

$$\lambda_{1111} = \lambda_{2222} = \lambda_{3333}, \quad \lambda_{1122} = \lambda_{1133} = \lambda_{2233}, \quad \lambda_{1212} = \lambda_{1313} = \lambda_{2323}.$$

Independent there are three modules of elasticity. If to accept as independent $(\lambda_{1111}, \ \lambda_{1122}, \ \lambda_{1212})$, then density of elastic energy of macrodeformation will be equal to

$$\begin{aligned} D_U &= \frac{1}{2}\lambda_{ikmn} e_{ik} e_{mn} = \frac{\lambda_{1111}}{2}\left(e_{xx}^2 + e_{yy}^2 + e_{zz}^2\right) + \\ &+ \lambda_{1122}\left(e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz}\right) + 2\lambda_{1212}\left(e_{xy}^2 + e_{yz}^2 + e_{yz}^2\right). \end{aligned} \tag{11}$$

Told about tensor λ_{ikmn} is fair and for a tensor k_{ikmn}. Density of elastic energy of microdeformation is

$$\begin{aligned} D_u &= \frac{1}{2}k_{ikmn}\varepsilon_{ik}\varepsilon_{mn} = \frac{k_{1111}}{2}\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2\right) + \\ &+ k_{1122}\left(\varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{xx}\varepsilon_{zz} + \varepsilon_{yy}\varepsilon_{zz}\right) + 2k_{1212}\left(\varepsilon_{xy}^2 + \varepsilon_{yz}^2 + \varepsilon_{yz}^2\right). \end{aligned} \tag{12}$$

From (11), (12) one can find a tensor of elastic macrotension

$$\sigma_{ik}^U = \frac{\partial D_U}{\partial e_{ik}} = \begin{cases} 2\mu e_{ik} + \lambda\delta_{ik}e_{\alpha\alpha} & (i = k), \\ 2\mu a_1 e_{ik} & (i \neq k) \end{cases} \tag{13}$$

and tensor of elastic macrotension

$$\sigma_{ik}^u = \frac{\partial D_u}{\partial \varepsilon_{ik}} = \begin{cases} 2k_1\varepsilon_{ik} + k_2\delta_{ik}\varepsilon_{\alpha\alpha} & (i = k), \\ 2k_1 a_2 \varepsilon_{ik} & (i \neq k). \end{cases} \tag{14}$$

Here new designations for elasticity modules are entered

$$\begin{aligned} &\lambda_{1111} = 2\mu + \lambda, \quad &\lambda_{1122} = \lambda, \quad &\lambda_{1212} = \mu a_1, \\ &k_{1111} = 2k_1 + k_2, \quad &k_{1122} = k_2, \quad &k_{1212} = k_1 a_2. \end{aligned} \tag{15}$$

The coefficients (a_1, a_2) characterize anisotropy according to macro- and microshifts

$$a_1 = \frac{2\lambda_{1212}}{\lambda_{1111} - \lambda_{1122}}, \qquad a_2 = \frac{2k_{1212}}{k_{1111} - k_{1122}}. \tag{16}$$

If $a_1 = 1$, then the continuum of macroshifts will be isotropic. If $a_2 = 1$, then the continuum of microshifts will be isotropic.

Components of a tensor e_{ik} have to satisfy relationships of compatibility of Saint-Venant

$$\Delta e_{ik} + e_{\alpha\alpha,ik} - (e_{i\alpha,k\alpha} + e_{k\alpha,i\alpha}) = 0. \tag{17}$$

3 Plane deformation of crystals of cubic symmetry

By definition, the field of shifts is called plane, parallel to the plane $x_3 = 0$, if

$$U_x = U_x(t, x, y), \qquad U_y = U_y(t, x, y), \qquad U_z = 0, \tag{18}$$

$$u_x = u_x(t, x, y), \qquad u_y = u_y(t, x, y), \qquad u_z = 0. \tag{19}$$

In the case of deformation of crystal media with a cubic lattice the symmetric tensor of mechanostriction s_{ik} has two components which don't equal to zero $s_{11} = s_{22}$, $s_{12} = s_{21}$. Owing to this fact the symmetric tensor of inelastic tension σ^p_{ik} is equal

$$\sigma^p_{xx} = \sigma^p_{yy} = s_{11}\Phi(u_R), \qquad \sigma^p_{xy} = \sigma^p_{yx} = s_{12}\Phi(u_R), \qquad \sigma^p_{xz} = \sigma^p_{yz} = \sigma^p_{zz} = 0. \tag{20}$$

