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HIGHLY NON-LINEAR THEORY OF BIFURCATION TRANSFORMATIONS OF CRYSTALLINE LATTICE STRUCTURES

E.L. Aero

Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vas.Ostrov, St.Petersburg 199178, Russia

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Abstract. A highly-nonlinear theory is elaborated which describes elastic and inelastic phenomena in media with complicated lattice structure consisting of two sublattices. In the framework of this approach, the standard linear theory of acoustic and optic oscillations of a complicated lattice is generalized, taking into account internal translational symmetry of relative shear of the sublattices taken into account. As a result, the interaction between the sublattices is characterized in terms of a non-linear periodic force described, in particular, as sine of relative shear of two atoms belonging to an elementary cell. The corresponding equations in the case of solids without a central symmetry contain terms that describe the interatomic interactions. We have the situation with quasistatic loading of solids. The dependence of effective stresses on macroscopic strains is found which has a bifurcation point responsible for a structural transformation of the twinning type. It is shown that the transformation is related to a transformation of the interatomic interaction potential, the namely occurrence of both an additional minimum of the potential and a new structure (which has mirror symmetry relative to the initial structure.

1. INTRODUCTION

Continuum mechanics postulates, in particular, that local topology of a strained medium is constant. It means that a material particle (a structural unit of the medium) has the same neighbouring material particles in its vicinity during deformation. In other words, structure of the medium and interparticle bindings are not rearranged during deformation.

With this postulate, a model of a continuum as a smooth manifold allowed to elaborate self-consistent effective methods of the phenomenological elasticity theory of continuum media. Recently, however, it has became evident that many inelastic phenomena in continuum media, which are related to structural transformations, phase transitions, generation of point defects, plastic deformation and failure processes, can not be adequately described using representations of the model of a strained medium with constant local topology. In an analysis of such phenomena, structural transformations of real solids should be definitely taken into consideration.

Attempts to generalize the model of smooth manifold, introducing internal degrees of freedom, have demonstrated that linear models based on the idea on such degrees of freedom, are not effective in a description of inelastic effects. Weak (linear) transformations of the internal structure take into account only small changes of continuum geometry, giving rise to only changes of material parameters figuring in standard equations of the classical continuum mechanics. In the framework of this approach, a model of the complicately arranged structure is reduced to the standard model of a simple structure. The approach in question allows to reveal the following new results: dispersion of elastic properties in both space and time, and boundary effects in statics, which are capable of playing the essential role in several cases.

In general, the phenomenological theory of elasticity can be formulated on the basis of the linear

Corresponding author: E.L. Aero, e-mail: aero@microm.ipme.ru

microscopic theory [1,2] that takes into account the crystal lattice structure. Internal degrees of freedom can be introduced in the framework of the model of a complicated crystal lattice (consisting of two or more sublattices), in which case optical oscillation modes come into play. However, the linear microscopic theory, with internal degrees of freedom involved into consideration, does not describe dramatic transformations of the structure and properties of strained solids. The main aim of this paper is to suggest a new approach based on use of non-linear optical oscillations, which is effective in a theoretical description of dramatic structural transformations in strained crystalline solids.

2. BASIC EQUATIONS

2.1. Linear equations

For definiteness and simplicity, we consider a crystalline polyatomic solid consisting (in equal parts) of atoms of two types. Its crystalline lattice is composed of two periodic sublattices each consisting of atoms of one type (Fig. 1a). The sublattices have the same geometry and coincide in space when one of them is shifted by vector a_i, the crystal lattice vector (Fig. 1a).

Oscillations of the crystal lattice consisting of atoms of two types can be divided into acoustic and optical modes which are respectively oscillations of the lattice as a whole and oscillations of the sublattices relative each other. In these circumstances, the linear theory of crystal lattices consisting of atoms of two types operates with two equations for acoustic and optical oscillations, based on the so-called harmonic approximation of the energy that characterizes interatomic pair interactions:

$$\Phi = \sum_{nl}\sum_{pq} \alpha_{ik}^{pq}(n-l)U_i^p(n)U_k^q(l). \qquad (1)$$

Here the tensor $\alpha_{ik}^{pq}(n-l)$ with tensor indices i and k describes the constants of the interactions between atoms n and l belonging to the p-th and q-th sublattices, respectively; U_i^p and U_k^p are the displacement vectors of atoms belonging to the p-th and q-th sublattices, respectivley. In our case with two sublattices, we have $p,q = 1, 2$.

