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Essentially nonlinear theory of microdeformations in medium with periodic structure

E. L. Aero *

Abstract

Essentially nonlinear theory of micro and macro deformations of a medium with cardinally rearranging periodic structure is presented using a new model of double continuum with variable local topology. In a frame of proposed model there are two deformation modes (macroscopic and microscopic) when some threshold is reached. Some problems such as twin transitions, catastrophic deformation waves, shock and tilting bifurcation waves are considered. An exact solution describing elasto plastic fragmentation of medium is constructed also when double periodic domain superstructure are formed. There are solid rotons of opposite signs with singular defects between them. They appear in a critical field of macroscopic deformations of pure shear. When this bifurcation point is overcome then dimensions of domains are stabilized. The letter depend on value of macroscopic deformations. Some criterion of global stability is established.

1 Introduction

One of postulate in a classical continuum theory of deformation is that a local topology remains unchanged - the nearest environment of each

*Institute of Mechanical Engineering Problems, Russian Academy of Sciences, St. Petersburg, Russia (e-mail: aero@microm.ipme.ru)

material particle is conserved without any rearrangement of interatomic bonds.

Using a continual model as smooth manifold it is possible to construct elegant theory of elasticity. But now it is not adequate conception. intrinsically is connected with rather complex phenomena such as plasticity, defects formation, phase transitions, damage and other structural rearrangements. It is evident that local topology cannot be conserved and must be introduced in a model directly.

If these processes are possible due to cooperative but no diffusion atomic rearrangements (ex. mastering transitions, twinning, etc.) then deformation theory may be developed but in some generalized form.

Some attempts to generalize the model of smooth manifold was connected with introduction of inner degrees of freedom. It seems to be adequate but as it became clear later not in linear approximation [1,2]. Small distortions of inner structure directly connected with small deformations and may by excluded - a complex model may be reduced to a model with a simple structure (smooth manifold).

A phenomenological theory of elasticity may be derived from linear microscopic theory [2] of crystalline lattice as a long wave approximation. Introduction of inner degrees of freedom is possible in the last one using the model of complex lattice consisting of two or more sublattices. As a result additive modes of vibration (optical modes) may be predicted.

In spite of it in linear theory local topology variations cannot be introduced. New effects are space-time dispersion of elastic properties, scale and boundary effects at most [1,2]. Only essentially nonlinear deformations when some bifurcations are achieved and overcome may realize cardinal structural rearrangements.

Let us consider at the beginning a model of complex lattice consisting of two sublattices (Fig.1).

Then in the linear theory of crystalline bodies [2,3] two equations may be introduced - for so called acoustic and optical modes. In harmonic approximation for an energy Φ of pair interactions of atoms one has

$$\Phi = \sum_{nl} \sum_{pq} \bar{\alpha}_{pq}(n-l)\vec{U}_p(n)\vec{U}_q(l) \tag{1.1}$$

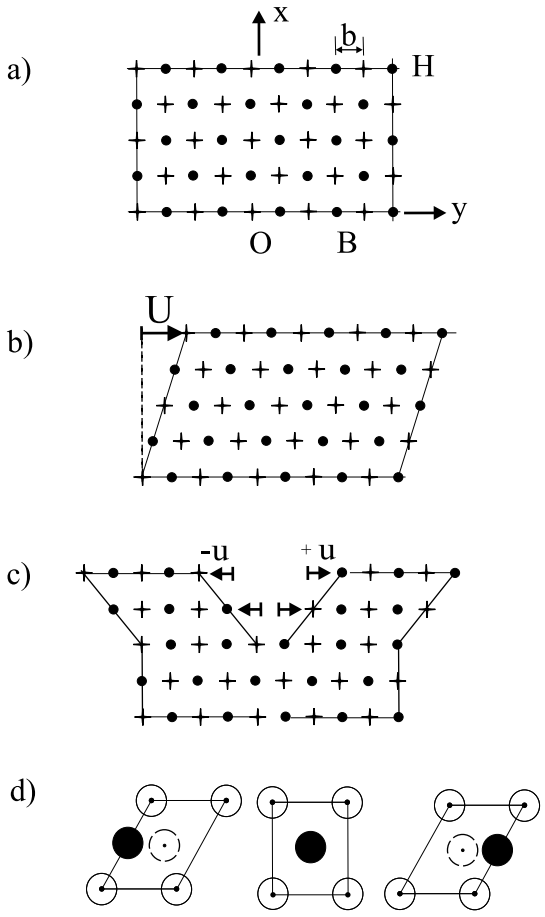

Figure 1:

