Chapter 13
Nonlinear Theory of Cardinal Rearrangement of the Solid Body Structure in the Field of Intensive Pressure

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Abstract A nonlinear theory of microscopic and macroscopic strains is developed for the case of large inhomogeneous relative displacements of two sublattices making up a complex crystal lattice. The standard linear theory of acoustic and optical oscillations of a complex lattice is generalized, taking into account new additive principle of internal translational symmetry—relative shear of two sublattices leaving deformation energy invariant. As a result, the force interaction between the sublattices is characterized by a nonlinear periodic force of its mutual displacements. The theory describes large microdisplacements due to bifurcation transitions of atoms into neighboring cells. As a result, the theory predicts defect formations, switching interatomic bonds, phase transitions, formation of nanoclasters, etc. Some examples of resolutions of nonlinear equations of equilibrium are presented.

13.1 Introduction

Now considerable attention is called to the problem of structural and phase transitions in nano-structured materials, degradation of material properties under loading (ageing and fatigue) and to with it connected processes of generations of defects of the structure and other damages of it. A well-developed approach to the solution of the problem is based on an artificial introduction of concrete, previously designed elements of a damage of a crystalline structure with subsequent monitoring of their evolution under intensive power and temperature influence. A more universal approach, following a remarkable work of Cosserats [7], is based on an introduction of

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internal degrees of freedom into a continuum model of a solid. Numerous attempts of its realizations revealed new effects in the framework of linear theory. Main new results concern an appearance of new optical oscillations, spatial–temporal dispersion of elastic features and border effects in statics.

However, this approach is not adequate enough to the new problems arising while studying the formation and control of the structure of new materials. Small variations in the internal structure described by the linear theories, simple precise variations in the macroscopic geometry of the lattice, giving only re-normalization of material constants. Hence a model of a complex structure is reduced to that of a simple one. The cardinal rearrangements of the structure appear beyond the linear approach. The transition to the essentially nonlinear equations yields a possibility to predict drastic structural rearrangements, lowering of the potential barriers, switching of interatomic connections, arising of singular defects and other damages, phase transitions.

There is a limitation of a phenomenological theory. Indeed, internal parameters, like micro-strains describing structural deviations, may be incorporated into the theory, they could be even estimated. However, their physical sense might be understood provided that an initial structural state of the body is defined, and material scales of length and time are introduced. The last is skipped in the continua theory.

It turns out that simultaneous description of discreteness and nonlinearity of the model allows us to formulate a new principle of translation invariance of the energy. A similar principle was introduced for the first time by E. and F. Cosserat for a medium with rotational degrees of freedom. A model of complex lattice may be used as a base of a suggested theory. The complex lattice consists of two sub-lattices which coincide or merge into one by a shift for a constant structural vector $\mathbf{u}_0$, appearing as a parameter of the complex lattice (Fig. 13.1). The model is known in the physics of solid state, however, it was developed in a linear and anharmonic limit. Two equations arise in the linear theory of crystalline lattice of Karman and Born-Huang [6], one for the acoustic ($\mathbf{U}$) and the other for the optical ($\mathbf{u}$) displacement. The physical mechanics of non-ideal crystalline lattice with defects has been developed in the works of Kosevich [8]. A linear nonlocal theory of complex crystalline lattice was developed by Kunin [9] where a long-range action was refined.

Here, in the local nonlinear theory [1, 3, 2, 4, 5, 10], the main attention is paid to the effects of a short-range action responsible for the cardinal variations in the structure, in particular, for the generation of defects, new phases and the so-called reconstructive transitions or changing of the class of lattice symmetry. The employment of essentially nonlinear equations gives rise to predicting the lowering of potential barriers and switching of interatomic connections.