Symmetric tensor of elastic macrotension σ^U_{ik} takes the form

$$\begin{aligned} \sigma^U_{xx} &= 2\mu e_{xx} + \lambda(e_{xx} + e_{yy}), \qquad \sigma^U_{yy} = 2\mu e_{yy} + \lambda(e_{xx} + e_{yy}), \\ \sigma^U_{xy} &= 2\mu a_1 e_{xy}, \qquad \sigma^U_{xz} = \sigma^U_{yz} = 0, \qquad \sigma^U_{zz} = \lambda(e_{xx} + e_{yy}). \end{aligned} \tag{21}$$

The symmetric tensor of elastic microtension σ^u_{ik} will have the same form

$$\begin{aligned} \sigma^u_{xx} &= 2k_1\varepsilon_{xx} + k_2(\varepsilon_{xx} + \varepsilon_{yy}), \qquad \sigma^u_{yy} = 2k_1\varepsilon_{yy} + k_2(\varepsilon_{xx} + \varepsilon_{yy}), \\ \sigma^u_{xy} &= 2k_1 a_2 e_{xy}, \qquad \sigma^u_{xz} = \sigma^U_{yz} = 0, \qquad \sigma^u_{zz} = k_2(\varepsilon_{xx} + \varepsilon_{yy}). \end{aligned} \tag{22}$$

Taking into account the form of tensors $(\sigma^p_{ik}, \sigma^U_{ik}, \sigma^u_{ik})$, we will receive the equations describing flat deformation of crystal media of cubic symmetry

$$\rho \ddot{U}_x = \sigma^-_{xx,x} + \sigma^-_{xy,y}, \tag{23}$$

$$\rho \ddot{U}_y = \sigma^-_{yx,x} + \sigma^-_{yy,y}, \tag{24}$$

$$\mu \ddot{u}_x = -P\frac{u_x}{u_R}\Phi'(u_R) + k_1\Delta u_x + k_2\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) + \bar{k}_1\frac{\partial^2 u_x}{\partial x^2}, \tag{25}$$

$$\mu \ddot{u}_y = -P\frac{u_y}{u_R}\Phi'(u_R) + k_1\Delta u_y + k_2\frac{\partial}{\partial y}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) + \bar{k}_1\frac{\partial^2 u_y}{\partial y^2}. \tag{26}$$

Here

$$\sigma^-_{ik} = \sigma^U_{ik} - \sigma^p_{ik}, \qquad \bar{k}_1 = \frac{2}{a_2}(1 - a_2)k_1, \qquad u_R = \sqrt{u_x^2 + u_y^2}, \tag{27}$$

The motion equations (23)–(26) are the system of four nonlinear coupled equations. The last two are nonlinear Klein-Fock-Gordon equations with a variable amplitude. Some approaches to the solution of such equations are stated in [11], [12]. Finding of analytical solutions of the system is a complex mathematical problem. Therefore simplifying assumptions are justified.