From (1) one finds the following equations of motion of atoms belonging to the two sublattices:

$$m_1\ddot{U}_i^1(n) = -\sum_{iq} \alpha_{ik}^{1q}(n-l)U_k^q(l),\ (q = 1,2), \qquad (2)$$

$$m_1\ddot{U}_i^2(n) = -\sum_{iq} \alpha_{ik}^{2P}(n-l)U_k^P(l),\ (p = 1,2). \qquad (2a)$$

Here m_p is the mass of an atom belonging to the p-th sublattice, and $\ddot{U}$ means the second derivative of function U in time.

The interaction constants obey the following conditions of symmetry [2]:

$$\begin{aligned} &\alpha_{ik}^{pq}(n) = \alpha_{ki}^{qp}(-n),\\ &\sum_{n,p}\alpha_{ik}^{pq}(n) = \sum_{n,q}\alpha_{ik}^{pq}(n) = 0,\\ &\sum_{n,p}\alpha_{ik}^{pq}(n)R_j^p(n) = \sum_{n,q}\alpha_{ik}^{pq}(n)R_k^p(n). \end{aligned} \qquad (3)$$

with $R_j^p(n)$ being the vector of initial position of the n-th atom belonging to the sublattice p. The second and third relationships in formula (3) represent symmetry of the lattice relative to respectively rigid body translation and rotation of the lattice as a whole. The first relationship in (3) comes into play in the only case of pair interatomic interactions. The interactions of non-pair character in the general situation can be reduced to triple interactions [4]. (In doing so, the sum of energies that characterize triple interatomic interactions appears on the r.h.s. of Eq. (1).

The discrete Eqs. (2) of motion of atoms are transformed into equations operating with continuous functions characterizing a strained lattice. To do so, it is assumed that displacements of neighbouring atoms relative each other are infinitesimal, in which case a short-range order in arrangement of atoms in a strained crystalline lattice is the same as in a non-strained lattice. In other words, in the approximation under consideration, every sublattice represents a subcontinuum being a smooth manifold. To define such a subcontinuum, one assumes that there is smooth and differentiable function, $r_i^p(n)$ and $R_i^p(n)$, of spatial positions of atoms belonging to the p-th sublattice in its initial (non-strained) and final (strained) states, respectively.

This description of the discrete structure by smooth function is not absolutely adequate: spectrum of Fourier harmonics of the function under consideration does not contain high spatial frequences [3]. However, it is inessential in the case of our long-wave model. The important specific feature of the model is the continuous character of the displacement field that characterizes only atoms belonging to one sublattice. At the same time, even neighbouring atoms of the crystal lattice in its initial state can be essentially displaced relative each other, if they belong to different sublattices. The linear theory does not take into consideration such

displacements; it deals with only small displacements.

We have by definition:

$$U_i^p(n) = R_i^p(n) - r_i^p = U_i^p(r_k). \tag{4}$$

Smooth character of vector function $U_i^p(r_k)$ allows us to represent it as the following decomposition in vicinity of any point of the *p*-th subcontinuum:

$$U_i^p(r_n + \delta r_n) = U_i^p(r_n) + \delta r_k U_{i,k}^p(r_n) + \frac{1}{2}\delta r_m \delta r_k U_{i,mk}^p(r_n) + O(\nabla^3), (p = 1,2). \tag{5}$$

Here $(\,)_{,i}$ denotes $\partial(\,)/\partial r_i$, $(\,)_{,ij}$ denotes $r_j\partial(\,)/\partial r_i$, and by $O(\nabla^3)$, are meant small terms containing gradients of the third (or more) power .

With decomposition (5) used in discrete Eqs. (2) and (3), one obtains their continuum versions to be as follows:

$$m_1\ddot{U}_i^1 = \sum_q \left(C_{ik}^{1q}U_k^q + C_{ikj}^{1q}U_{k,j}^q + C_{ikjm}^{1q}U_{k,jm}^q\right) + O_1(\nabla^3), (q = 1,2), \tag{6}$$

$$m_2\ddot{U}_i^2 = \sum_q \left(C_{ik}^{2p}U_k^p + C_{ikj}^{2p}U_{k,j}^p + C_{ikjm}^{2p}U_{k,jm}^p\right) + O_2(\nabla^3), (p = 1,2). \tag{7}$$

At the stage discussed, two sublattices are represented as two mutually penetrating subcontinuums. The sublattices in their initial state are shifted relative each other by vector a_i. The relative displacement of the sublattices in a strained state is a spatially inhomogeneous vector field considered below in detail.

