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Micromechanics of a double continuum in a model of a medium with variable periodic structure

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Abstract. A new model of a double continuum with variable local topology is used to develop an essentially nonlinear theory of a medium with a cardinally rearranged periodic structure. This theory is based on a continualization of the periodic structure of a complex crystalline lattice consisting of two sublattices. In the long-wave approximation, the standard linear theory of acoustic and optic oscillations of the complex lattice is generalized. In this generalization, an internal translational symmetry of relative shear of the sublattices is taken into account. As a result, the interaction between the sublattices is expressed in terms of a nonlinear periodic force described, in particular, as a sine of the relative shear of two atoms belonging to an elementary cell. The corresponding equations describe elastic and inelastic catastrophic deformations due to the structural instability which accompanies phase transitions, twinning, defect formation, etc. Some static and dynamic problems are analyzed.

Key words: bifurcations, cardinal structure rearrangements, complex lattice, inelastic deformations, inner translation invariance

1. Introduction

Continuum mechanics postulates, in particular, that deformation does not affect the local topology of the medium. This means that a material particle (a structural unit of the medium) in the deformed medium has the same neighboring material particles as in the undistorted one. In other words, the structure of the medium and the interparticle bonds are not rearranged in the deformed state. Using this postulate, modeling the continuum as a smooth manifold, allows one to elaborate self-consistent effective methods of the phenomenological theory of elasticity of continuous media. However, it is now evident that many inelastic phenomena in continuous media, which are related to structural transformations, phase transitions, generation of point defects, plastic deformation and failure processes, can not be adequately described within a framework of the standard model of the deformed medium with constant local topology. In an analysis of such phenomena, structural transformations of real solids should definitely be taken into account. Attempts to generalize linear models of smooth manifold based on introducing internal degrees of freedom have been unable to describe inelastic effects in solids. Weak (linear) transformations of the internal structure are connected only with small changes of the continuum geometry. Therefore, such transformations only give rise to changes in material parameters involved in the standard equations of classical continuum mechanics. As a result, by this approach, the model of the complexly arranged structure is reduced to the standard model of a simple structure. An actually required approach should allow one to obtain new results, namely, dispersion of elastic properties in both space and time, and boundary effects in statics which could play an essential role in several cases.

In general, the phenomenological theory of elasticity can be formulated on the basis of a linear microscopic theory [1, Chapter 3, Section 11], [2, Chapter 3, Section 8] that takes into account the crystalline lattice structure. Internal degrees of freedom can be introduced in the model of a complex crystalline lattice consisting of two or more sublattices. In this case, optical oscillation modes are also involved in processes occurring in the medium. However, such a linear microscopic theory with internal degrees of freedom 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 which is based on the use of nonlinear optical oscillations and 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 portions) of atoms of two types. Its crystalline lattice is composed of two periodic sublattices, and each sublattice consists of atoms of only one type (Figure 1a). The sublattices have the same geometry and coincide in space when one of them is shifted with respect to another by the crystalline lattice vector vector a_i (Figure 1a).

Oscillations of the crystalline lattice consisting of atoms of two types can be separated into acoustic and optical modes, *i.e.*, oscillations of the lattice as a whole and oscillations of the sublattices with respect to each other, respectively. In these circumstances, the linear theory of crystalline lattices consisting of atoms of two types operates with two equations for acoustic and optical oscillations, respectively, which can be derived from the so-called harmonic approximation of the energy. In this approximation, the total potential energy of the medium is given by

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

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 pth and qth sublattices, respectively, and

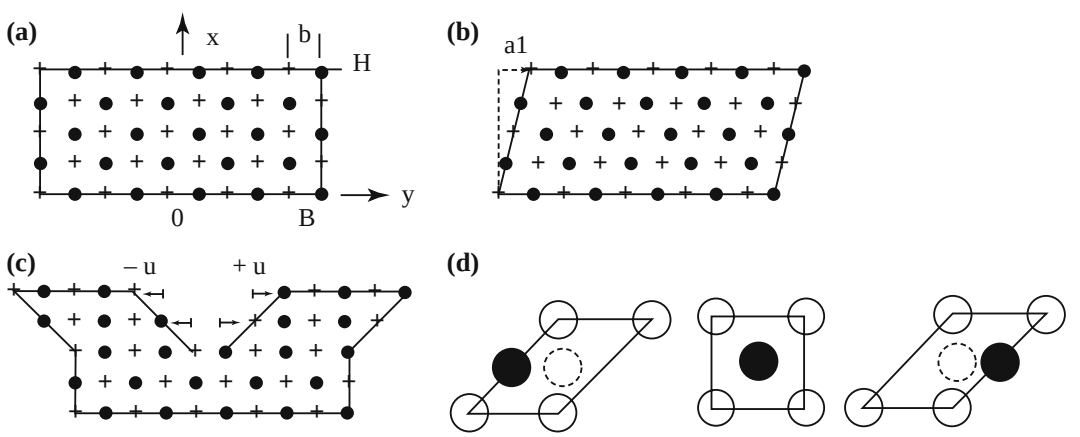

Figure 1. (a) The complex crystalline lattice consisting of two sublattices. (b) Macroscopic deformation without a relative shear of sublattices. (c) Microdeformations at twinning. (d) Bifurcation of the structure of an elementary cell during microdeformation.