The introduction of variations of a local topology in the theory by means of internal degrees of freedom ($\mathbf{u}$) turns out efficient, provided that the generation of the linear approach is done as follows. Consider arbitrarily large displacements of sub-lattices $\mathbf{u}$ and put an additional element of translational symmetry, typical for complex lattices but have not used before in physics of solid state. Certainly, the relative displacement of one sub-lattice for one period (or for its integer number) yields a merge of the sub-lattice with itself, and the structure of the complex lattice is reproduced. It means that its energy should be a periodic function of the

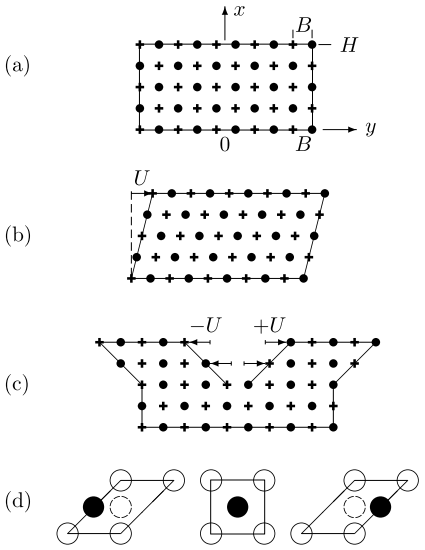

Fig. 13.1 (**a**) The complex crystalline lattice consisting of two sublattices. (**b**) Macroscopic deformation without a relative shear of sublattices. (**c**) Microdeformations at twinning. (**d**) Bifurcation of the structure of an elementary cell during microdeformation

relatively tough displacements of sub-lattices $\mathbf{u}$ which are invariant to such a translation. Certainly, a classical principle of translational symmetry is kept, that yields an invariance of the energy of the lattice to the shared translation $\mathbf{U}$ of both sublattices for one period of the complex lattice. The approach allows us to introduce new parameters of a crystal in micromechanics, that makes possible a description of micromechanisms of the cardinal rearrangements of the lattice such as characteristics of the short-range order, potential barriers, typical sizes of the elements of structure and interphase boundaries, bifurcation parameters.

13.2 General Equations

Let us introduce a displacement $\mathbf{U}$ of the center of inertia of a pair of atoms (elementary cell) and their relative displacement u inside the cell (due to variation of $\mathbf{u}_0$) as follows

$$\mathbf{U} = \frac{m_1\mathbf{U}_1 + m_2\mathbf{U}_2}{(m_1 + m_2)}, \qquad \mathbf{u} = \frac{\mathbf{U}_1 - \mathbf{U}_2}{a}. \tag{13.1}$$

Here $\mathbf{U}_1$ and $\mathbf{U}_2$ are the displacements of atoms with masses m_1 and m_2 of the first and the second sub-lattices, respectively, a is the period of a sub-lattice.

The development of a three-dimensional theory requires explicit introduction of an energy invariant both to the mutual displacements and rotations of sub-lattices. The basic idea is in the development of a scalar periodic function of the simplest rotation invariants of the vector field. This might be done by choosing it as

$$\Phi \to \left(1 - \cos\sqrt{u_i\alpha_{ik}u_k}\right), \quad \alpha_{ik} = a_1^{-2}k_ik_i + a_2^{-2}m_im_i + a_3^{-2}n_in_i, \tag{13.2}$$

where α_{ik} is a tensor of inverse periods of the lattice (a_1, a_2, a_3), while $\mathbf{k}$, $\mathbf{m}$, $\mathbf{n}$ are the unit vectors of crystallographic directions.

The force of interaction of neighboring atoms reads

$$P_i = \frac{\partial \Phi}{\partial u_i} - \frac{\partial \Phi}{\partial u_R}\frac{\partial u_R}{\partial u_i} - \frac{\partial u_R}{\partial u_i}\sin(u_R), \quad u_R = (u_i \alpha_{ik} u_k)^{1/2}. \tag{13.3}$$

Simpler relationships arise for the crystals of cubic symmetry ($a_1 = a_2 = a_3 - a$),

$$\begin{aligned} &\alpha_{ik} = a^{-2}(k_i k_i + m_i m_i + n_i n_i), \qquad u_R^2 = u^2; \\ &P_i = l_i \sin(u), \quad l_i = u_i/u, \\ &u = \left(u_x^2 + u_y^2 + u_z^2\right)^{1/2}. \end{aligned} \tag{13.4}$$

Here u is the absolute value of the vector of micro-displacements, l_i is its basic vector.