It is worth noting that equations (6) and (7) can be re-written in the different way as equations operating with new functions, the namely displacement U_i of mass center of atom pairs (elementary cells) and a relative displacement of the atoms in the cell:

$$U_i = \frac{m_1U_i^1 + m_2U_i^2}{m_1 + m_2}, \qquad u_i = \frac{U_i^1 + U_i^2}{b}. \tag{8}$$

Here *b* is one of periods of Bravais lattice. In doing so, from Eqs. (6) and (7) one obtains the following system:

$$\rho\ddot{U}_i = c_{ikj}u_{k,j} + \lambda_{ikjm}U_{k,jm} + O_1, \tag{9}$$

$$\mu\ddot{u}_i = -p_{ik}u_k - c_{kij}U_{k,j} - \hat{c}_{kij}u_{k,j} + k_{ikjm}u_{k,jm} + O_2. \tag{10}$$

Here ρ (the mean atomic density per elementary cell) and μ are given as follows:

$$\rho = \frac{m_1 + m_2}{v}, \qquad \mu = \frac{m_1m_2}{(m_1 + m_2)v} \tag{11}$$

with *v* being the elementary cell volume.

The tensors of elastic constants are invariant relative to the following permutations of indexes: $p_{ik} = p_{ki}$; $\hat{c}_{kij} = -\hat{c}_{ikj}$; $\lambda_{ikjm}=\lambda_{kijm}=\lambda_{kimj}=\lambda_{ikmj}$. This property follows from symmetry (3) of the tensor a_{ik}^{pq} of force constants from which all tensors of material characteristics are derived [2]. Symmetry relative pair permutations of indexes of the tensor λ_{ikjm} is absent, if interatomic forces are of either non-pair or non-central type [5].

Hereinafter we will divide the magnitude u_i of the vector of relative displacements of atoms (belonging to different sublattices) of an elementary cell by period *b* of Bravais lattice. In these terms, the case of $|u_i|=1$ corresponds to a displacement of the sublattices along the *i*-th direction by a period.

Terms O_1 and O_2 are non-linear terms including high powers of gradients, which are not taken into account in our theory. They are as follows:

$$O_1 = C_{ikjm}u_{k,jm} + \Lambda_{ikjml}U_{k,jml} + \ldots, \tag{12}$$

$$O_2 = C_{ikjm}u_{k,jm} + K_{ikjml}U_{k,jml} + \ldots. \tag{13}$$

First, let us consider formulas (9) and (10). The terms in these formulas, describing the local interaction of modes are non-zero in only the case of crystals without center of symmetry due to odd rank of the corresponding tensor coefficients c_{ikn}. Similar terms (describing local interaction of modes) of higher orders are written in formulas (12) and (13). Some of them are non-zero (in crystals without center of symmetry) due to the even rank of the corresponding tensor coefficients.

Equation (9) of acoustic oscillations in the case of media with central symmetry is reduced (with terms O_1 of high power of gradients being neglected) to the macroscopic equation of oscillations of a continuous medium without a dispersion of its elastic properties. In this situation, the macroscopic displacements U_i characterize changes in dimensions and shape of a solid as a whole.

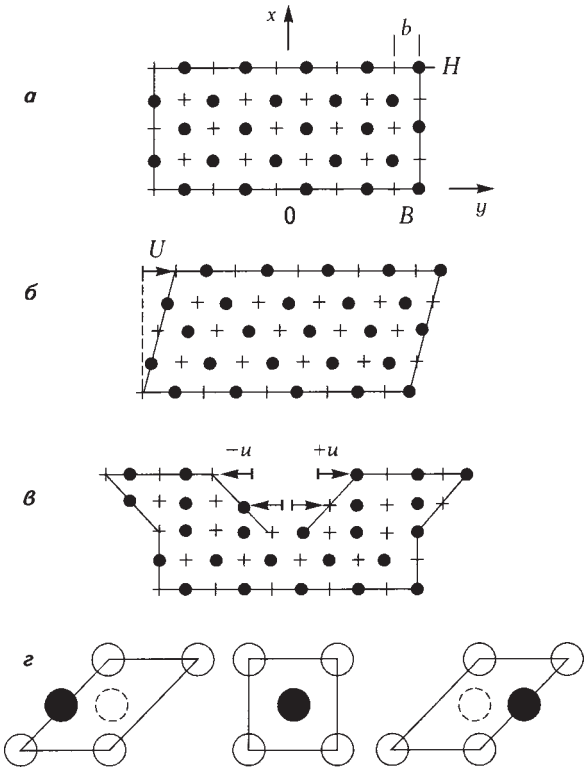

Fig. 1. (a) Complicated crystalline lattice consisting of two sublattices. (b) Macroscopic deformation without a relative shear of sublattices. (c) Microdeformations at twinning. (d) Bifurcation of the structure of an elementary cell during microdeformation.