U_i^p and U_k^q are the displacement vectors of atoms belonging to these sublattices. In our case of two sublattices, we have $p, q = 1, 2$. From (1) one can obtain the following equations of motion of atoms belonging to these sublattices:

$$\begin{aligned} m_1 \ddot{U}_i^1(n) &= -\sum_{lq} \alpha_{ik}^{1q}(n-l) U_k^q(l), \quad (q = 1, 2), \\ m_2 \ddot{U}_i^2(n) &= -\sum_{lq} \alpha_{ik}^{2p}(n-l) U_k^p(l), \quad (p = 1, 2). \end{aligned} \tag{2}$$

Here m_p is the mass of an atom belonging to the pth sublattice, and $\ddot{U}$ is the second time derivative of the function U. The interaction constants obey the following symmetry conditions [2]:

$$\alpha_{ik}^{pq}(n) = \alpha_{ki}^{qp}(-n), \quad \sum_{n,p} \alpha_{ik}^{pq}(n) = \sum_{n,q} \alpha_{ik}^{pq}(n) = 0, \quad \sum_{n,p} \alpha_{ik}^{pq}(n) R_j^p(n) = \sum_{n,q} \alpha_{ij}^{pq} R_k^p(n), \tag{3}$$

with $R_j^p(n)$ being the vector of the initial position of the nth atom belonging to the sublattice p. The second and third relationships in Equation (3) represent, in that order, symmetry of the lattice relative to rigid-body translations and rotations of the lattice as a whole. The first relationship in (3) is valid only in the case of pair interatomic interactions. In the general situation, the non-pair interactions can be reduced to only triple interactions [3]. In this case, the sum over the energies of triple interatomic interactions should appear on the r.h.s. of Equation (1).

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

Such a description of a discrete structure by means of smooth functions is not entirely adequate: a spectrum of Fourier harmonics of the function under consideration does not contain high spatial frequencies [4, Chapter 1Y, Section 1]. However, it is not essential for our long-wave model. The important specific feature of the model is the continuous character of the displacement field that characterizes only atoms that belong to one sublattice. At the same time, even neighboring atoms of the whole crystalline lattice in its initial state can be situated sufficiently far from each other if they belong to different sublattices. In linear theories, such a situation is not considered. By definition we have

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

The smooth character of the vector function $U_i^p(r_k)$ allows us to expand it in Taylor series in the vicinity of any point of the pth subcontinuum, namely,

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

Here $()_{,i}$ denotes $\partial()/\partial r_i$, $()_{,ij}$ denotes $\partial^2()/\partial r_i r_j$, and $O(\nabla^3)$ denotes small terms containing higher derivatives. Using the expansion (5) in the discrete equations (2) and (3), one can obtain their continuum version as follows:

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

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

Now, two sublattices are represented as two mutually penetrating subcontinuums. In the initial state, these sublattices are shifted with respect to each other by vector a_i. The relative displacement of the sublattices in a strained state is described by a spatially inhomogeneous vector field considered in detail below.

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

$$U_i = (m_1 U_i^1 + m_2 U_i^2)/(m_1 + m_2), \quad u_i = (U_i^1 - U_i^2)/b. \tag{8}$$

Here b is one of periods of the Bravais lattice. As a result, from Equations (6) and (7) we obtain the following set of equations:

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

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

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

$$\rho = (m_1 + m_2)/v, \quad \mu = m_1 m_2/(m_1 + m_2)v, \tag{11}$$

where v is the volume of the elementary cell.

The tensors of the elastic constants are invariant with respect to permutations of the indices, namely, $p_{ik} = p_{ki}$; $\hat{c}_{kij} = -\hat{c}_{ikj}$; $\lambda_{ikjm} = \lambda_{kijm} = \lambda_{kimj} = \lambda_{ikmj}$. This property follows from the symmetry (3) of the tensor of the force constants α_{ik}^{pq}. All tensorial material characteristics of the solid are expressed in terms of these tensors; see [2]. The symmetry with respect to pair permutations of the indices of the tensor λ_{ikjm} is absent if the interatomic forces are either of non-pair or non-central type [5].

In the following we will use the ratio of the magnitude u_i of the vectors of relative displacements of atoms (belonging to different sublattices) within each elementary cell to the period b of the Bravais lattice. Thus, the case of $|u_i| = 1$ corresponds to a displacement of the sublattices along the ith direction by the period b.

The terms O_1 and O_2 are nonlinear terms that are proportional to higher derivatives, and, hence, these are omitted here. They can be represented as follows:

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

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

Let us now consider Equations (9) and (10). The crossed terms in these equations, which describe the local interaction of modes, are non-zero only in the case of crystals without a center of symmetry due to the odd rank of the corresponding tensorial coefficients c_{ikn}. The crossed terms representing interactions of higher order are given by Equations (12) and (13). Some of these are non-zero for crystals without a center of symmetry due to the even rank of the corresponding tensorial coefficients.

Equation (9), which describes the acoustic oscillations, for media with central symmetry, is reduced (by neglecting terms O_1 of higher order) to the macroscopic equation for oscillations of a continuous medium without dispersion of its elastic properties. Then, the macroscopic displacements U_i characterize changes in dimensions and shape of the solid as a whole (its external geometry).

Equation (10), which describes the optic oscillations, contains the gradient-independent term (the first term on its r.h.s.). This term describes forces between two neighboring atoms of the elementary cell or, in other words, the interaction between different 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 was noted above, these changes are unambiguously related, by means of Equation (10), to gradients of the macroscopic (acoustic) displacement field U_i. Therefore, these changes can be excluded from the macroscopic equation, and, hence, we return to the model of a smooth manifold with constant local topology.