It is easy to see that both functions are periodic along the directions $\mathbf{k}$, $\mathbf{m}$, $\mathbf{n}$ with periods equal to a_1, a_2, a_3, respectively.

General equations for macro- and micro-displacements $\mathbf{U}(t, x, y, z)$, $\mathbf{u}(t, x, y, z)$ follow using the Lagrangian

$$\begin{aligned} L = \int_0^t \int_V \Big[&\frac{1}{2}\rho \dot{U}_n \dot{U}_n + \frac{1}{2}\mu \dot{u}_n \dot{u}_n - \frac{1}{2}\lambda_{ikmn} U_{(i,k)} U_{(m,n)} \\ &- \frac{1}{2} K_{ikmn} u_{i,k} u_{m,n} + s_{ik} U_{(i,k)} \Phi(u_R) - p\Phi(u_R) \Big] \mathrm{d}V \end{aligned} \tag{13.5}$$

and they read (due to the variations of $\dot{U}_i$, $\dot{u}_i$, $U_{(i,k)}, u_{i,k}, u_i$)

$$\rho \ddot{U}_i = \lambda_{ikmn} U_{(km),n} - s_{in}\left[\Phi(u_R)\right]_{,n}, \tag{13.6}$$

$$\begin{aligned} &\mu \ddot{u}_i = K_{ikmn} u_{k,mn} - P l_i \frac{\partial \Phi}{\partial u_R}; \\ &l_i = \frac{\partial u_R}{\partial u_i}; \qquad P = p - s_{ik} U_{(i,k)}. \end{aligned} \tag{13.7}$$

Here commas in interlinear indices denote spatial derivatives, their inclusion in parentheses denotes symmetrization, and a period on top corresponds to the temporal derivative.

The first equation is useful in rewriting the equation of mechanics of a continuum medium in the standard form:

$$\rho \ddot{U}_i = \sigma_{ik,k}, \tag{13.8}$$

where the stress tensor σ_{ik} is introduced as

$$\sigma_{ik} = \lambda_{ikmn} U_{(m,n)} - s_{ik}\Phi(u_R). \tag{13.9}$$

Equations (13.7)–(13.9) correspond to the translation invariant equations of the dynamics of the double continuum. Equation (13.9) allows us to consider the stress as a sum of an elastic part (the first term) and an inelastic part caused by a microstructure of the lattice. The latter disappears at small micro-displacements and achieves a maximum value equal to s_{ik}, when $u = \pi$, or at the shift of atoms from the potential holes to the peaks of interatomic potential barriers. Certainly, the value of the material tensor s_{ik} is the limit of inelastic stresses corresponding to the loss of stability of the lattice. The plastic strains as well as interphase transitions and other bifurcation processes are possible further. They are defined by the field of micro-displacements that is obtained from (13.7).

The value of P in (13.7) corresponds to an effective potential barrier of the rearrangement of the lattice, depending on the strain gradient $U_{i,k}$. It might be excluded expressing through σ_{ik}. This gives another representation for P

$$P = p - s_{mn}\lambda^{-1}_{mnik}\sigma_{ik}. \tag{13.10}$$

Choosing the periodic function Φ according to (13.2) and taking into account (13.3), the governing equations are rewritten as

$$\rho\ddot{U}_i = \lambda_{ikmn}U_{(mn),k} - s_{ik}l_k\sin(u_R), \quad u_R = (u_i\alpha_{ik}u_k)^{1/2}, \tag{13.11}$$

$$\mu\ddot{u}_i = K_{ikmn}u_{k,mn} - Pl_i\sin(u_R), \quad P = p - s_{ik}U_{(ik)}. \tag{13.12}$$

These equations correspond to the crystal of any class of symmetry but they are too complicated for an analysis. Therefore, a more simple case will be considered further.