Eq. (10) of optic oscillations contains the first term on its r.h.s., which is independent on gradient(s). This term describes interatomic forces between two atoms composing an elementary cell or, in other words, the interaction between sublattices. The corresponding microdisplacement vector u_i describes changes in the short-range order of the lattice or, in other words, rearrangements of its internal structural geometry. However, as it has been noted above, these changes are unambigiously related with the help of Eq. (10) to gradients of the macroscopic (acoustic) displacements field U_i. Therefore, the changes in question can be excluded from the macroscopic equation, in which case we come back to the model of smooth manifold with a constant local topology.

2.2. Non-linear theory

Changes of the local topology are effectively involved (with the help of internal degrees of freedom, described by field u_i) into the theory, if we make the following generalization of Eq. (10). We consider arbitrary large relative displacements u_i of sublattices, which are described by a non-linear term $P_i(u_n)=-P_i(-u_n)$, instead of previously used linear term. The non-linear term represents a non-linear odd periodic vector function with period corresponding to period of Bravais lattice along direction of the displacement u_i. The crystal lattice in its ideal, non-strained state is characterized by u_i and $P_i=0$.

The discussed non-affine changes of geometry of the crystal lattice are realized at polyamorphic transformations of the non-diffusional type, accompanied by changes in the short-range order of atomic arrangement or, in other words, by changes of the local topology under extreme conditions of mechanical load.

Figs. 1c and d schematically shows large displacements of neighbouring atoms of a complicated lattice at twinning and a transformation of bcc-lattice, occurring due to large shear transformations of sublattices. Transformations of the short-range order in atomic arrangement evidently come into play in the situations shown in Fig. 1c and d.

In these circumstances, instead of Eqs. (9) and (10), we have the following system of equations:

$$\rho\ddot{U}_i = c_{ikj}u_{k,j} + \lambda_{ikjm}U_{k,jm} + O_1, \qquad (14)$$

$$\mu\ddot{u}_i = -P_i(u_j) - c_{kij}U_{k,j} - \hat{c}_{kij}u_{k,j} - + k_{ikjm}u_{k,jm} + O_2. \qquad (15)$$

Here terms O_1 and O_2 are given by expressions (12) and (13).

Since displacement u_i is formulated in units of periods of Bravais lattice in the *i*-th direction, periods of this displacement function are integers. In particular, if $P \to \sin(2\pi u)$, the displacement $u=|u_i|=1$ corresponds to the transformation of sublattices into a new structural state which is crystallographically equivalent to the initial state. During the transformation, the interatomic bindings and neighbouring atomic arrangement change. That is, the local topology changes. (These topological changes do not occur, if microdispalcements $u \le 1/2$.) As a corollary, in a description of the situation discussed, it is necessary to take into account highly non-linear effects which come into play at microdisplacements $u \le 1$. Hereinafter we will focus our consideration to namely such microdisplacements. (In general, however, there are also multiple structural transformations of complicated crystal lattices, described by $u \ge 2$. For instance, such transformations can occur during either the formation of domain superstructures or microphase polymorphic decomposition.)

The vector function $P_i(u_n)$ can be derived from the scalar periodic function of the energy f^p that characterizes a solid shear of sublattices and is invariant relative to coordinate transformations. More precisely, $P_i=\partial f^p/\partial u_i$.

In the general situation, the energy f^p is a function of the three projections, $u^1=u_n\, m_n^{\,1}$, $u^2=u_n\, m_n^{\,2}$, $u^3=u_n\, m_n^{\,3}$, of the vector u_i onto unit vectors of crystallographic axes ($m_n^{\,1}$, $m_n^{\,2}$, $m_n^{\,3}$). They are invariant relative to transformations of the general coordinate system. In these circumstances, we have:

$$P_i = \frac{\partial f^p}{\partial u_i} = \frac{\partial f^p}{\partial u^1} m_i^1 + \frac{\partial f^p}{\partial u^2} m_i^2 + \frac{\partial f^p}{\partial u^3} m_i^3 . \qquad (16)$$

In the general situation under consideration, f^p is a periodic function with three periods b_1, b_2 and b_3; it is invariant relative to translations over periods b_1, b_2 and b_3 along directions m_1, m_2 and m_3, respectively.