At the beginning we will be limited to static deformation. For problems of a statics Eqs. (23), (24) will assume the form

$$\sigma^{-}_{xx,x} + \sigma^{-}_{xy,y} = 0, \quad \sigma^{-}_{yx,x} + \sigma^{-}_{yy,y} = 0. \tag{28}$$

Eqs. (28) are satisfied identically, if a tensor σ^{-}_{ik} to write with help Airy function

$$\sigma^{-}_{ik} = -\frac{\partial^2 Q}{\partial x_i \partial x_k} + \delta_{ik}\Delta Q. \tag{29}$$

Through Airy function it is possible to express a tensor of macrodeformations e_{ik}

$$e_{xx} = \frac{1+\sigma}{E}\left[\frac{\partial^2 Q}{\partial y^2} - \sigma\Delta Q + (1-2\sigma)s_{11}\Phi(u_R)\right], \tag{30}$$

$$e_{yy} = \frac{1+\sigma}{E}\left[\frac{\partial^2 Q}{\partial x^2} - \sigma\Delta Q + (1-2\sigma)s_{11}\Phi(u_R)\right], \tag{31}$$

$$e_{xy} = \frac{1+\sigma}{a_1 E}\left[-\frac{\partial^2 Q}{\partial x \partial y} + s_{12}\Phi(u_R)\right]. \tag{32}$$

For plane deformation from six Saint-Venant equations of compatibility (17) only one remains

$$\frac{\partial^2 e_{xx}}{\partial y^2} + \frac{\partial^2 e_{yy}}{\partial x^2} = 2\frac{\partial^2 e_{xy}}{\partial x \partial y}. \tag{33}$$

Having substituted (30)–(32) in (33), we will receive the equation for finding of Airy function

$$(1-\sigma)\Delta\Delta Q + \frac{2(1-a_1)}{a_1}\frac{\partial^4 Q}{\partial x^2 \partial y^2} = (2\sigma - 1)s_{11}\,\Delta\Phi(u_R) + \frac{2s_{12}}{a_1}\frac{\partial^2 \Phi}{\partial x \partial y}. \tag{34}$$

As we can see from (34), function of Erie, unlike the classical theory of elasticity, satisfies to the non-homogeneous equation. The role of a source is played by plastic deformations of a lattice. In general case the solution of the equation (34) can be written in the form of the sum of two functions

$$Q = Q^0 + Q^p, \tag{35}$$

where Q^0 is a solution of homogeneous equation, and Q^p is a partial solution of the non-homogeneous equation. For isotropic media the methods of finding of Q^0 are stated in [8], and for anisotropic media in [9]. The partial solution Q^p can be expressed through Green's functions.

Relationships (30)–(32) allow to rewrite an effective potential barrier through $Q(x, y)$ function

$$P = p - s_{ik}e_{ik} = p\left[\bar{P}_1 + 2\bar{P}_2(1 - \Phi(u_R)\right]. \tag{36}$$

Here

$$\bar{P}_1 + 2\bar{P}_2 = 1 - \frac{1+\sigma}{pE}\left[s_{11}(1-2\sigma)\Delta Q - \frac{2s_{12}}{a_1}\frac{\partial^2 Q}{\partial x \partial y}\right], \tag{37}$$

$$\bar{P}_2 = \frac{1+\sigma}{pE}\left[s_{11}^2(1-2\sigma) + \frac{s_{12}^2}{a_1}\right]. \tag{38}$$

We will note that only coefficient $\bar{P}_1$ is expressed through $Q(x,y)$ function. Therefore, generally $P_1 = P_1(x,y)$. Coefficient P_2 is constant because it depends only on material parameters of the medium.

4 Solution of the one-dimensional equations of statics

Eqs. (23)–(26) are a system of the coupled nonlinear equations in partial derivatives. Their analytical integration is coupled to overcoming of great mathematical difficulties. The simplest case is the one-dimensional deformation. For it it is possible to receive exact solutions of the equations of statics at arbitrary potential of interaction of sublattices $\Phi(u_R)$, that allows to find dependence between the potential of $\Phi(u_R)$ and features structures of microdeformations.