2.2. Nonlinear theory

Using the internal degrees of freedom described by the field u_i, the changes in the local topology may be effectively incorporated into the theory, if we make the following generalization of Equation (10). Let us consider arbitrary large relative displacements u_i of the sublattices, which are described by the nonlinear term $P_i(u_n) = -P_i(-u_n)$, instead of the previously used linear one. The nonlinear term should be a nonlinear odd periodic vector function with a period corresponding to that of the Bravais lattice along the direction of the displacement u_i. The crystalline lattice in its initial, non-strained state is characterized by the conditions $u_i = 0$ and $P_i = 0$.

The discussed non-affine changes in geometry of the crystalline lattice are realized by polyamorphic transformations of the non-diffusion type accompanied by changes in the short-range order of the atomic arrangement or, in other words, by changes in the local topology under extremely large mechanical loads.

Figures 1c and d show schematically large displacements of neighboring atoms of the complex lattice at twinning and a transformation of the bcc-lattice occurring due to large shear transformations of sublattices. A rearrangement of the short-range order is clearly observed.

Then, instead of Equations (9) and (10), we have the following set of equations:

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

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

where terms O_1 and O_2 are given by expressions (12) and (13). Since the displacement u_i is measured in units of periods of the Bravais lattice in the ith direction, the periods of this 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, for an infinitely large sample, is crystallographically equivalent to the initial one. However, this transformation gives rise to changes in interatomic bonds, in the arrangement of neighboring atoms, and in the local topology. Such topological changes do not occur, if the microdisplacements are relatively large, but still $u_i < 1/2$. This means that in this situation we should take into account essentially nonlinear effects which can occur even at the microdisplacements $u \ll 1$. In the following, we will consider such microdisplacements. In general, however, one can also imagine multiple structural transformations of complex crystalline lattices corresponding to $u \geq 2$. For

instance, such transformations can occur at either the formation of domain superstructures or microphase polymorphic decomposition.

Large interatomic microdisplacements were introduced for the first time in the one-dimensional Frenkel-Kontorova model of a crystalline chain. In spite of its simplicity, this model attracts some attention up to the present day.

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 with respect to coordinate transformations, namely, $P_i = \partial f^p / \partial u_i$. 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 the crystallographic axes (m_n^1, m_n^2, m_n^3). They are invariant with respect to transformations of the general coordinate system. So, we have

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

In this general case, f^p is a periodic function with three periods b_1, b_2 and b_3, and it is invariant with respect to translations of the Bravais sublattices over periods b_1, b_2, and b_3 along the directions m_1, m_2, and m_3, respectively. In the case of media with central symmetry, this function is odd. In particular, when the directions of the force and the 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. Thus, P_i is given as follows:

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

This case is realized when interactions between atoms belonging to one elementary cell are of the central type, and the structural vector a_i of the complex lattice defines the directions of vectors P_i and u_i. If these interactions are not of central type, and, moreover, vectors a_i and u_i are orthogonal, a pair of atoms is rotated. Actually, this situation occurs in molecular crystals with rigid molecules when the rotational degrees of freedom are essential. In this case, rotations of the structural vector a_i with constant length, similar to those in the model reported in [6], should be taken into account. Here we will not introduce such a restriction, and will not consider this case separately.

3. Strong interaction between modes in media without central symmetry

3.1. Basic equations

Let us consider some crystals of pyroelectric and piezoelectric classes which have no center of symmetry. Equations (14) and (15) for a lattice without central symmetry can be formulated in their simplest form in the so-called long-wave approximation. In this approximation, the terms in Equation (15) containing gradients can be neglected, and it is reasonable to restrict our consideration to low-frequency oscillations of the medium, and neglect high-frequency oscillations of the crystalline lattice. Within the framework of this approach, Equations (14) and (15) are written in the following reduced form:

$$\rho \ddot{U}_i = c_{ikj} u_{k,j} + \lambda_{ikjm} U_{k,jm}, \tag{18}$$

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

This is a rather crude approximation because boundary conditions or domain walls are neglected. A more adequate description will be presented in Subsection 3.4. Besides, the gradient terms were considered in [7, 8] for a medium with central symmetry where, however,

terms (the first right-hand ones in (12), (13)) describing the local interaction between modes were not taken into account.

Equation (18) can be written in the form of the classic equation of continuum mechanics

$$\rho \ddot{U}_i = \sigma_{ij,j}, \tag{20}$$

if we assume that the quantity

$$\sigma_{ij} = \lambda_{ikjm} U_{k,m} + c_{ikj}(u_k - u_k^o) \tag{21}$$

plays the role of an effective stress tensor. Here u_k^0 (integration constant) is the vector representing the relative translation of sublattices without any deformations due to the natural modification of the crystalline structure (its symmetry). For ionic crystals, $u_k^0 \sim P_0$. Here P_0 is the vector of the natural polarization of the pyroelectric crystal. The corresponding term $c_{ikj}u_k^0$ in Equation (21) denotes the inner stresses $\sigma^0 = \lambda_{ikjm}\varepsilon_{km}^0$, where ε_{km}^0 is the spontaneous deformation tensor.

