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CATASTROPHIC MICRODEFORMATIONS IN CRYSTALLINE LATTICE. STRUCTURAL STABILITY AND MODIFICATIONS

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Abstract. Essentially nonlinear theory of three-dimensional lattice subjected to the intensive shear is presented. Two, acoustic and pseudo optical, branches of deformations are considered. The deformation energy is shown to consist of periodic and gradient terms. The equilibrium equation in the sine-Helmholtz form is exactly solved. It demonstrates some effects of bifurcations. The first effect is the transformation of homogeneous macrodeformation into inhomogeneous one, in which case a superstructure with large periods and a new translation order are formed. The second bifurcation effect is associated with occurrence of two deformed, elastic and elastoplastic, states, in which case the short-range atomic order is altered and a new modification of crystalline lattice is formed. Some criteria of local and global structural stability are revealed.

1. GENERAL EQUATIONS

One of the postulates in the continuum theory of deformations is that the local topology remains unchanged in the course of structural transformations. The nearest environment of atoms is conserved without any rearrangement of interatomic bonds. However, sometimes, the so called martensite transitions take place in solids. In doing so, the lattice structure is modified and polymorphic (bimorphic) transitions are possible due to cooperative (but not diffusional) atomic rearrangements. Another example is the twin formation. In order to describe these and other cases where the classical model approximations are not effective, it is worth to combine a continuum approach and a discrete lattice model. It is the main subject of this paper.

Let us suppose that discrete degrees of freedom are presented by a specific lattice potential – a periodic function of interatomic displacements u – and their gradients. Interatomic or microscopic displacements are introduced in the theory of optical vibrations of ionic crystals, too. In this case, however, they are formulated in only terms of the infinitesimal approach. As for the macroscopic displacements U of acoustic branch, they correspond to a half sum of absolute atomic displacements. The macroscopic field U obeys equations of the continuum theory.

In the framework of the suggested model, three-dimensional crystalline lattice consists of atoms of one type and is imaginary divided into mutually penetrating sublattices which are identical in the non-deformed state. The sublattices in the non-deformed state can be displaced relative each other along crystallographic axes by a constant value $u = n$ (where n is integer, and the microdisplacement u is expressed in units of crystal lattice parameter b), in which case the structure of the lattice as a whole is uncharged. We are interested in the case with $u = u(x,y)$, that corresponds to a deformed state of the crystalline lattice. In doing so, misfit occurs between the sublattices composing the lattice, which are either completely coherent or not. We have the standard continuum when the sublattices are coherent. If $u = 1/2$, $U = 0$, the lattice structure is in an unstable state. Transitions from a continual state, $u = 0$, $U = U(x,y)$, to demorphic state, $u = u(x,y)$, $U = U(x,y)$, may be realized due to bifurcation. If $u(x,y) > 1/2$, then the effect of bond switching takes place. It may be accompanied by local structural (morphological) transitions, formation of defects and other variations of lattice topology.

Here we will develop a mesoscopic theory taking into account both degrees of freedom. (Some results in this area were presented early in [1-3].) Let us put both atomic periodic and continual gradient terms into the total energy of deformation E.

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One can consider here the simplest example of polyatomic layer with thickness *H* subjected to shear along the OY axis. The structure of the layer represents the two-dimensional periodic lattice with period *b* and nonlinear interatomic interactions. In these circumstances, the energy of a layer fragment of length *B* is given as:

$$\overline{E} = \int_0^H \int_0^B \left[\frac{1}{2} k_1 \left(\frac{\partial u}{\partial x} - \frac{\varepsilon}{b} \right)^2 + \frac{1}{2} k_2 \left(\frac{\partial u}{\partial y} \right)^2 + p(1 - \cos 2\pi u) \right] dxdy. \quad (1.1)$$

Here u is the microdisplacement (in units of b) along the Y direction, k_1, and k_2 are the shear micromodulus and the strength, respectively. A positive value p is the amplitude of the periodic interparticle potential or force. The constant ε is the macroscopic shear deformation or x-gradient of macrodisplacement field U.