For one-dimensional case

$$U_x = U(x), \quad U_y = 0, \quad U_z = 0, \quad u_x = u(x), \quad u_y = 0, \quad u_z = 0, \quad u_R = u. \tag{39}$$

The equations of a statics will assume a form

$$\left[(\lambda + 2\mu)U_{,x} - s\Phi(u)\right]_{,x} = 0, \qquad s = s_{11}, \tag{40}$$

$$ku_{,xx} = (p - sU_{,x})\Phi(u), \qquad k = k_{1111}. \tag{41}$$

The coupled system (40), (41) can be divided and the separate equations for microshift $u(x)$ and macrodeformation $\varepsilon = U_{,x}$ can be found. The equation for $u(x)$ will be found if to integrate (40)

$$(\lambda + 2\mu)U_{,x} - s\Phi(u) = \sigma, \tag{42}$$

and then from (41) with the help (42) to exclude $U_{,x}$. As a result for $u(x)$ we will receive the separate nonlinear differential the equation of the second order, which first integral has a form

$$u_{,\xi}^2 = 2g + 2\beta\Phi(u) - \beta_0\Phi^2(u), \qquad \xi = \frac{x}{l_0}. \tag{43}$$

Here (σ, g) are the integration constants, l_0 is length of coherence of the lattice, playing role of material nanoscale, and (β, β_0) are parameters of the model,

$$l_0^2 = \frac{k}{p}, \quad \beta = 1 - \frac{\sigma}{\sigma_t}, \quad \beta_0 = \frac{s}{\sigma_t}, \quad \sigma_t = \frac{p}{s}(\lambda + 2\mu). \tag{44}$$

From Eq. (43) the field of microdeformation $u(x)$ can be found. If $\Phi(u) = 1 - \cos u$, then it will assume a form

$$u_{,\xi}^2 = 2g + 2\beta(1 - \cos u) - \beta_0(1 - \cos u)^2. \tag{45}$$

For potential $\Phi(u) = 1 - \cos u + \delta(1 - \cos u)^2$

$$u_{,\xi}^2 = 2g + a_1\beta(1 - \cos u) - a_2(1 - \cos u)^2 + a_3\beta(1 - \cos u)^3 - a_4(1 - \cos u)^4, \quad (46)$$

$$a_1 = 2\beta(1 + 4\delta), \quad a_2 = 4\beta\delta + \beta_0(1 + 4\delta)^2, \quad a_3 = 4\beta_0\delta(1 + 4\delta), \quad a_4 = 4\beta_0\delta^2. \quad (47)$$

From (45), (46) it is visible that in the first case a field of microdeformation of $u(x)$ is given by the inversion of elliptic integral

$$\int \frac{du}{\sqrt{\left(1 + a^2\sin^2\frac{u}{2}\right)\left(1 - b^2\sin^2\frac{u}{2}\right)}} = \sqrt{2g}(\xi + C), \quad (48)$$

$$a^2 - b^2 = \frac{2\beta}{g}, \qquad a^2b^2 = \frac{2\beta_0}{g}, \quad (49)$$

and in the second case — by inversion of hyperelliptic integral

$$\int \frac{du}{\sqrt{1 + \overline{a}_1(1 - \cos u) - \overline{a}_2(1 - \cos u)^2 + \overline{a}_3(1 - \cos u)^3 - \overline{a}_4(1 - \cos u)^4}} = \sqrt{2g}(\xi + C), \quad (50)$$

$$\overline{a}_i = \frac{a_i}{2g}, \qquad i = 1, \ldots, 4. \quad (51)$$

The separate equation for macrodeformation $\varepsilon = U_{,x}$ will be obtained, if to write the derivative du/dx through $d\varepsilon/dx$ from Eq. (40)

$$(\lambda + 2\mu)\frac{d\varepsilon}{dx} = s\Phi'(u)\frac{du}{dx}, \quad (52)$$

and from Eq. (42) to express $\Phi(u)$ through ε.