3.2. Structural transformations and bifurcations in statics

Let us consider a stationary version of our equations, namely,

$$0 = \sigma_{ij,j}, \tag{22}$$

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

In the two-dimensional case, the former equation can be solved in general form by introducing a stress function ψ that obeys the special equation

$$\sigma_{xx} = \partial^2\psi/\partial y^2, \quad \sigma_{yy} = \partial^2\psi/\partial x^2, \quad \sigma_{xy} = -\partial^2\psi/\partial x\,\partial y. \tag{24}$$

The stress function ψ is more general than an Airy function, however. It obeys the equation

$$\nabla\nabla\psi = c_{nkn}u_k - (\lambda_1 + \lambda_{12} - \lambda_2)(\lambda_1 + \lambda_{12} + \lambda_2)^{-1}c_{ikj}u_{k,ij}. \tag{25}$$

Here $\nabla\nabla\psi \to \psi_{,nn}$. Then, for three functions (u_x, u_y, ψ) we have a set of equations, namely (23), (25). Equation (22) is satisfied by the introduction of the stress function. It is worth while to notice that in Equation (23) the gradient term $U_{i,j}$ may be expressed through σ, on account of (21):

$$\lambda^{-1}\sigma = \varepsilon - \lambda^{-1}cu, \quad \lambda^{-1}\lambda = 1 \tag{26}$$

where λ^{-1} is the fourth-order inverse tensor of λ. Let us express σ trough ψ here and then exclude from (25) the gradient term $U_{i,j}$. As a result, we find the components of the vector u_i and the tensor $U_{i,j}$. In doing so, we must take into account that the periodic function $P_i(u_k)$ should be either defined initially or derived from a periodic scalar energetic function, as was shown in Section 2.

Let us consider the simple case of a one-component movement when all the vectors have only one component, for example,

$$u_y = u(x), \quad P_y = p\sin(2\pi u), \quad U_y = U(x), \quad 2\varepsilon = U_{y,x}, \quad \sigma = \sigma_{yx}, \quad c = c_{yyx}. \tag{27}$$

If OZ and OX coincide with the axes of symmetry (of the third and second order), respectively, in piezoelectric crystals belonging to the D_{3h} and D_3 classes, then the third term in Equation (23) vanishes because of the antisymmetry of the tensor $\hat{c}_{kij}$ over permutations of k and i. The same result is valid for the piezoelectric crystal of the C_{3h} class.

The basic equations can now be written for this case as follows:

$$\sigma = \lambda\varepsilon + c(u - u_o), \quad 0 = p\sin(2\pi u) + c\varepsilon \tag{28}$$

This equation is valid also for the following one-component cases (axes OX, OZ are directed as before):

I. $U_x = U_x(x)$, $u_x = u_x(x)$, $\varepsilon = U_{x,x}$, $\sigma = \sigma_{xx}$, $c = c_{xxx}$ for the C_{3h}, D_{3h}, D_3 and piezoelectric classes, and the C_{3v} pyroelectric class;

II. $U_x = U_x(y)$, $u_x = u_x(y)$, $2\varepsilon = U_{x,y}$ and $\sigma = \sigma_{xy}$, $c = c_{xyy}$. This is possible only for piezoelectric crystals belonging to the C_{3h} class;

III. $U_y = U_y(y)$, $u_y = u_y(y)$, $\varepsilon = U_{y,y}$, $\sigma = \sigma_{yy}$, $c = c_{yyy}$ only for the piezoelectric C_{3h} class.

It is worthwhile to discuss Equations (28). Vector u_k may be interpreted as an order parameter. For ionic crystals it is evident because $u_k \sim P_k$, where P_k is the vector of electric polarization. Then the second equation in (28) represents the low of electrostriction. For nonionic crystals it is simply the striction, or more exactly, the mechanical striction, *i.e.*, a deformation due to the order (disorder) of the crystal. But in our theory an opposite effect, namely, ordering due to the deformation is also analyzed (see the first equation in (28)). The fields ε and u are selfconsistent. As a result, using the second equation, one can derive an effective material relationship excluding the parameter u from the first equation. Then we have

$$\sigma = (\lambda p/c)e - c \arcsin e, \quad e = \varepsilon/\varepsilon_{b2}, \quad \varepsilon_{b2} = p/c. \tag{29}$$

This relationship is presented graphically in Figure 2 for

$$\gamma = p\lambda/c^2 > 1. \tag{30}$$

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

$$e_{b1}^2 = 1 - 1/\gamma^2. \tag{31}$$

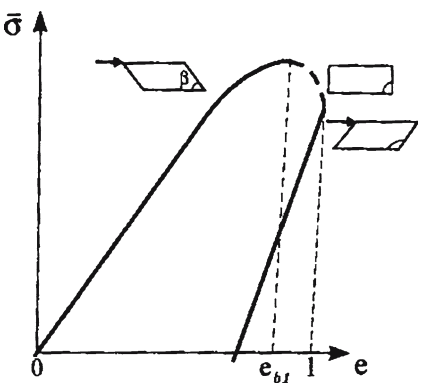

Figure 2. Dependence of stress on relative deformation accompanied by structural transformation (schematically). The upper branch corresponds to the initial structure exhibiting softening. The lower branch corresponds to the secondary structure exhibiting strengthening. The dashed fragment of the curve corresponds to the transitional region of instability.

The lower branch corresponds to relaxation of the secondary structure. Its appearance is caused by a bifurcation and is accompanied by a jump of the strain from e_{b1} to the maximum value of the relative strain $e=1$, *i.e.*, $\varepsilon=\varepsilon_{b2}=p/c$. This means that the second limit ε_{b2} of the stability of the secondary structure represents the limit of the structural stability of the lattice; when the deformation exceeds this limit, the lattice fails. The area of the hysteresis loop corresponds to the latent energy required for the formation of a new (secondary) structure.

The lower branch corresponds to relaxation of the secondary structure until complete relaxation of the stresses for $e \to e^p$. Here, e^p is the residual (plastic) deformation that accompanies the process of structural relaxation. This branch extends to the point of its intersection with the stress axis. At this point we have $\varepsilon=0$, and the stresses reach some values of opposite sign. These stresses are required for an elastic relaxation of the residual strains.