The third term on the r.h.s. of Eq. (1.1) represents the energy of a finite shear of rigid monolayers (chains), while the first and the second terms on the r.h.s. of Eq. (1.1) account for their compliance (elasticity of the D lattice under shear and tension) along the Y axis. They represent continuum forces which are smooth over the mesoscopic scales defined below.

If monolayers are rigid, then the simple condition that the field u is constant means that the shear microdeformation is homogeneous and equal to microdisplacement (in units of b), but not equal to macrodeformation ε.

The equilibrium equation corresponding to a minimum of functional (1.1) (when ε is constant) has the form:

$$k_1 \frac{\partial^2 u}{\partial x^2} + k_2 \frac{\partial^2 u}{\partial y^2} - p \sin 2\pi u = 0. \quad (1.2)$$

This nonlinear equation, known as the sine-Helmholtz one, defines two characteristic coherent lengths of the lattice as follows:

$$l_1 = \sqrt{\frac{k_1}{p}}, \qquad l_2 = \sqrt{\frac{k_2}{p}}. \quad (1.3)$$

They determine the mesoscopic length scales appearing in the suggested theory in contrast to scaleless continuum theory. For $l_1 \to 0$, we have the Frenkel-Kontorova one-dimensional model dealing with elastic chain of atoms on a periodic rigid substrate. Our model is concerned with a system of parallel atomic chains with interaction between them. At the same time, the chains do not interact with the substrate which, therefore, may be ignored. The chains can slip relative to one another and be deformed continuously. We can see that the single Frenkel-Kontorova's solitons in two-dimensional lattice coalesce into special domain boundaries.

In fact, we deal with high-gradient fields. Macroscopic, low-gradient fields U can be approximated (with very high accuracy which corresponds to uncertainty in U, being lower than b) as follows: $U = Nb$, where N is integer. It may be a weak discrete function of x and y. This approximation may be called as quantization of macrofield. With this approximation, macrofield obey not only the continuum equilibrium equation, but the Eq. (1.2), too. Actually, $\sin(2\pi Nb) = 0$, in which case Eq. (1.2) transforms into the equation of the continuum theory of elasticity. At the same time, microfield u obeys Eq. (1.2), too. Consequently, both macrofield and microfield obey Eq. (1.2). It means that there is some bifurcation point of coexistence of these two modes of deformation.

Let us take into account a maximum in the functional (1.1) also. The corresponding condition of the maximum is different from (1.2) by a sign before the sine term, that is,

$$k_1 \frac{\partial^2 u_+}{\partial x^2} + k_2 \frac{\partial^2 u_+}{\partial y^2} + p \sin 2\pi u_+ = 0, \quad (1.4)$$

$$u_-(x,y) = u_+(x,y) - \frac{1}{2}. \quad (1.5)$$

Here u_+ and u_- are solutions of Eqs. (1.4) and (1.2), respectively. There is obvious relation (1.5) between them which means that the fields, u_+ and u_-, differ by $b/2$. As a result, the lattice passes from a stable to unstable configuration: some atoms are shifted from local wells to tops of a potential atomic relief, while others atoms, on the contrary, are shifted from tops to wells. It formally corresponds to the change in sign of interatomic forces. It is clear that these processes are accompanied by bond rearrangements and changes in the nearest neighbor environment of atoms. Such processes are beyond a description of the continuum mechanics.

The second (excited) configuration may be stabilized due to some boundary conditions. Therefore, both configurations will be considered next sections.

2. ELASTIC CRITICAL SHEAR

First, we will find solutions of Eqs. (1.4) and (1.5). From these equations one can find a critical elastic shear when plastic deformations are absent. Let us suppose that the critical elastic shear reaches a maximum value on the boundaries, such as

$$u_-(0,y) = -\frac{1}{2},$$
$$u_-(nH,y) = \frac{2n-1}{2}, \qquad (2.1)$$
$$n = \pm 1, 2, \ldots$$