This function is odd in the case of media with central symmetry. In particular, when directions of the force and displacement vectors coincide with that of the structural vector a_i, we have: $f^p = f(u^2)=f(u)$, with u being the length of u_i. In doing so, P_i is given as follows:

$$P_i = \frac{\partial f^p}{\partial u_i} = \frac{\partial f^p}{\partial u}\frac{\partial u}{\partial u_i} = \frac{\partial f^p}{\partial u}\frac{u_i}{u}. \qquad (17)$$

This case is realized, if the forces of the interatomic of atoms belonging to one elementary cell are of the central type, and the structural vector a_i of the lattice causes directions of vectors P_i and u_i. If these forces are not of central type, and, more than that, vectors a_i and u_i are orthogonal, a pair of atoms is rotated. The situation in question occurs in molecular crystals with solid molecules, where rotation degrees of freedom (corresponding to rotations of the structural vector a_i without changes of its length) should be taken into consideration, similar to the model [6]. Here we will not consider this situation originated from the restrictive condition discussed above.

3. STRONG INTERACTION BETWEEN MODES IN MEDIA WITHOUT CENTRAL SYMMETRY

3.1. Basic equations

Eqs. (14) and (15) of the lattice without central symmetry are formulated in their simplest form in the so-called long-wave approximation. In doing so, terms containing gradients in Eq. (15) can be neglected. In the long-wave approximation it is reasonable to restrict our consideration to only low-frequency oscillations of the medium, neglecting high-frequency oscillations of the crystal lattice. In the framework of this approach, Eqs. (14) and (15) are written in the following reduced form:

$$p\ddot{U}_i = c_{ikj}u_{k,j} + \lambda_{ikjm}U_{k,jm}, \qquad (18)$$

$$0 = -P_i - c_{kij}U_{k,j} - \hat{c}_{kij}u_{k,j}. \qquad (19)$$

Consideration of terms containing gradients has been done in papers [7,8] in the case of a medium with central symmetry where terms describing the local interaction between modes are not taken into account.

Eq. (18) can be written in the form of the classic equation of continuum mechanics:

$$\rho\ddot{U}_i = \bar{\sigma}_{ij,j} \qquad (20)$$

if we assume that quantity

$$\bar{\sigma}_{ij} = \lambda_{ikjm}U_{k,m} + c_{ikj}(u_k - u_k^0) \qquad (21)$$

plays the role as the effective stress tensor. Here u_k^0 (integration constant) represents the vector (colinear to the vector u_i) of relative translation of sublattices over integer of periods, which keeps the crystal structure to be unchanged. Its value is chosen in such a way as to make the stress tensor to be invariant relative to the translation considered. This integration constant can be excluded from our consideration, if we initially suggest that $|u_i| \le 1$ (see a discussion in section 2).

3.2. Structural transformations and bifurcations in statics

Let us consider a stationary version of our equations, that is:

$$0 = \bar{\sigma}_{ij,j}, \qquad (22)$$

$$0 = -P_i - c_{kij}U_{k,j} - \hat{c}_{kij}u_{k,j}. \qquad (23)$$

In the two-dimensional case, the former equation can be solved in its general form, with stress function introduced as that obeying biharmonic equation:

$$\bar{\sigma}_{xx} = \frac{\partial^2\psi}{\partial y^2},\ \bar{\sigma}_{yy} = \frac{\partial^2\psi}{\partial x^2},$$
$$\bar{\sigma}_{xy} = \frac{\partial^2\psi}{\partial x\partial y},\ \nabla\nabla\nabla\nabla\psi = 0. \qquad (24)$$

In this case, after we have found the solution of the corresponding boundary problem, with Eqs. (21) and (23), we will have a system of algebraic equations which allow one to find components of the vector u_i and tensor $U_{i,j}$. In doing so, it is worth to take into account that the periodic function $P_i(u_k)$ should be either defined in advance or derived from a periodic scalar function of the energy, as it has been shown in section 2.

Let us examine a simple case of one-component movement with all the vectors having one component:

$$\begin{aligned} u_y &= u(x,y), \\ P_y &= p\sin(2\pi u), \\ U_y &= U(x,y). \end{aligned} \tag{25}$$

In this case, the basic equations can be written as follows:

$$\begin{aligned} \bar{\sigma} &= \lambda\varepsilon - c(u - u_0), \\ 0 &= p\sin(2\pi u) + c\varepsilon. \end{aligned} \tag{26}$$

Here $c = c_{yyx}$, $2\varepsilon = u_{x,y}$ and $\bar{\sigma} = \bar{\sigma}_{xy}$ are the shear strain and stress, respectively. The third term of Eq. (23) is equal to 0, because of antisymmetry of the tensor $\hat{c}_{kij}$ over permutations of k and i.