An example of a transformation of this kind is the twinning or, in other words, the transformation of the structure to its mirror image. The second initial branch corresponds to an elastic change of the twinning angle ($\tan\beta=2\varepsilon$) of the pre-existent crystal to 90° at the point of maximum stress. Then the structure spontaneously starts increasing the twinning angle of opposite sign corresponding to a twinning structure.

The existence of two branches of stable strains (the initial and secondary structures), connected to each other by a region of intermediate unstable states, can be described in terms of the effective elastic modulus:

$$\Lambda=\partial\sigma/\partial\varepsilon=\lambda-c(\arcsin e)_{,e}=\lambda--+c/\sqrt{(1-e^2)}. \tag{32}$$

Here, $()_{,e} \to \partial()/\partial e$. The signs + and − of the second term on the r.h.s. of Equation (31) mean the existence of two branches of the dependence $\Lambda(e)$. This dependence is presented in Figure 3.

The solid line in Figure 3 corresponds to stable structures with $\Lambda>0$. The lower branch corresponds to the initial structure. It intersects the axis $y=0$ at the point $e=e_{b1}$ which is a bifurcation point where the local elastic modulus $\Lambda=0$. The dashed line below the axis $y=0$ describes an 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 also an important characteristic of the deformation process in dynamics. This will be demonstrated below.

3.3. Stability and instability of initial state

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

In our theory we can reveal an atomic mechanism of the above-mentioned phenomenon. Let us consider the interatomic potential of the strained lattice when $\gamma=1$ in the simple case of the one-component movement (26). In this case, the elastic energy density D is given by

$$D=(1/2)\lambda\varepsilon^2+c(u-u_o)\varepsilon+p[1-\cos(2\pi u/b)]. \tag{33}$$

Here we have neglected the gradient terms $k\nabla u\nabla u$, *i.e.*, an energy of domain boundaries.

By use of the second relationship in (27), it can be expressed in terms of the microdisplacement u, namely,

$$D/p = (1/2)\gamma \sin^2(2\pi u/b) - (u - u_o)\sin(2\pi u/b) - \cos(2\pi u/b) + 1. \tag{34}$$

The third and fourth terms on the r.h.s. of Equation (33) represent the interatomic potential of the solid unstrained lattice. This potential, which is denoted above as ρf^p, is depicted by the dashed curve in Figure 4. The total potential given by Equation (33) is presented in Figure 4 for $\gamma > 1$ (curves 1 and 2) and $\gamma < 1$ (curve 3). The curves 1 and 2 have minima in the coordinate origin. This means that the lattice is stable in its unstrained state. Curve 3 has its maximum in the coordinate origin (the unstrained lattice is unstable) and a minimum in the vicinity of $u/b \to \approx 1/4$. This displacement corresponds to a spontaneous deformation of the lattice at $\gamma < 1$. This phenomenon is well known as the ferroelastic transition in some crystals [9]. It occurs at certain temperature when the above inequality is valid.

Now let us analyze curve 1 corresponding to the stable structure with a minimum in the coordinate origin. Its minima nearest to the above-mentioned curve exist for $u/b < 1$; this is in contrast to the dashed curve of the interatomic potential of the solid lattice. It corresponds to the second (lower) branch of the hysteresis loop shown in Figure 2. The upper branch of the hysteresis loop corresponds to a fragment of curve 1 in Figure 2, between the initial minimum and the maximum. This maximum, in turn, corresponds to the maximum of the hysteresis loop, *i.e.*, to the bifurcation point.

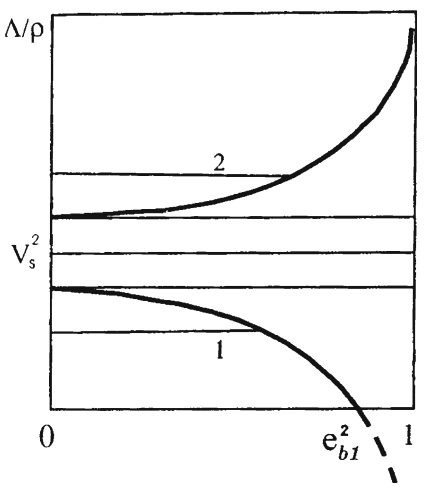

Figure 3. The pseudo-elastic effective modulus. The lower and upper branches correspond to soft initial and solid secondary structures, respectively.

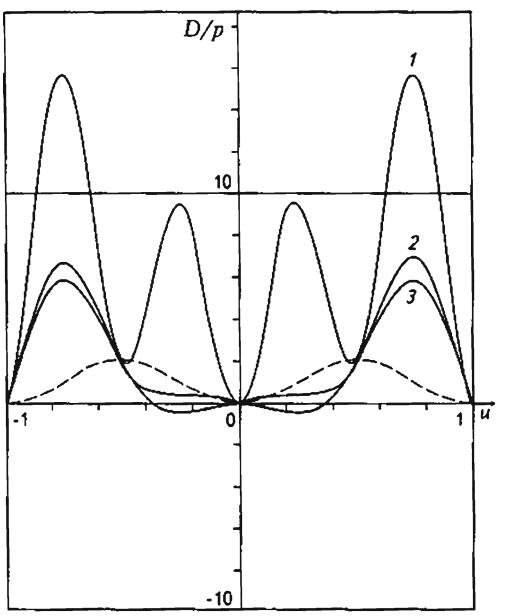

Figure 4. Dependence of the elastic potential on microdisplacement. The dashed curve corresponds to solid relative shear of unstrained sublattices. Curves 1 and 2 correspond to the potential at $\gamma = 4$ and $\gamma = 2$, respectively. Curve 3 describes the potential with maximum at coordinate origin for $\gamma = 0{\cdot}5$. It corresponds to a ferroelastic crystal.