Evidantly we have an interchain rigid shear (on the boundaries) by a *b/2*, with *b* being the interatomic distance. Inside of the layer of thickness *H*, the interchain shear is low. It becomes zero at some curve inside of the layer under consideration. The shear is elastic, because $u \le 1/2$. The solution obeying these boundary conditions is presented as (1.5), where u_+ is a solution of the Eq. (1.4). This equation may be solved by separation method [3] that gives us the following doubly periodic function to be the solution in question:

$$\operatorname{tang}\frac{\pi u_+}{2} = \frac{\pm \operatorname{tn}\frac{xK_1}{H}\operatorname{dn}\frac{yK_2}{B}}{A\operatorname{cn}\frac{yK_2}{B}},$$
$$A^2 = \frac{\nu_2}{\sqrt{1-\nu_1^2}}. \qquad (2.2)$$

Two signs in Eq. (2.2) correspond to two opposite equivalent directions of microshear.

Here 2*H* and 4*B* are periods of the functions figuring on the right-hand side of Eq. (2.2), i.e. the elliptic tangent (tn) and the elliptic cosine (cn), respectively. As for the delta-function of Jacoby (dn), it has the period 2*B*. K_1 and K_2 are the complete elliptic integrals of the first kind, which depend on the magnitudes of ν_1 and ν_2 in the conventional manner. Asymptotic behavior of the elliptic functions is as follow [4]:

$$K \to \ln\frac{4}{\sqrt{1-\nu^2}}, \quad \operatorname{tn} \to \sin x,$$
$$\operatorname{dn} \to \operatorname{cn}, \quad \operatorname{cn} \to \frac{1}{\cosh}, \quad \nu \to 1,$$
$$K \to \pi/2, \quad \operatorname{tn} \to \tan, \qquad (2.3)$$
$$\operatorname{dn}^2 \to (1-\nu^2\sin^2), \quad \nu \to 0.$$

Using the properties of the elliptic tangent function tn0 = 0 and $\operatorname{tn}K \to \infty$, one can see that solution (2.2) and (2.3) satisfies the boundary conditions (2.1).

Obviously, this solution is satisfied by periodic boundary conditions (with period 4*B*) along the *Y* axis. Thus we have double periodic solution and double periodic superstructure. It consists of rectilinear cells (domains) divided by domain walls or boundaries.

3. LOCAL STABILITY CONDITIONS

Periods of the superstructure are not arbitrary. They depend not only on ε, but on some properties of the lattice as well. Indeed, there are two algebraic relations, the so called dispersion equations derived in [5]. They may be realized by the substitution of the solution (2.2) and (1.5) into the Eq. (1.2). In doing so, we have

$$S\left(\frac{k_1K_1^2}{H^2A^2} + \frac{k_2K_2^2}{B^2}\right) = -2p,$$
$$S = (A^2-1)\left(1-\frac{\nu_2^2}{A^2}\right), \qquad (3.1)$$

$$\frac{k_1K_1^2}{H^2} = \frac{A^2k_2K_2^2}{B^2}, \qquad (3.2)$$
$$p \ge 0.$$

Equations (3.1) and (3.2) specify the existence conditions for the stable solution (2.2) and (1.5). A local stability is taken into account. Evidently, it takes place at *A*<1, because *p*>0.

The analysis of the relations under consideration allows one to reveal all points of structural transformations at arbitrarily large nonlinear displacements. One should exclude the constants of integration ν_1 and ν_2. These can be expressed through *H* and *B* using Eqs. (3.1) and (3.2). As a result, we obtain *A* as a function of *H* and *B*. The relations between *A*, *B* and *H* can be conveniently visualized by plotting

H as a function of B at various values of the bifurcation parameter A, which can be formally called the inverse amplitude of the displacement field, according to its position in the expression (2.2).