13.3 Two-Component Two-Dimensional Micro-Fields in Cubic Crystals

Consider a plane problem with the strain field of the form

$$\begin{aligned} &U_x = U_x(x,y,t), \qquad U_y = U_y(x,y,t), \qquad U_z = 0,\\ &u_x = u_x(x,y,t), \qquad u_y = u_y(x,y,t), \qquad u_z = 0. \end{aligned} \tag{13.13}$$

According to (13.4) for cubic crystals $u_R = u = (u_x^2 + u_y^2)^{1/2}$, (13.11), (13.12) read as

$$\mu\ddot{u}_x = -Pl_x\sin\left(u_x^2 + u_y^2\right)^{1/2} + K_1u_{x,xx} + K_{23}u_{y,xy} + K_3u_{x,yy}, \tag{13.14}$$

$$\mu\ddot{u}_y = -Pl_y\sin\left(u_x^2 + u_y^2\right)^{1/2} + K_1u_{y,yy} + K_{23}u_{x,yx} + K_4u_{y,xx}, \tag{13.15}$$

$$\rho\ddot{U}_x = \sigma_{xx,x} + \sigma_{xy,y}, \qquad \rho\ddot{U}_y = \sigma_{yy,y} + \sigma_{yx,x}. \tag{13.16}$$

Here the components of the strain tensor are expressed according to (13.9)

$$\sigma_{xx} = \lambda_1 U_{x,x} + \lambda_2 U_{y,y} - s_{xx}\big(1 - \cos\big(u_x^2 + u_y^2\big)^{1/2}\big), \tag{13.17}$$

$$\sigma_{yy} = \lambda_2 U_{x,x} + \lambda_1 U_{y,y} - s_{yy}\big(1 - \cos\big(u_x^2 + u_y^2\big)^{1/2}\big), \tag{13.18}$$

$$\sigma_{yx} = \lambda_3 (U_{x,y} + U_{y,x}) - s_{yx}\big(1 - \cos\big(u_x^2 + u_y^2\big)^{1/2}\big). \tag{13.19}$$

Further simplifications are needed for obtaining analytical solutions.

13.4 Thin Layer Assumption. Statics

Consider a static version of (13.16) with the defining parities given by (13.17)–(13.19).

Assume that a layer is directed along the OY axis, while the solution is localized in the vicinity of this axis, then besides the conditions $\ddot{U} = \ddot{u} = 0$ a natural assumption may be suggested

$$U_x \ll U_y, \qquad u_x \ll u_y, \qquad l_x \ll l_y, \qquad \partial()/\partial y \ll \partial()/\partial x. \tag{13.20}$$

Equations (13.20) allow us to write leading order equations defining two-dimensional stationary fields of macro- and micro-strains $U_x(x, y), U_y(x, y); u_x(x, y), u_y(x, y)$. The substitution of (13.17)–(13.19) into (13.16) allows simplifying them with the help of (13.20). Neglecting the terms with derivatives $U_{x,yy}, U_{y,xy}, u_{x,y}$ in the equation for the x projection and terms $U_{y,yy}, u_{y,y}$ in the equation for y projection, one obtains two equations of the second order that may be integrated once with respect to x, giving

$$\lambda_1 U_{x,x} + (\lambda_2 + \lambda_3) U_{y,y} - s_{xx}\big(1 - \cos(u_y)\big) = \varepsilon_0(y), \tag{13.21}$$

$$\lambda_3 U_{y,x} - s_{yx}\big(1 - \cos(u_y)\big) = \sigma_0(y). \tag{13.22}$$

Here $\sigma_0(y), \varepsilon_0(y)$ are the constants of integration with respect to x. Then the system of two equations appears for the macroscopic fields $U_x(x, y), U_y(x, y)$ connected with the micro-field $u(x, y)$. Then a consideration of the static reduction of (13.14), (13.15) is needed. Leaving the left-hand side in (13.14) and changing u with u_y in (13.15), we rewrite the system (13.14)–(13.15) as

$$0 \approx K_1 u_{x,xx} + K_{23} u_{y,xy}, \tag{13.23}$$

$$\mu \ddot{u}_y \approx -P l_y \sin(u_y) + K_1 u_{y,yy} + K_{23} u_{x,yx} + K_4 u_{y,xx}. \tag{13.24}$$