Here the second rank tensors $\bar{\alpha}_{pq}(n-l)$ (marked by upper bars) are force constants of atoms $n \quad l$, belonging to sublattices p and q Besides $\vec{U}_p$, $\vec{U}_q$ are displacements of atoms including to sublattices p and q respectively. In our case $p, q \to 1, 2$.

Then one has two equations of motion of atoms of both sublattices

$$m_1 \partial^2 \vec{U}_1(n)/\partial t^2 \; = \; -\sum_{l,q} \bar{\alpha}_{1q}(n-l)\vec{U}_q(l), \; (q=1,2), \tag{1.2}$$

$$m_2\partial^2\vec{U}_2(n)/\partial t^2 \;=\; -\sum_{l,p}\bar{\alpha}_{2p}(n-l)\vec{U}_p(l),\ (p=1,2). \tag{1.3}$$

Here m_p is a mass of an atom n belonging to the sublattice p.

After all some procedure of continualization is realized. In this connection one supposes that neighboring atoms (belonging to a single sublattice!) undergo to small displacements. In this case each sublattice is deformed as continuum (smooth manifold) without rearrangement of nearest order. But the neighboring atoms belonging to different sublattices may undergo to great displacements! This interesting possibility was not used in classic linear theories.

After this procedure one has a model of complex continuum consisting of two subcontinua. But each of them is not proper continuum but pseudo continuum because they must penetrate to each other without concur of their points!. They are two compatible manifolds as well as compatible two sublattices. Instead of single smooth manifold one has so called double (complex) manifold consisting of two pseudo continua. A correct definition of a pseudo continuum was done in [1] but interesting possibilities of double manifold were not used.

By the way it is possible to introduce a smooth differentiable function of displacements of particles in each pseudo continuum.

By definition

$$\vec{U}_p(n) \;=\; \vec{R}_p(n)-\vec{r}_p(n) \;=\; \vec{U}_p(\vec{r}) \;=\; \vec{U}_p(\vec{R}_p) \tag{1.4}$$

Here $\vec{R}_p(n)$ and $\vec{r}_p(n)$ define position of atom n belonging to a lattice p in reference and actual configuration respectivly.

If a function $\vec{U}_p$ is smooth it may be presented as Tailor series in vicinity of an arbitrary point $\vec{r}$ of sucontinuum p

$$\vec{U}_p(\vec{r}+\delta\vec{r}) \;=\; \vec{U}_p(\vec{r})+\delta\vec{r}\nabla\vec{U}_p(\vec{r})+\frac{1}{2}\delta\vec{r}\delta\vec{r}\nabla\nabla\vec{U}_p(\vec{r})+\vec{O}(\nabla^3),\ (p=1,2) \tag{1.5}$$

Here ∇ is vectorial gradient operator.

Using this expansion in discrete equations (1.2),(1.3) one has its continual approximation

$$m_1\partial^2\vec{U}_1/\partial t^2 \;=\; \sum_q (c_{1q}\vec{U}_q + C_{1q}\nabla\vec{U}_q + \Lambda\nabla\nabla\vec{U}_q) + O_1(\nabla^3), \quad (q=1,2) \tag{1.6}$$

$$m_2\partial^2\vec{U}_2/\partial t^2 \;=\; \sum_p (c_{2p}\vec{U}_p + C_{2p}\nabla\vec{U}_p + \Lambda\nabla\nabla\vec{U}_p) + O_2(\nabla^3), \quad (p=1,2) \tag{1.7}$$