To each A value corresponds some (H vs. B) curve which has the only asymptote, $B = B_i$, and arrives at the terminal point H_c, B_c, approaching the asymptote in such a way that

$$H \geq H_c, \qquad B_c \leq B < B_i. \tag{3.3}$$

The limits are as follows:

$$H_c = \frac{\pi l_1 (1 - A^2)}{2A}, \qquad B_c = l_2 (1 - A^2) K_{22}, \qquad B_i = \frac{\pi l_2 \sqrt{1 - A^2}}{2}. \tag{3.4}$$

Here K_{22} is the value of the function $K_2(\nu_2)$ in the point $\nu_2 = A^2$. It is clear that not all values of H and B are allowable; obvious limitations follow these inequalities. The main result is that there are the upper limit of all lengths of modulation B. It equals to B_i, when $A = 0$, i.e. we have $B \leq (\pi l_2/2)$. As a corrollary, the only modulated microshear is stable as soon as inequalities (3.3) take place. As for a homogeneous elastic microshear ($B \to \infty$), it can not occur at all, because it does not satisfy either Eq. (3.3) or Eq. (1.2). Notice that the continuum theory of elasticity does not impose any restrictions on H and B. It is interesting to present the inequalities (3.3) in the following form:

$$\frac{\pi^2 k_1}{\dfrac{4H^2}{A^2}} (1 - A^2)^2 \leq p, \qquad \frac{k_2}{B^2} (1 - A^2)^2 K_{22}^2 \leq p, \tag{3.5}$$

$$k_2 \left(\frac{\pi}{2B} \right)^2 (1 - A^2) > p. \tag{3.6}$$

The first and second inequalities present the conditions of local stability of microdeformations. The third inequality is the criterion of their formation. In other words, the energy of nonhomogeneous elongation along Y-direction must exceeds potential barriers of a lattice due to the effect of incompatibility of neighbouring chains, as with the Frenkel-Kontorova's (one-dimensional) model. If it is not valid, microdeformations can not occur; only macrodeformations come into play. However, from Eq. (3.6) it follows that deformed configuration becomes stable, when barriers are large enough to prevent the destroying of the superstructure, the translational crystalline order.

Evidently, the wide spectra of mean space frequencies $1/B$ and $1/H$ are allowable, that is, a set of private solutions takes place. However, only some of these solutions are preferable under the action of an external macrofield. It will be demonstrated later.

4. BIFURCATION AND TEMPERATURE / DEFORMATION TRANSITIONS

If inequalities (3.5) are not realized, a transition of the initial lattice structure into a new structure (with the new topology) can occur. This process is going through some bifurcation point where a continuum model is effective. If the crystalline potential p tends to zero (due to temperature, for example), then the set of Eqs. (2.4) and (2.5) becomes a uniform homogeneous system of two variables, $H^2/k_1 K_1^2$ and $B^2/k_2 K_2^2$. If these variables become zero (trivial solution) - which is not physically meaningless - solution (2.2) corresponds to a uniform shear in a continuum. A nontrivial solution of Eq. (2.4) and (2.5) can be found by equating the corresponding determinant to zero, i.e.

$$S = 0. \tag{4.1}$$

With the corresponding expression for S in (3.1), we find two roots of Eq. (4.1):

$$A = 1, \quad \nu_1^2 + \nu_2^2 = 1; \qquad A = 1, \quad \nu_1 = 0, \quad \nu_2 = 1 \tag{4.2}$$

Under these conditions, (2.2) degenerates into a series of partial solutions, in which case some solutions coincide with those in the continuum model (nonuniform shear), while other soltions do not. Without going into details, we focus ourselves on a more essential aspect of the problem. Indeed, at $A = 1$, there is a bifurcation of solutions. At this point, from the left-hand side of equation (2.4) we have S=0. The same situation occurs when the crystalline potential $p = 0$. As mentioned above, this situation implies a transition from a minimum to maximum of energy functional, i.e. from a stable to unstable lattice configuration. It becomes stable at $A > 1$, if one shifts the microdisplacement by 1/2, according to (1.5). The aforesaid will allow us to construct a new solution of elasto-plastic deformation in the following.