The term $u_{x,yy}$ is skipped in (13.23) due to smoothness along the layer. It is integrated once with respect to x, giving the first order equation

$$B \approx K_1 u_{x,x} + K_{23} u_{y,y}. \tag{13.25}$$

Here B is a constant of integration. Differentiating (13.25) with respect to y, one excludes from (13.23) the mixed derivative $u_{x,yx}$; this gives rise to

$$\mu\ddot{u}_y \approx -Pl_y \sin(u_y) + K_4 u_{y,xx} + K_5 u_{y,yy}. \tag{13.26}$$

Its right-hand side may be simplified using (13.23) and the assumption $l_y \approx 1$. Due to the smallness of the component u_x, the equation may be finally written as

$$\mu\ddot{u}_y \approx -P\sin(u_y) + K_5 u_{y,yy} + K_4 u_{y,xx}, \qquad K_5 = K_1 - K_{23}^2/K_1. \tag{13.27}$$

Here P is an effective potential, depending on deformation gradients according to (13.7). For cubic crystals we get

$$P = p - s_{xx}U_{x,x} + s_{yy}U_{yy} + (s_{xy} + s_{yx})(U_{x,y} + U_{y,x}). \tag{13.28}$$

Then the equations for macro- and micro-fields become coupled, which strongly complicates their analysis. However, according to (13.21) and (13.22), the deformation gradients are expressed through two arbitrary functions $\sigma_0(y)$ and $\varepsilon_0(y)$ that may be replaced with constants. Then only one of the three functions $U_{x,x}$, $U_{y,y}$, $U_{x,y}$ remains in (13.28). It simplifies a choice of useful hypothesis for obtaining solutions.

It is useful to transform to the dependence of the effective potential barrier P on the stresses according to its equivalent definition (13.10). For cubic crystals, following (13.17), (13.18) and (13.19), we have

$$P = p - \bar{\sigma}; \qquad \bar{\sigma} = \varepsilon_1\sigma_{xx} + \varepsilon_2\sigma_{yy} + \varepsilon_3\sigma_{yx} + \widehat{S}\big(1 - \cos(u)\big). \tag{13.29}$$

Here ε_1, ε_2, ε_3, $\widehat{S}$ are complicated combinations of the material constants (λ_1, λ_2, λ_3) and coefficients of striction (s_{xx}, s_{yy}, s_{yx}). The three components of stresses are expressed through two constants σ_0, ε_0 according to (13.21) and (13.22). Then the useful hypothesis may be chosen for construction of particular solutions, assuming P does not depend on the coordinates under certain boundary conditions. The stress is a constant in the one-dimensional case when only dependence of one coordinate is taken into account.

13.5 Some Particular Solutions

One of the solutions of (13.26) reads

$$\tan(u_y/4) = \frac{A\,\mathrm{cn}(xK_1/H)}{\mathrm{sn}(xK_1/H)\,\mathrm{dn}(yK_2/B)} \approx \frac{A}{\mathrm{sh}(x/L)\,\mathrm{dn}(yK_2/B)}. \tag{13.30}$$

Here $\bar{K}_1 = \bar{K}_1(\nu_1)$, $\bar{K}_2 = \bar{K}_2(\nu_2)$ are complete elliptic integrals of the first kind. The arguments ν_1, ν_2 play the role of constants of integration in the present theory, while $\mathrm{sn}()$, $\mathrm{cn}()$, $\mathrm{dn}()$ are the standard notations for the Jacobi elliptic functions.