Having substituted du/dx and $\Phi(u)$ in (43), we find the separate equation for ε. If potential is $\Phi = 1 - \cos u$, then it has a form

$$\int \frac{du}{\sqrt{(\varepsilon - \alpha_1)(\varepsilon - \alpha_2)(\varepsilon - \alpha_3)(\varepsilon - \alpha_4)}} = \sqrt{\frac{\lambda + 2\mu}{k}}(x + C). \quad (53)$$

Here roots $(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$ are the values

$$\left(\frac{\sigma}{\lambda + 2\mu}, \quad \frac{\sigma + 2s}{\lambda + 2\mu}, \quad \frac{\sigma + 2s/b^2}{\lambda + 2\mu}, \quad \frac{\sigma - 2s/a^2}{\lambda + 2\mu}\right).$$

According to algorithm of the inversion of elliptic integral they have be ordered. We will accept that

$$\alpha_1 > \alpha_2 > \alpha_3 > \alpha_4.$$

For potential $\Phi(u) = 1 - \cos u + \delta(1 - \cos u)^2$ macrodeformation ε can be found by inversion of the ultraelliptic integral (under a root in (53) a polynom of the sixth degree is situated).

The problem of inversion of elliptic integral was solved by Abel, Jacobi, Weierstrass and Riemann. They introduced into the analysis doubly periodic functions (theta-functions, elliptic functions) of one complex variable. Problem of the inversion of ultraelliptic integral was solved by Göpel and Rosenhain. They developed the theory of theta-functions of two complex variables and showed that formulas of the inversion of ultraelliptic integral are expressed through the relations of the introduced theta-functions. The inversion of ultraelliptic integral by the Rosenhain method gives in [10]. The theory of theta-functions of two complex variables is a very complicated and in modern mathematics practically isn't known. That is why, it is expedient to use methods of qualitative research of the equations (45), (46).

Arrangement of roots α_i determines model parameters. Two of them β_0, l_0 describe properties of a crystal. We will consider them fixed. Parameter β depends on external stress σ. It can change over a wide range. Different values can accept and a dimensionless constant of integration g. In particular, if microshifts ($u_s = 0$) are equal to zero on the border, then maginitude pg is surface energy of microgradients on border

$$pg = \frac{k}{2}(u_{,x}^2)_s, \qquad u_s = 0, \qquad x = x_s. \tag{54}$$

In this case $g \geq 0$. If $u_s \neq 0$, then g can be negative. We will note that at certain ratios between parameters the elliptic integral becomes pseudo-elliptic. The last is expressed through elementary functions.

Solutions of Eq. (43) are considered in [5]. In the present work we will be limited only by quality comparison of solutions of equations (43) and (50).

Phase portraits of the equation (43) are represented on Fig. 1—3 for the case, when $\beta = 0.5$, $\beta_0 = 0.75$. On a vertical axis value of a microgradient of $u_{,\xi}$, and on hor-

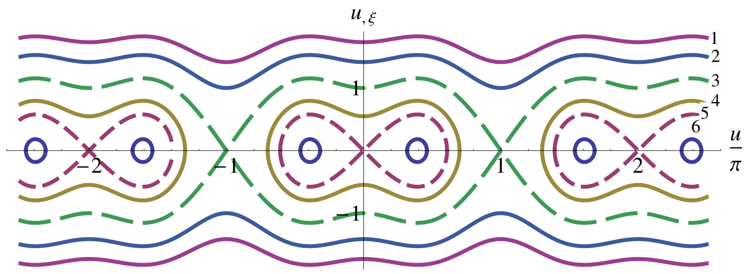

Figure 1: Phase portraits at value of parameter $\delta = 0$.

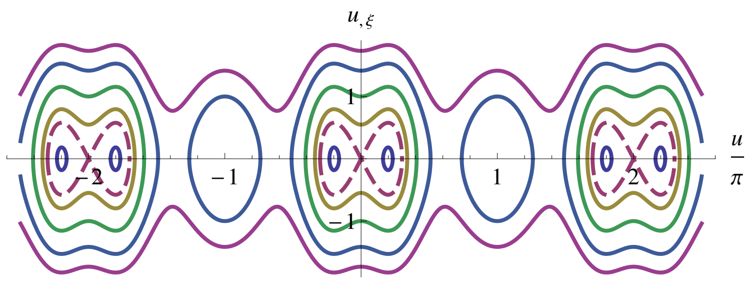

Figure 2: Phase portraits at values of parameter $\delta = 0.7$.