Essentially, a similar bifurcation occurs when the crystalline potential does not change, but some parameters reach some asymptotic values. Let us define effective potentials as follows:

$$P_1 = \frac{pH^2}{k_1K_1^2} = \left(\frac{H}{K_1l_1}\right)^2,$$
$$P_2 = \frac{pB^2}{k_2K_2^2} = \left(\frac{B}{K_2l_2}\right)^2. \qquad (4.3)$$

These potentials may become zero at constant p when either $H^2/k_1K_1^2$ or $B^2/k_2K_2^2$ becomes zero, which corresponds to the transition to the continuum field u, because $S = 0$. Then we have two acoustic modes (U, u). In spite of the interaction between sublattices ($p \neq 0$), they are deformed as two continua. With the new designations, the dispersion relations (2.4) and (2.5) take the following form

$$-S = P_2 = A^2P_1 \quad \text{or}$$
$$-S\left(\frac{K_1}{A}\right)^2 = \left(\frac{H}{l_1}\right)^2,$$
$$-SK_2^2 = \left(\frac{B}{l_2}\right)^2. \qquad (4.4)$$

It is evident that the bifurcation point (A =1 or S = 0) can be attained, but only asymptotically, when the effective potentials (at constant p) are defined by (4.3) and tend to zero. If atomic potential p characterizes stability of the undeformed rigid lattice in response to shear, the values P_1 and P_2 can be thought of as being potentials (or stability) of the collective interaction between chain segments of length H and B belonging to neighbouring deformed chains or stability (strength) of deformed lattice. The transition from individual to collective potentials is associated also with deformation-induced changes of translational order in the system, in which case the atomic-scale periodicity gives rise to a mesoscopic-scale structure with larger periods.

Let us analyze the second conditions in (4.4). They demonstrate universal scaling effects – the ratio of lengths (H/l_1 or B/l_2) is a function of $S \sim (A^2\text{-}1)$, i.e. of a "distance" from bifurcation point $A = 1$. In other words, a decrease in similitude takes place. The left-hand side parts of these conditions are the scaling parameters. Taking into account that $l = (\sqrt{k/p})$ is a function of temperature, one can say that a bifurcation point (transition from region A <1 to region A >1) may be reached due to temperature ($p = 0$) as well as due to deformation ($A = 1$), according to (4.4) described by our model. All processes obey these universal conditions.

The first and second two conditions in (4.4) demonstrate anisotropy of domain form. Each of them (H- and B- domain) have different scale parameters such that $Bl_1/Hl_2 = A(K_2/K_1)$.

5. ELASTO-PLASTIC SHEAR WITH SLIDING

If the bifurcation point $A = 1$ is overcome, then the solution (2.2) becomes unstable. However, this solution can be modified, for A >1, by removing translation $b/2$ from (1.5). Then one can have

$$\operatorname{tang}\frac{\pi u_-}{4} = \frac{\pm \operatorname{tn}\dfrac{xK_1}{H}\operatorname{dn}\dfrac{yK_2}{B}}{A\operatorname{cn}\dfrac{yK_2}{B}},$$
$$A^2 = \frac{\nu_2}{\sqrt{1-\nu_1^2}}. \qquad (5.1)$$

In this case the other boundary conditions may be satisfied. Using the properties of the elliptic tangent function tn0 = 0 and tn$K \to \infty$, one can see the following:

$$u_-(0,y) = 0, \quad u_-(nH,y) = m \quad m, n = \pm1,2,\ldots \qquad (5.2)$$

It is obviously that we deal with a rigid interchain shear (sliding) by one interatomic distance b on the boundaries, $x = +nH$ and $x = -nH$. However, the interchain shear becomes zero at $x = 0$. If $u_- \leq 1/2$, then plastic deformations are negligible, in which case elastic shear occurs. It takes place in some zone near the boundary $x = 0$. The elasto-plastic frontier is defined by a condition $\operatorname{tn}((\pi u)/2) = 1$. However, it is not rectilinear. Rearrangements of interatomic bonds occur in the two plastic regions and do not in the elastic region.

It is interesting that sliding is irregular, because the microfield $u_-(x,y)$ is not uniquely defined by formula (5.1); m may by a stochastic function of n. In these circumstances, the so called shuffling mode of plastic deformation, as in the theory of martensite transitions, takes place.

Obviously, the solution (5.1) is satisfied by periodic boundary conditions (with period $4B$) along the Y axis. Thus we have double periodic solution and double periodic superstructure. It consists of rectilinear cells (domains) divided by domain walls

or boundaries. They consist of Frenkel-Kontorova's solitons or misfit solitons. It is possible that due to them but dislocations the above mentioned shuffling mode may be realized due to such misfit solutions (instead of dislocations).