Now let us analyse the expression (21) for the effective stress tensor, considering it as a material relationship. With the second Eq. in (26), one can relate the stresses through strains as follows:

$$\begin{aligned} \bar{\sigma} &= \frac{\lambda p}{c} e - c\arcsin e, \\ e &= \frac{\varepsilon}{\varepsilon_{b2}}, \\ \varepsilon_{b2} &= \frac{p}{c}. \end{aligned} \tag{27}$$

This relationship is graphically presented in Fig. 2, provided

$$\gamma = \frac{p\lambda}{c^2} > 1. \tag{28}$$

The curve in Fig. 2 represents a hysteresis loop. Its upper branch corresponds to deformation of the initial structure. This branch extends to the stress maximum, that is, point $e = e_{b1}$ which is the first limit of stability (existence) of the initial structure:

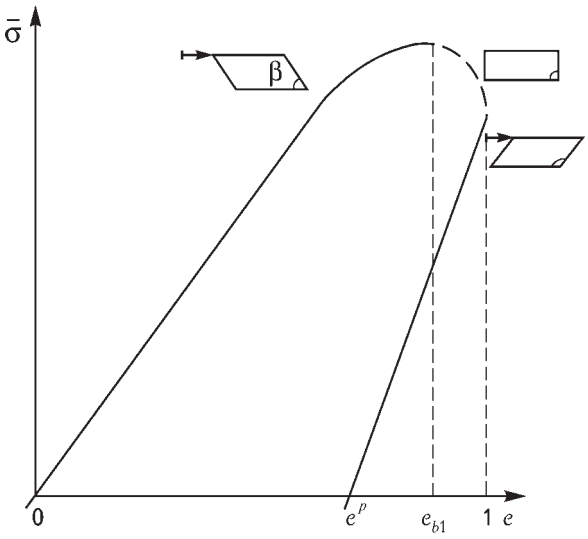

Fig. 2. Dependence of stress on relative deformation accompanied by structural transformation. The upper branch corresponds to the initial structure exhibiting softening. The lower branch corresponds to the secondary structure exhibiting strengthening. Dashed fragment of curve corresponds to the transition region of unstabitity.

$$e_{b1}^2 = 1 - \frac{1}{\gamma^2}. \tag{29}$$

The lower branch corresponds to relaxation of the secondary structure. It is resulted from a jump of strain from value of e_{b1} to the maximum value of relative strain $e = 1$, that is, $\varepsilon = \varepsilon_{b2} = p/c$. It means that the second limit (barrier) ε_{b2} of stability of the secondary structure represents the limit of structural stability of the lattice; it is failured at very large strains. The area of the hysteresis loop corresponds to the latent energy spent to the formation of the new (secondary) structure.

The lower branch corresponds to relaxation of the secondary structure until complete relaxation of the stresses at $e \to e^p$. Here e^p is the residual (plastic) deformation that accompanies the process of structural relaxation. This branch extends to a point where it intersects the stress axis. At this point we have $\varepsilon = 0$, and the stresses reach some value of the opposite sign. These stresses cause elastic relaxation of the residual strains.

An example of the transformation of such a kind is the twinning or, in other words, the transformation resulting in the formation of a structure being a mirror of the initial structure. The second initial branch

corresponds to elastic change of the twinning angle ($tg\beta = 2\varepsilon$) of the pre-existent crystal until value of 90 ° in the point of the maximum stress. Then the structure spontaneously starts increasing the twinning angle of opposite sign, that corresponds to twinning structure.

The existence of the two branches of stable strains (the initial and secondary structures) joined by a range of intermediate intermediate unstable states can be described in terms of the local elasticity modulus:

$$\Lambda = \frac{\partial\overline{\sigma}}{\partial\varepsilon} = \lambda - c(\arcsin e)_{,e} = \lambda - + \frac{c}{\sqrt{(1-e^2)}}. \quad (30)$$

Here $(\,)_{,e} \to \partial(\,)/\partial e$. The signs + and - of the second term on the r.h.s. of Eq. (30) mean the existence of the two branches of the dependence $\Lambda(e)$. This dependence is presented in Fig. 3.