izontal — microshifts is postponed u. Parameter of curves is the integration constant $2g = -0.3$, 0, 0.3, 1, 2, 3. The entire set of solutions is divided into three groups by separatrixes which are designated by shaped lines. "Small" separatrixes ($g = 0$) limit domains in which there are two subdomains of the closed curves with the centers of stable equilibrium. The closed curves are satisfied by periodic solutions $u(x)$. These are the modulated domain nanostructures. They are limited both in size of microshifts, and in size of micro-gradients. Between "small" and "big" separatrixes the periodic solutions are realized. They

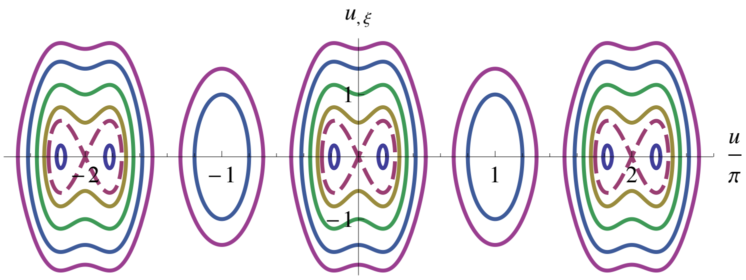

Figure 3: Phase portraits at values of parameter $\delta = 0.9$.

describe the big microshifts of the near atoms which aren't going beyond an elementary cell. Outside "big" separatrix the domain of non-closed curves lies. They are answered by solutions not limited by the size of microshifts. They describe a plastic current of a lattice.

The phase portrait of the equation (46) qualitatively doesn't differ from the phase portrait of Eq. (43) if amplitude of the second harmonica (δ) is small. With increase δ qualitatively change non-closed trajectories. They in turn (everyone at the critical value δ) begin to become the closed (Fig. 2). There is a limit critical value δ, above which all trajectories become closed (Fig. 3). Thus, qualitative analysis of Eqs. (43) and (46) allows to draw a conclusion that existence of the second harmonica in potential of interactions of sublattices $\Phi(u)$ promotes (in process of growth δ) to transformation of acyclic nuclear structures into the periodic. At big δ only periodic structures are realized.

Acknowledgements

This work was supported by RFBR, grants 12-01-00521-a and 13-01-00224-a.

References

[1] E.L. Aero, Phys. Solid State **42** (2000) 1147–1153.

[2] E.L. Aero, Uspekhi Mekhaniki **1** (2002) 130–176.

[3] M. Born, K. Huang. Dynamical Theory of Crystal Lattices. Oxford Univ. Press, Oxford, 1954.

[4] E.L. Aero, A.N. Bulygin, Mech. Solids **45** (2010), 670–688.

[5] E.L. Aero, A.N. Bulygin, Mech. Solids **42** (2007), 807–822.

[6] E.L. Aero, Phys. Solid State **45** (2003) 1557–1565.

[7] A.L. Korzhenevskii, E.L. Aero, A.N. Bulygin, Izvesyiya RAN, Ser. Fizicheskaya, **69**, (2005) 1271–1281.

[8] N.I. Muskhelishvili, Some Main Mathematical Problems of Elasticity Theory (In Russian). Nauka, Moscow, 1966.

[9] S.G. Lekhnitskii, Elasticity Theory of Anisotropic Body (In Russian). Nauka, Moscow, 1977.

[10] E.L. Aero, A.N. Bulygin, Yu.V. Pavlov, *Nonlinear Klein-Fock-Gordon equation and Abelian functions*. Proc. Int. Conference "Days on Diffraction 2013", St.Petersburg, Russia, pp. 5–10.

[11] E.L. Aero, A.N. Bulygin, Yu.V. Pavlov, Differential Equations **47** (2011) 1442–1452.

[12] E.L. Aero, A.N. Bulygin, Yu.V. Pavlov, Appl. Math. Comput. **223** (2013) 160–166.

E. L. Aero, A. N. Bulygin, Yu. V. Pavlov, N.A. Reinberg
Institute of Problems in Mechanical Engineering, RAS,
61 Bol'shoy, V.O., Saint Petersburg, 199178, Russia