The periods of the superstructure depend on the external field e or s (in the elastic case they depend on the properties of lattice). Indeed, there are two algebraic relations, the so called dispersion equations. They may by derived by the substitution of the solution (5.1) to the equation (1.2). In doing so, we have

$$S\left(\frac{k_1K_1^2}{H^2A^2}+\frac{k_2K_2^2}{B^2}\right)=2p,$$
$$S=(A^2-1)\left(1-\frac{\nu_2^2}{A^2}\right), \tag{5.3}$$

$$\frac{k_1K_1^2}{H^2}=\frac{A^2k_2K_2^2}{B^2}, \tag{5.4}$$
$$p\geq 0.$$

The first condition is different from (2.4) only by the sign of the right-hand side. Therefore, it is satisfied by the inequality $A > 1$. Both expressions specify the existence conditions for the stable solution (5.1). In doing so, the local stability is taken into account. The global stability will be considered later.

As for the conditions (4.3) and (4.4), they get opposite signs before the value S only. One can use the total conditions introducing notation IISII for the absolute value. Then, in both the cases discussed, we have

$$\|S\|=A^2P_1=P_2. \tag{5.5}$$

Evidently, the universal scale principle is valid in the case A >1, too.

The analysis of the relations in question allows one to reveal all points of structural transformations at arbitrarily large nonlinear displacements. In this case, one should exclude the constants of integration ν_1 and ν_2. These can be expressed through H and B using (5.3) and (5.4). As a result, we obtain A as a function of H and B. The relations between A, B and H can be conveniently visualized by plotting H as a function of B at various values of the bifurcation parameter A.

To each A value some (H *vs.* B) curve corresponds, which resembles a hyperbola with the asymptotes given by

$$H>H_t,\quad H_t=(l_1(A^2-1)K_{11})/A^2, \tag{5.6}$$

$$B>B_t,\quad B_t=\frac{\pi}{2}l_2\sqrt{A^2-1}. \tag{5.7}$$

Here K_{11} is the value of the function $K_1(\nu_1)$ in the point $\nu_1=\sqrt{1-1/A^4}$.

The domain square HB is minimal when H and B are approximately equal to each other and larger then H_t and B_t. The density of energy E/BH is maximal when the square HB is minimal. It is obvious that the very anisotropic domains are preferable. If $B\to\infty$, than $H\to H_t$. As for the last value, it corresponds to the minimum of the total energy E/BH. Short periods B are impossible. There is an essential difference from the elastic case A<1. This rather simple results are realized when A^2>2. For A^2<2, the coexistence region takes place where short domains ($B < (\pi l)/2$) are formed.

Energetic restrictions become visible, if one presents (5.7) and (5.6) in the following form:

$$k_1\frac{K_{11}^2}{H^2}\left(1-\frac{1}{A^2}\right)^2<p,$$
$$\left(1-\frac{1}{A^2}\right)^2<P_1<\left(1-\frac{1}{A^2}\right), \tag{5.8}$$

$$k_2\left(\frac{\pi}{2B}\right)^2(A^2-1)<p,$$
$$\frac{(A^2-1)^2}{A^2}<P_2<(A^2-1). \tag{5.9}$$

It is evident that the elasto-plastic deformation becomes stable and a long-scale translation order exists, if the atomic potential barriers exceed a local deformation energy; the right-hand side of this inequalities. The second inequalities in (5.8) and (5.9) are presented via effective potentials P_1 and P_2. They give us the criteria of microstructure stability. If the second inequalities in (5.8) and (5.9) are not satisfied, deformations destroy the translational order completely. If $A\approx 1$, both effective barriers stabilizing the structure are low. When $A >> 1$, there is just a very high barrier P_2, i.e. very stable long domains exist.