Solid line in Fig. 3 corresponds to stable structures with $\Lambda>0$. The lower branch corresponds to the initial structure. It intersects axis $y=0$ in point $e=e_{b1}$, the bifurcation point where the local elastic modulus $\Lambda=0$. The dashed line below axis $y=0$ is shown which describes unstable state where the local elastic modulus $\Lambda<0$. Another (upper) branch with $\Lambda>0$ corresponds to the stable secondary structure.

The local elastic modulus is an important characteristic of the deformation process in dynamics, too. It was demonstrated in paper [8].

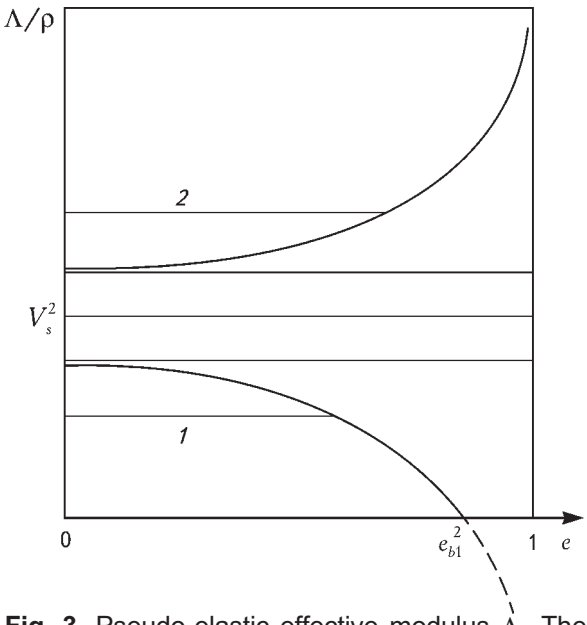

Fig. 3. Pseudo-elastic effective modulus Λ_i. The lower and upper branches correspond to soft initial and solid secondary structures, respectively.

3.3. Stability and instability of initial state

It is worth to consider the situation where the lower branch as a whole is below the axis $y=0$, with the bifurcation point corresponding to $e_{b1}=0$ and $\gamma=1$. It means that the unstrained solid is structurally unstable and has to undergo a transformation. This situation is described by the hysteresis loop in Fig. 2, which is located below axis $y=0$ and has 0 as a value of its derivative at coordinate center. The derivative becomes <0 at $\gamma\geq1$. In this context, it is interesting to know, if such values are realized in real system, and what is their nature?

In our theory we can describe the aforesaid phenomenon, using terms of the atomic structure. Let us consider the interatomic potential of the strained lattice when $\gamma=1$ in the simple case of one-component movement (25). In these circumstances, the elastic energy density D is given as:

$$D = \frac{1}{2}\lambda\varepsilon^2 + c(u-u_0)\varepsilon + p\left[1-\cos\frac{2\pi u}{b}\right]. \quad (31)$$

D can be expressed through microdisplacement u, using the second relationship in (26). In doing so, we get:

$$\frac{D}{p} = \frac{1}{2}\gamma\sin^2\frac{2\pi u}{b} - (u-u_0)\sin\frac{2\pi u}{b} - \cos\frac{2\pi u}{b} + 1. \quad (32)$$

The third and fourth terms on the r.h.s. of formula (32) represent the interatomic potential of a solid unstrained lattice. This potential (designated as ρf^p; see above) is shown as dashed curve in Fig. 4. The complete potential given by formula (32) is presented in Fig. 4, for $\gamma>1$ (curves 1 and 2) and $\gamma<1$ (curve 3). Curves 1 and 2 have a minimum in the coordinate center; the lattice in its unstrained state is stable. Curve 3 has its maximum in coordinate center (the unstrained lattice is unstable) and a minumum in vicinity of $u/b \to \approx 1/4$. This displacement corresponds to spontaneous deformation of the lattice at $\gamma<1$. The phenomenon discussed is known as a ferroelastic transition in some crystals [9]. It occurs at certain temperature when the above inequality becomes valid.