Let us introduce new functions: U-a displacement of center of inertia of elementary cell (pair of different atoms) and u- a relative atomic displacement (inner displacement) in such a way

$$\vec{U} \;=\; (m_1\vec{U}_1 \,+\, m_2\vec{U}_2)/(m_1 \,+\, m_2), \qquad \vec{u} \;=\; (\vec{U}_1 \,-\, \vec{U}_2)/b \tag{1.8}$$

Then instead of (1.6), (6.2) one has equations

$$\rho\partial^2\vec{U}/\partial t^2 \;=\; \tilde{c}\nabla\vec{u} \,+\, \hat{\lambda}\nabla\nabla\vec{U} \,+\, O_1(\nabla^2\vec{u},\, \nabla^3\vec{U}) \tag{1.9}$$

$$\mu\partial^2\vec{u}/\partial t^2 \;=\; -\tilde{c}\nabla\vec{U} \,-\, \bar{p}\vec{u} \,+\, \hat{k}\nabla\nabla\vec{u} \,+\, O_2(\nabla^2\vec{U},\, \nabla^3\vec{u}) \tag{1.10}$$

Here ρ is a mean density of two atomic masses, μ - a density of reduced mass, v - a volume of elementary cell:

$$\rho \;=\; (m_1 \,+\, m_2)/v, \qquad \mu \;=\; m_1m_2/(m_1 \,+\, m_2)v \tag{1.11}$$

Mutual displacement of two different atoms $\vec{u}$ will be mesured in units of b - period of sublattice (Bravai lattice). Then $|\vec{u}| = 1$ means mutual displacement of sublattices on one period.

Besides in equations (1.9), (1.10) there are coefficients - tensors: $\bar{p}$ (the second rank), $\tilde{c}$ (the third rank) and $\hat{k}$, $\hat{\lambda}$ (the fourth rank). In addition O_1, O_2 -high gradient members which will not be taking into account in long wave approximation such as

$$O_1 \;=\; \hat{C}_1\nabla\nabla\vec{u} \,+\, \Lambda\nabla\nabla\nabla\vec{U} \,+\, \ldots \tag{1.12}$$

$$O_2 = \hat{C}_2 \nabla\nabla\vec{U} + K\nabla\nabla\nabla\vec{u} + \dots \quad (1.13)$$

Here $\hat{C}_1, \hat{C}_2$ - material tensors of the fourth rank and Λ, K - tensor of the fifth rank.

Let us consider for the first time (1.9), (1.10). The first members at right are crossed members due to local mode interaction. They exist only for crystal without center of symmetry.

Some crossed high order members presented in (1.12), (1.13). They dont equal to zero for crystals without center of symmetry due to even rank of tensors $\hat{C}_1, \hat{C}_2$.

The first equation (of acoustic vibrations) (1.9) contains only gradient members at right. It means that only long range forces are taken into account.

The second equation of microvibrations (1.10) contains gradientless member (the second at right). This member presents short range interactions between neighboring different atoms in elementary cell. A microdisplacement vector $\vec{u}$ give us nearest order (local topology) distortion - structural rearrangement. In linear theory this variation may be expressed through macroscopic gradients $\nabla\vec{U}$ using eigenfunctions. Then microscopic gradients may be excluded from the first equation (1.9). As a result the first equation (1.9) may be reduced to a macroscopic equation of classi continuum if one neglects of high gradient members O_1. Then a field U give us a distortion of macroscopic dimension of a body, i.e. its external geometry. It returns us to a classic model of medium.

2 General equations

Inner degrees of freedom may be effective for local topology if in a frame of a model of complex lattice (and double continuum) one introduces essentially nonlinear short range interactions. It may be achieved due to following generalization of (1.9).

Let us consider arbitrary microdisplacements of sublattices $\vec{u}$. Then one must exchange linear member in it by nonlinear $\vec{P}(\vec{u})=-\vec{P}(-\vec{u})$. The main idea that due to inner translation symmetry of complex

lattice this vectorial function must be periodic one. Its period is equal to the period of mutual translation of sublattices $\vec{b} = const$.