3.4. Stationary waves of structure rearrangements

Let us consider the following one-component, one-dimensional motion

$$U_i \to U(x,t), \quad u_i \to u(x,t). \tag{35}$$

The directions of the vectors U_i and u_i are arbitrary but fixed. Then, ε may be considered as a shear, stretch deformation or a volume deformation. The equations of motion (14), (15) may be rewritten as

$$\rho\ddot{U} = \lambda U_{,xx} + cu_{,x}, \tag{36}$$

$$\mu\ddot{u} = -p\sin u + cU_{,x} + ku_{,xx}. \tag{37}$$

Here U denotes U_x or U_y and u – u_x or u_y, respectively.

Now we consider the second equation, taking into account both (time and spatial) second derivatives. In the case of a stationary wave with the wave argument given by

$$q = n(x - Vt), \quad V > 0, \quad V < 0, \tag{38}$$

where n is a wave number, V is a phase velocity (positive and negative signs of V correspond to two waves spreading in opposite directions, respectively). Then one has a set of ordinary differential equations

$$(\rho V^2 - \lambda)nU_{,qq} = cu_{,q}, \tag{39}$$

$$(\mu V^2 - k)n^2 = -ncU_{,q} - p\sin u, \quad U_{,q} \to \partial U/\partial q, u_{,q} \to \partial u/\partial q. \tag{40}$$

Upon integration, the first equation can be rewritten as

$$(\rho V^2 - \lambda)nU_{,q} = cu + \sigma_o, \tag{41}$$

where σ_o is an integrating constant. Excluding the derivative $U_{,q}$ from Equation (39) by using expression (40), one can obtain an equation with respect to the single unknown function $u(q)$, namely

$$(\rho V^2 - \lambda)(\mu V^2 - k)n^2 u_{,qq} = -p(\rho V^2 - \lambda)\cos u - c^2 u - c\sigma_o. \tag{42}$$

The first integral of this equation has the form

$$(\rho V^2 - \lambda)(\mu V^2 - k)n^2 u_{,q}^2 = d_o - \hat{d}, \tag{43}$$

where d_o is an arbitrary constant and $\hat{d}$ is the effective microscopic potential given by

$$\hat{d} = 2p(\rho V^2 - \lambda)\cos u - c^2 u^2 + c\sigma_o u. \tag{44}$$

The first term on the right-hand side of this expression is the lattice atomic potential. But the second and third ones express the influence of the acoustic mode (macroscopic deformations) on the structure of a lattice, due to the striction effect. In other words, Equation (43) describes the potential of the deformed lattice.

Although there is no exact analytical solution to Equation (42), except for the cases when $\sigma_o = d_o = 0$, this equation has by now been well-investigated by asymptotic methods and some properties of its solutions are known. Let us consider some of these.

The Figures 5a and b demonstrate the potential energy (43) in the case of low wave velocity ($V^2 < \lambda/\rho < k/\mu$) and for middle wave velocity ($\lambda/\rho < V^2 < k/\mu$), respectively. The

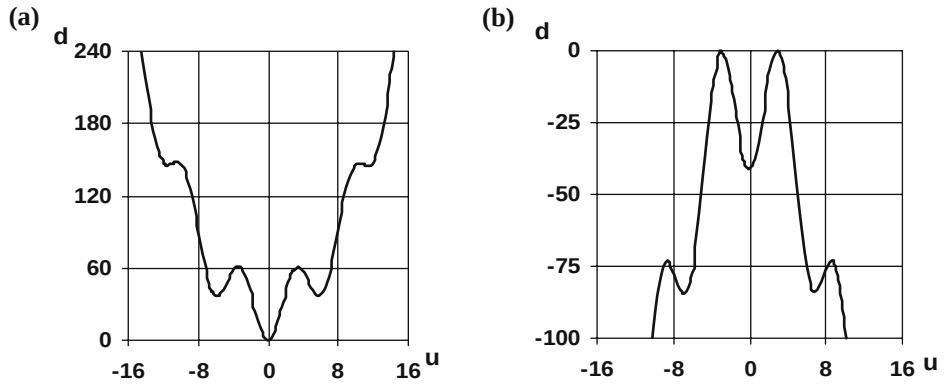

Figure 5. Effective potential d for low velocity (a) and for middle velocity (b).

difference between these curves is connected with the sign before the term with $\cos u$ on the right part of expression (43).

In the first case (low velocities), we can have some particular solutions corresponding to a kink (a motion between low maxima) and two solitons (motion from the right maximum in the right direction and from the left maximum – in the left one), respectively. Soliton-like solutions occur also in the region between high and low maxima.

In the second case, we also have a kink-like solution (a motion between high maxima) and two solitons. These solitons correspond to a motion from the right low maximum to the left and from the left low maximum to the right, respectively. On both curves the maxima are bifurcation points, and a number of these points are determined by the ratio between periodical and nonperiodical terms in Equation (43).

3.5. Bifurcation waves

The dynamics of structural transformations is also interesting. A few of such problems were analyzed in [8]. Nonstationary waves with variable profile can be regarded as some solutions of the Equations (36), (37). Let us consider a high-frequency approximation from which the dynamic terms in the acoustic Equation (36) have been omitted. Then we have the set of equations

$$0 = \lambda U_{,xx} + c u_{,x}, \tag{45}$$

$$\mu \ddot{u} = -p \sin u + c U_{,x} + k u_{,xx}. \tag{46}$$

Integration of the first equation gives the following expression:

$$\lambda U_{,x} = c u + \sigma_{oo}, \tag{47}$$

where σ_{oo} is an arbitrary constant.