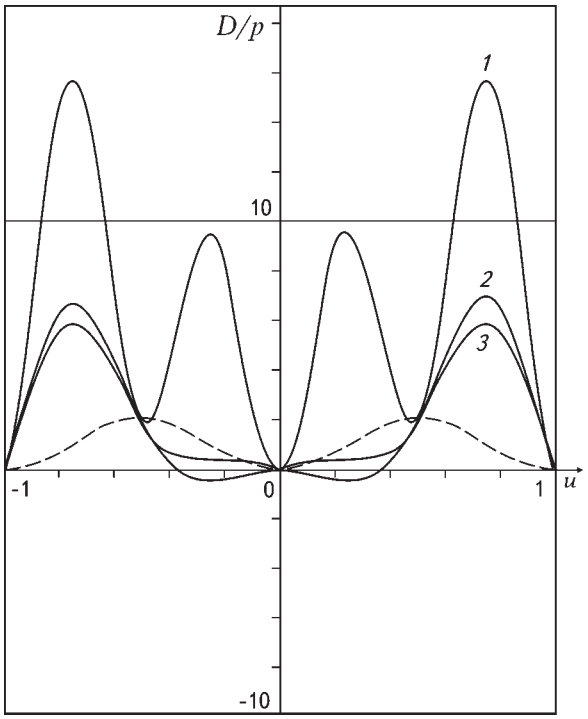

Fig. 4. Dependence of elastic potential on microdisplacement. Dahsed curve corresponds to solid relative shear of unstrained sublattices. Curves 1 and 2 correspond to the potential at $\gamma = 4$ and $\gamma=2$, respectively. Curve 3 describes the potential with maximum at coordinate center, for $\gamma=0,5$. It corresponds to ferroelastic crystal.

Now let us analyze curve 1 (corresponding to the stable structure) with a minumum in coordinate center. Its minima nearest to the above minumum are at u/b <1, in contrast to dashed curve of the interatomic potential of the solid lattice. It corresponds to the second (lower) branch of the hysteresis loop in Fig. 2. The upper branch of the hysteresis loop corresponds to a fragment of curve 1 in Fig. 2, between the initial minimum and maximum. The maximum, in its turn, corresponds to maximum at hysteresis, that is, bifurcation point.

Dynamics of structural transformations is interesting, too. Some problems in this area have been analyzed in paper [8].

4.CONCLUDING REMARKS

Thus, classical model of smooth manifold, based on the condition that the local topology is unchanged, can be generalized using the notion of double (in general, multiple) continuum with a complicated structure. Its discrete analog is a solid with a complicated crystalline lattice whose elementary cells contain atoms of two types. The lattice is represented as either superposition of two sublattices (Bravais sublattices) or a result of periodic arrangement of an atomic group (elementary cell). Atoms of the cell can be of different types or can be distinguished by their position in the elementary cell and, as a corollary, their neighbouring atomic arrangement.

Linear models are not sufficient to describe a variable local topology. Such models are well-known in both physical theory of optic oscillations and continuum mechanics of multicomponent systems. Local topology (elementary cell) undergoes changes not only at large, but also at small deformations. However, such changes of local topology, described as internal degrees of freedom, are unambigiously caused by small deformations. Therefore, the changes can be removed from equations of motion of the medium, which are transformed into classical equations with re-normalized values of elastic constants. That is, equations of a medium with a complicated structure are reduced to those of a medium with a simple structure.

In the case of occurrence of new properties (for instance, extension of matrix of elastic properties or occurrence of their time-spatial dispersions), several new effects can come into play such as boundary layers, scale effects, and new branches of oscillations. However, many phenomena of inelasticity, structural transformations, defect formation, mixing (alloying), transformations of lattice crystallography and other dramatic transformations in solids under extreme conditions of loading can not be described as those associated with small changes of their elastic properties.

The important feature of adequate theory of dramatic transformations of crystals with complicated lattices should be a high non-linearity of the processes which may reach bifurcation points and lead to radical changes of the existent properties and occurrence of new properties. Up to now, the general axiomatic theory of a complicated continuum has been not elaborated. An alternative to this theory can be the phenomenological theory of inelastic phenomena, taking into account structural transformations and using the notion of Eshelby tensor [10]. The approach suggested here is the structural-phenomenological theory whose linear basis is the theory of optical and acoustic oscillations of a complicated crystalline lattice. Internal periodic structure of the lattice essentially simplifies mathematical methods of its description. At the same time,

there is a simple procedure of transformation of discrete equations into continuum ones. The discrete type of the structure allows one to take into account in a rather simple way several effects of local topology of a continuum serving, for example, as a model of the discrete lattice of a polyatomic solid. A simple hypothesis of the non-linear interaction between the sublattices is automatically described in terms of the complicated continuum. This hypothesis allows one to describe a number of interesting mechanisms of structural transformations, using exact analytical solutions of non-linear equations.

In this paper we have analyzed several examples of these mechanisms. In doing so, we first have described such non-trivial effects as catastrophic deformations, bifurcations, structural transformations, twinning, inelastic non-diffusional deformations, violations of short- and long-range order, and rearrangements of interatomic binding.

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