6. INTERACTION OF MODES AND STABILITY UNDER ACTION OF EXTERNAL FIELD

The equation (1.2) does not contain macrodeformations ε and macrodisplacements *U*. They depend on equilibrium conditions for macroscopic body and, generally speaking, play the role of "external field" for the microdeformations. In papers [1,2] we considered the problem without external fields. Indeed, the expression (1.1) may be presented after integration as

$$\frac{\bar{E}}{BH} = \frac{\bar{k}_1\left(\varepsilon^2 - \dfrac{2\varepsilon\delta u b}{H}\right)}{2} + \frac{E}{BH}, \tag{6.1}$$

$$E = \int_0^H \int_0^B \left[\frac{1}{2}k_1\left(\frac{\partial u}{\partial x}\right)^2 + \frac{1}{2}k_2\left(\frac{\partial u}{\partial y}\right)^2 + p(1-\cos 2\pi u)\right] dxdy. \tag{6.2}$$

Here $\bar{k}_1 = k_1/b^2$ denotes the macroscopic shear modulus, and δu the difference of values of microdisplacements on neighbouring boundaries, for example, for $x = 0, H$. In the cases considered below, we have $\delta u = 1$. Then $(1/H)$ is a mean microdeformation per a half period H. However, one can accept $\delta u = -1$ supposing the opposite sign of microshear, i.e. $-(b/H)$.

The second (crossed) term in (6.1) means that micro and macrodeformations are mutually dependent. Let us define the macrostresses σ as follows:

$$\sigma = \frac{\partial\left(\dfrac{\bar{E}}{HB}\right)}{\partial\varepsilon} = \bar{k}_1\left(\varepsilon - \frac{b}{H}\right). \tag{6.3}$$

Taking into account that $\delta u = 1$, we find that the first and the second terms in the brackets are the inner and external deformations, respectively. The external deformation is evidently equal to $\partial U/\partial x$. If the microdeformations are absent, we have macrofields, σ and ε, only.

We suppose that the interaction between the macrofield and the longitudinal modulations is absent, because the mean microdeformations are zero. In these circumstances, the modulations must be generated spontaneously in accordance with the energy minimum conditions:

$$\frac{\partial\left(\dfrac{E}{BH}\right)}{\partial B} = 0, \qquad \frac{\partial^2\left(\dfrac{E}{BH}\right)}{\partial B^2} > 0. \tag{6.4}$$

If the conditions (6.4) are valid, one can find an equilibrium value of modulation half period $2B_m$. Thus, in the elastic case ($A < 1$) $B_m = B_c$. For $A > \sqrt{2}$, $B_m \to \infty$. Let us consider the case with $A < 1$. In this case, B_m should be substituted to Eqs. (6.1) and (6.2). Then we have the energies E_m and $\bar{E}_m$ as some functions of two variables, H and ε. This allows one to define the mean microdeformation b/H as a function of ε or σ.

Let us establish the relation between them. In doing so, we suppose that external microstresses are absent, i.e.

$$\frac{\partial\left(\dfrac{\bar{E}_m}{HB_m}\right)}{\partial\left(\dfrac{b}{H}\right)} = -\bar{k}_1\varepsilon + \frac{\partial\left(\dfrac{E_m}{HB_m}\right)}{\partial\left(\dfrac{b}{H}\right)} = 0. \tag{6.5}$$

It is the necessary condition of an extremum of the total energy. It can be re-written as the following condition of equilibrium between macro and microfields:

$$\varepsilon = \frac{1}{\bar{k}_1}\frac{\partial\left(\dfrac{E_m}{B_m H}\right)}{\partial\left(\dfrac{b}{H}\right)}. \tag{6.6}$$

This equation allows us to define the second period H as a function of ε.

Now let us consider some conditions of the superstructure stability in a macrofield as a function of two variables, ε and (b/H). In doing so, one should accept

$$D = \bar{k}_1\frac{\partial^2\left(\dfrac{E_m}{B_m H}\right)}{\partial\left(\dfrac{b}{H}\right)^2} - \bar{k}_1^2 > 0. \tag{6.7}$$

where D is the determinant of (2x2) matrix with elements being second derivatives of the total energy E_m. If

$k_1 > 0$,

$$\frac{\partial^2\left(\frac{E_m}{HB_m}\right)^2}{\partial\left(\frac{B}{H}\right)^2} > 0, \qquad (6.8)$$

the energy density E_m/BH is minimal.