Excluding $U_{,x}$ from the second equation we have

$$\mu \ddot{u} = k u_{,xx} - p \sin u + (c^2/\lambda) u + \sigma_{oo}/\lambda. \tag{48}$$

This is the generalized sine-Gordon equation that has been investigated in the literature by perturbation methods for small enough coefficient c^2/λ. The exact Equations (36), (37) may be analyzed numerically. We demonstrate some results, taking into account that, for some critical value of the coefficient c^2/λ, solutions do not exist.

Let us consider a Cauchy problem for longitudinal oscillations of a very thin beam (with length 1) having an inner structure. The acoustic (macroscopic) displacements of its points are $U = U_x(x,t)$. The microdisplacements are $u = u_x(x,t)$. In dimensionless form the equations for the coupled modes are

$$\ddot{U} = U_{,xx} + 0,4u_{,x}, \tag{49}$$

$$0{\cdot}01\ddot{u} = 0{\cdot}01u_{,x} - \sin u - 0{\cdot}4U_{,x}, \tag{50}$$

where here the coupling coefficient is 0·4 while its critical value is 0·65.

We will not introduce new cumbersome notations for the dimensionless coefficients and U. The boundary conditions are the following:

$$U(0,t) = U(1,t) = 0, \quad u(0,t) = u(1,t) = 0, \quad u(x,0) = 0, \dot{u}(x,0) = 0, \quad \dot{U}(x,0) = 0. \tag{51}$$

The function $U(x,0)$ is a triangle shown in Figure 6a ($t = 0$). Figures 6b, c, d demonstrate the evolution of the initial distributions $U(x,t)$ (thin curves) and $u(x,t)$ (bold curves) at the instants $t = 0{\cdot}02; 0{\cdot}17$ and $0{\cdot}55$.

Obviously, the effect of excitation of microscopic (inner) oscillations and energy exchange between modes take place. If we do not know anything about inner oscillations and observe only macroscopic ones, it is possible to interpret this result as an effect of mechanical losses. But there is no dissipation in our system!

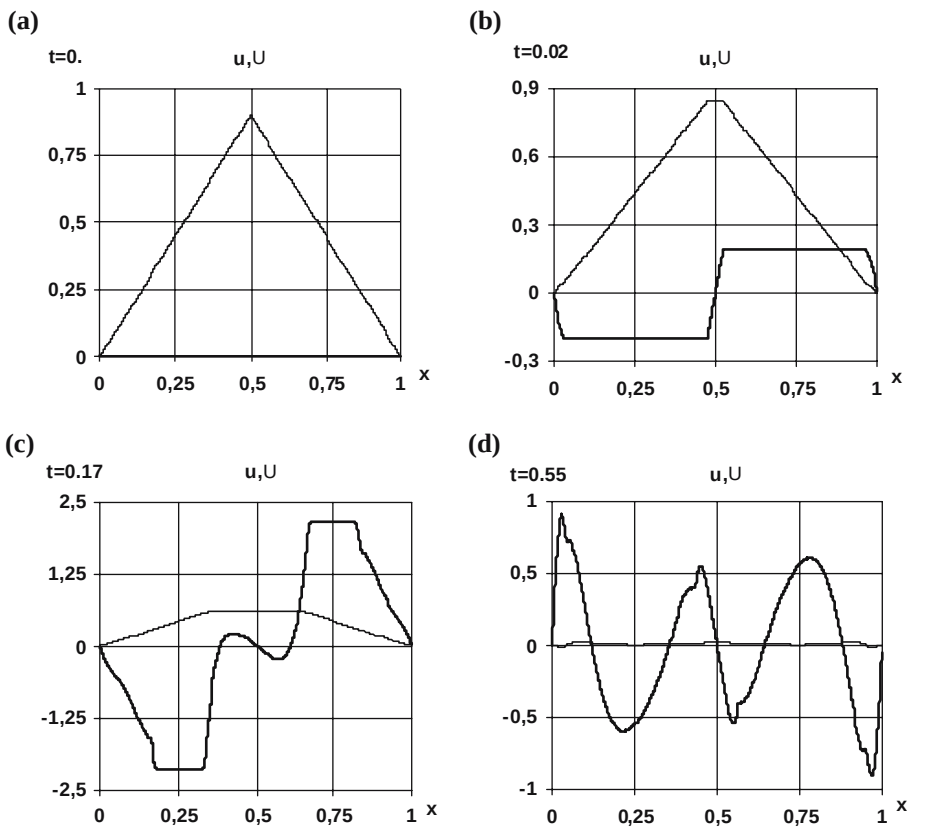

Figure 6. Some stages of evolution of free oscillations of an acoustic (U) and an optic (u) modes. The last is exited but the second disappears due to energy exchange.

The other example demonstrates a peaking regime of oscillations when the coupling coefficient is large enough, *i.e.*, $c^2/\lambda > 0{\cdot}65$, where $0{\cdot}65$ is the critical value. Let us consider the following set of coupled equations:

$$\ddot{U} = U_{,xx} + 0{\cdot}7u_{,x}, \tag{52}$$

$$0{\cdot}01\ddot{u} = 0{\cdot}01u_{,x} - \sin u - 0{\cdot}7U_{,x}, \tag{53}$$

with the boundary and initial conditions

$$U(0,t) = U(1,t) = 0, \quad u(0,t) = u(1,t) = 0, \tag{54}$$

$$u(x,0) = 0,\ \dot{u}(x,0) = 0, \quad U(x,0) = A\sin x, \quad \dot{U}(x,0) = 0. \tag{55}$$

Some results of a numerical simulation are presented in Figures 7a–d.