The second equality in (13.29) is obtained in the particular case $\nu_1 \to 1$, $\nu_2 \to 0$, when the form of the elliptic functions is simplified. The function $\mathrm{sh}(x/L)$ describes a variation of the structure within a contact zone of the width L. One gets obvious limiting relationships

$$\begin{aligned} &|x| \to 0, \qquad |\,\mathrm{sh}()| \to 0, \qquad \tan(u_y/4) \to \pm\infty, \qquad u_y \to 2\pi, \\ &|x| \to \infty, \qquad |\,\mathrm{sh}()| \to \infty, \qquad \tan(u_y/4) \to 0, \qquad u_y \to 0. \end{aligned} \tag{13.31}$$

The first relationship means that structural variations in the center of contact zone $x = 0$ are maximal, and the atoms move for an integer number of the periods of the lattice. The second one means that the atoms remain in the initial state of equilibrium, $\pm u_y = 0$, far from the contact zone. These relationships are the basis for the statement of the boundary conditions.

Using the field found and substituting it into (13.24), one obtains the solution for the second component of the displacement of the form

$$K_1 u_x = K_{23} \int \left[\arctan(u_y/4)\right] \mathrm{d}x - \varepsilon_0 x. \tag{13.32}$$

Using these relationships for the dependence of macro-displacements on micro-strains and stresses, one can obtain the distortion of the size and shape of the plate, calculating the micro-displacement U_i. The employment of (13.16), (13.17) and (13.18) allows us to obtain the stresses σ_{xx}, σ_{yy}, σ_{xy}. A tribute of the structure in them is described by the formula

$$1 - \cos(u) = \frac{8A^2\,\mathrm{tn}^2(xK_1/H)\,\mathrm{dn}^2(yK_2/B)}{A^2 + \mathrm{tn}^2(xK_1/H)\,\mathrm{dn}^2(yK_2/B)}. \tag{13.33}$$

Another particular solution of (13.27) reads

$$\begin{aligned} &\mathrm{tg}(u_y/4) = A\ \mathrm{dn}(xK_1/H)\ \mathrm{dn}(yK_2/B), \\ &A^2 = 1/\big(1-\nu_1^2\big)\big(1-\nu_2^2\big). \end{aligned} \tag{13.34}$$

Some features of a super-structure are caused by the boundedness of the Jacobi function $\mathrm{dn}(*)$. Therefore, the right-hand side of the solution does not apply at infinity, though reaches large values at $\nu_1 \to 1$, $\nu_2 \to 1$. It means that $u_y < 2\pi$, and the atoms do not jump into the neighboring holes, as it happens at the appearance of singularities. The corresponding micro-structure has the form of two-dimensional periodic system of nanocrystals separated by wide boundaries, when the lattice is disordered to some extent. No singular defects arise, contrary to the previous case.

One can find more particular solutions in [1, 3, 2]. Similar solutions of (13.14) and (13.15) may be obtained in the dynamical case of plane waves propagating with constant velocities and depending on the phase variables $\chi = x - V_1 t$, $\eta = y - V_2 t$. Some dynamical problems were studied in [4, 5, 10].

13.6 Conclusions

An important feature of adequate structural rearrangements should be an essential nonlinearity of the processes that may reach the points of bifurcation of the structure and give rise to the cardinal variations in the existing properties and the arising of new ones, including possible description of the process of the defect generation. The development of a theory is possible on the base of the known model of a complicated lattice whose elementary cell contains more than one atom. Existing theories are linear as a rule, however, they could describe anharmonicities of low degree as a last resort. The presented theory allows describing some interesting mechanisms of structural rearrangements by the exact solutions of nonlinear governing equations. Some nontrivial effects are revealed for the first time, like switching of interatomic connections by lowering of potential barriers under an influence of external stresses. As a result, the theory predicts an appearance of surface defects in initially ideal structure, its fragmentation with singular boundaries, loss of stability of homogeneous strains beyond the threshold of intensive action on the body, inelastic diffusionless strains, loss of long-range and short-range orders which are the micro-mechanisms of the surface reconstruction. It is interesting to note that in the complex stressed state the lattice hardening is also possible besides an inverse effect of softening. The criteria of the transitions in the form of bifurcating dependencies of the amplitude of microscopic field on the stresses and the domain sizes at the surface are obtained in [3, 2]. Further development of the theory is required to connect with the problem of thermodynamical stability of defects both in the fields of stresses and temperatures.

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