In this situation, Eq. (6.6) plays the role of the condition of stable equilibrium between micro and macrodeformations. In other words, Eq. (6.6) defines mean microdeformations induced by an external "macrofield" ε. As a corollary, the value of thickness H is not arbitrary. Equilibrium thickness depends on ε and the lattice properties. It means that real rigid boundaries do not exist; there is the induced superstructure with inner "boundaries".

Using the condition (6.6) in (6.3), the macrostresses may be represented only via mean microdeformations as follows:

$$\sigma = \frac{\partial\left(\frac{E_m}{B_m H}\right)}{\partial\left(\frac{b}{H}\right)} - \frac{\bar{k}_1 b}{H}. \qquad (6.9)$$

It is the condition of the microshear generation in an external field of shear stresses. With b/H given by formula (6.6) and substituted into formula (6.9), σ as a nonlinear function of ε may be derived due to microdeformations.

The analysis of the function $E_m(H)$ shows the following: if $b/H = 0$, Eq. (6.6) gives a critical value of external "field" ε_t. Otherwise, the forced microdeformations occur, when the external "field" reaches a threshold which is as follows:

$$\varepsilon_t = \left[\frac{\partial\left(\frac{E_m}{B_m H}\right)}{\partial\left(\frac{b}{H}\right)}\right]_0. \qquad (6.10)$$

Here the index "0" on the r.h.s. of formula (6.10) means that either $b/H = 0$ or $H \to \infty$. For the spontaneous microdeformations, we have $\varepsilon_t = 0$. Notice that function $(E_m/B_m H)$ monotonically increases with rising (b/H). It means that microdeformations occur, if

$$\varepsilon \geq \varepsilon_t. \qquad (6.11)$$

Thus, in the framework of the proposed model, there are the two, macroscopic and microscopic, deformation modes, when the threshold (6.11) is reached. Then a lattice is decomposed into two sublattices, in which case microdisplacements occur. As it is well known for the ionic crystals, the electric field decomposes the lattice into two sublattices due to the splitting of charges.

Obviously, the wide spectrum of mean space frequencies $1/B$ and $1/H$ is allowed, i.e. a set of partial solutions takes place. However, only some of the partial solutions are preferable. Indeed, the expressions (6.4) or (6.6) define a single pair of periods B_m and H, if the macrofield ε or σ is fixed ($A < 1$). In the case with $A > \sqrt{2}$, we have $H = H_t$ and $B \to \infty$.

7. CONCLUSIONS

In this work we analyzed the extralarge relative displacements of atomic chains, i.e. the pseudo optical deformation mode. It can be resulted from instability of lattice. In these circumstances, some inner boundaries of shear sliding and spatial modulations appear.

If $u \leq 1/2$, an elastic nonuniform shear occurs. Then microdeformations destroy translational symmetry of a lattice at mesoscopic scales. Some global symmetry appears as a superstructure or a domain structure with periods $2H$ and $4B$. Transversal boundaries consist of Frenkel-Kontorova's solitons distant by $2B$. Microdeformations are inhomogeneous. They destroy translational lattice order at the nanoscale only inside the domains. Domains form the superstructure with large periods. When the external macrodeformations e exist, the interaction between the acoustic and pseudo optical modes takes place. In this situation, one pair *(B,H)* corresponds to the local and global stable superstructure which is formed when some threshold e_t is reached. It is the first bifurcation point.

The second bifurcation point is realized when parameter $A \to 1$. In this situation, the local stable pseudo optical mode is realized, if $u \geq 1$ on parallel boundaries distant by $2H$. Then the elastoplastic microshear takes place. The superstructure takes place, too, but the nearest atomic order is changed due to depinning. In other words, a catastrophic transformation of lattice occurs without destroying. The microdeformation (pseudo optical mode) is generated under the action of macroscopic shear deformation (acoustic mode), when some threshold is overcome. The aforesaid problems have been

analysed here using the exact solutions of the equilibrium equation of sine-Helmholtz type.

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