The thick curves correspond to $U(x,t)$ and the thin ones to $u(x,t)$. The effects of energy exchange between modes are also visible. But now the effect depends crucially on the value of the initial acoustic amplitude A. Its critical value is $A_c = 0{\cdot}6285$. If $A = 0{\cdot}628$ (Figures 7a,b), then $u < 0$ at $t > 0$. If $A = 0{\cdot}629$ (Figures 7c,d), then $u > 0$. Apparently, since the initial states (7a,7c) are almost identical, we have an instability effect of catastrophic type!

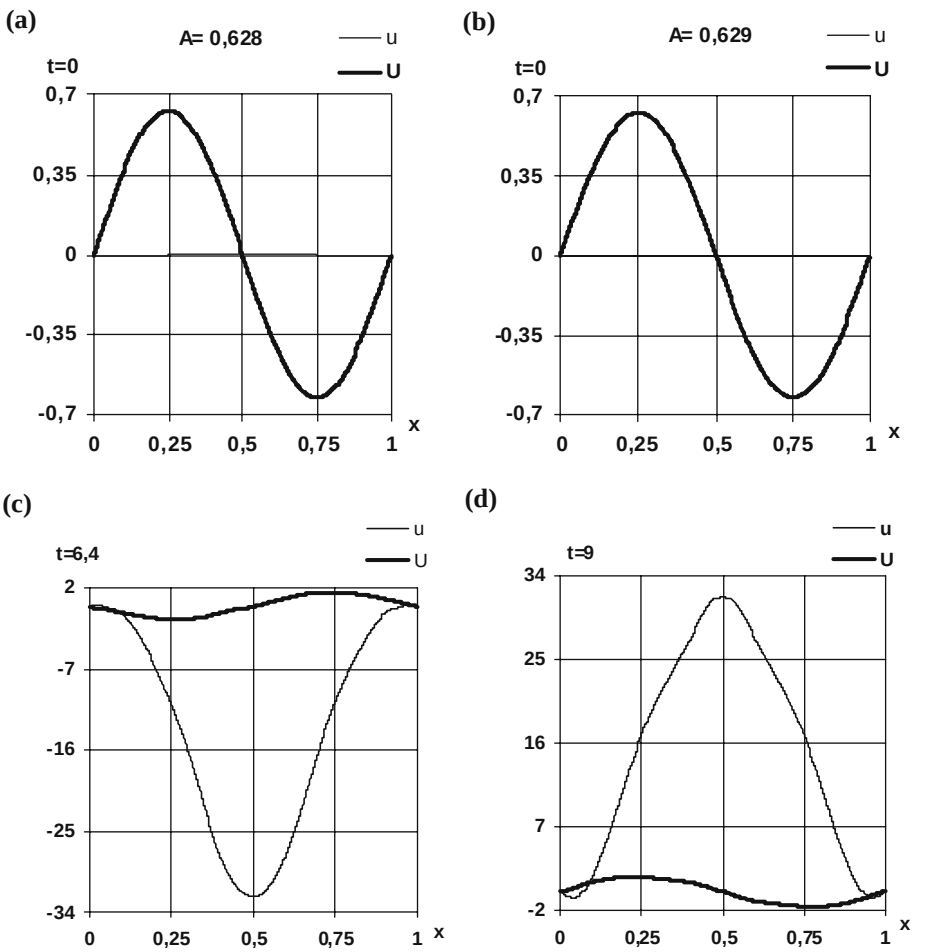

Figure 7. Crucial energy exchange when mode interaction is large enough. Inversion of optical mode near the critical value of initial acoustic amplitude $A = A_c$: $A < A_c$, $u < 0$ (a, b); $A > A_c$, $u > 0$ (c, d).

4. Conclusion

Many inelastic phenomena are connected with structural rearrangements. A range of famous mechanicists pay attention to a phenomenological theory that incorporates these effects adequately [10]. In this work we have made an attempt at defining the beginnings of a microscopic, atomistic model.

Our main attention has been directed towards the local topology of the continuum and to the diffeomorphic principle, taking catastrophic deformations into account. The question about their compatibility can be raised. Compatibility exists for a double pseudo-continuum model that is a proto-type of a complex lattice consisting of two or more sublattices.

It is necessary to consider strong nonlinear effects. Cardinal structural rearrangements can then be analyzed. We have generalized the classic linear micromechanics of complex lattices [1] by introducing a new symmetry element that is available for complex lattices. The structure (and energy!) of a complex lattice is invariant under a mutual shift of sublattices over a single period of the lattice. Because of this, its energy must be a periodic function of the relative displacements of sublattices.

As in the one-dimensional model of Frenkel and Kontorova, we have considered the simplest function, $\cos u$, to analyze corresponding cases. We tried the capabilities of the theory by studying simple, yet non-trivial examples involving dynamic effects. However, static phenomena are interesting too, if only to analyze certain bifurcation problems.

It is possible to predict certain phenomena that are associated with the effects of switching (or tearing) of atomic bonds, such as defect generation, fragmentation of the lattice, phase transitions, surface reconstruction, inner friction, to name a few. It is worth analyzing crystals that have centers of symmetry.

We have restricted ourselves to simple examples of one-dimensional and one-component microscopic fields. More general cases and further results can be found in [11, 12].

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