Then instead of (1.9), (1.10) one has the following equations

$$\rho\partial^2\vec{U}/\partial t^2 \,=\, \tilde{c}\nabla\vec{u} \,+\, \hat{\lambda}\nabla\nabla\vec{U} \,+\, O_1(\nabla^2\vec{u},\, \nabla^3\vec{U}) \qquad (2.1)$$

$$\mu\partial^2\vec{u}/\partial t^2 \,=\, -\tilde{c}\nabla\vec{U} \,-\, \vec{P}(\vec{u}) \,+\, \hat{k}\nabla\nabla\vec{u} \,+\, O_2(\nabla^2\vec{U},\, \nabla^3\vec{u}) \qquad (2.2)$$

Here the members O_1, O_2 may be presented as (1.12), (1.13). The value $\vec{u}$ is dimensionless -in units of lattice period b in any direction. Therefore it is pure number, integer. So if $P \to \sin(2\pi u)$, then the displacement $u = |\vec{u}| = 1$ corresponds to mutual translation of sublattices on one period. It is transition to an equivalent state of structure if and only if it takes place in homogeneous and endless medium. However this transition is accompanied by switching of atomic bonds and may form a new body with other boundaries. If $1/2 < |\vec{u}| < 1$, then nearest neighboring of each atom is rebuilt and a new structure is formed. It means that for cardinal variation of local topology essentially nonlinear effects are necessary.

Note that a vectorial periodic function $\vec{P}(\vec{u})$ may be constructed as a derivative of scalar periodic function E (energy) with respect to components of vector $u_i, (i \to x, y, z)$

$$P_i \,=\, \partial E/\partial u_i, \qquad I_1 = (\vec{u}\vec{l_1}),\; I_2 = (\vec{u}\vec{l_2}),\; I_3 = (\vec{u}\vec{l_3}). \qquad (2.3)$$

Here l_1, l_2, l_3 - cristallographic basic vectors and u_1, u_2, u_3 -their scalar products with $\vec{u}$.

Thus, in the frame of double continuum model the equations of motion of a medium with variable local topology are presented by relations (2.1), (2.2), (1.12), (1.13).

It is worthwhile to analyze media with center symmetry and without it as two special cases.

3 Some effects in media without center of symmetry

In that case it is necessary to take into account the cross members in these equations. The problem is not simple for analysis. Let us consider only long wave approximation neglecting gradient members in (2.2). It means that one disregards inner boundaries- between domains, for example. Then it is correct to neglect by microinertia too and one has the following equations

$$\rho\ddot{U}_i \;=\; c_{ikj}u_{k,j} \;+\; \lambda_{ikjm}U_{k,jm}, \tag{3.1}$$

$$0 \;=\; -P_i \;-\; c_{kij}U_{k,j} \;-\; \hat{c}_{kij}u_{k,j}. \tag{3.2}$$

Here a superimposed dot indicates the time derivative and the space derivative is denoted by coma in indexes as usual. It is possible to rewrite the first as the equation of classic theory of elasticity

$$\rho\ddot{U}_i \;=\; \bar{\sigma}_{ij,j}, \tag{3.3}$$

if one considers the expression

$$\bar{\sigma}_{ij} \;=\; \lambda_{ikjm}U_{k,m} \;+\; c_{ikj}(u_k - u_k^o) \tag{3.4}$$

as an effective stress tensor. Here $u_k^o = const$ (integration constant) is a collinear to u_k vector or its integer part which dont varies a crystal structure. This constant may be neglected if $|u_k| \leq 1$.

3.1 Structure transitions and bifurcations in static case

In two dimensional static case ($U = U(x, y)$) the equation (3.3) may be solved after introduction of so called Ary function ψ

$$\begin{gathered}\sigma_{xx} = \partial^2\psi/\partial y^2,\ \sigma_{yy} = \partial^2\psi/\partial x^2,\ \sigma_{xy} = -\partial^2\psi/\partial x\partial y,\\ \nabla\nabla\nabla\nabla\psi = 0.\end{gathered} \tag{3.5}$$

Consider more simple case of one-component displacements along OY axe when

$$u_y \;=\; u(x,y), \qquad P_y \;=\; p\,sin(2\pi u), \qquad U_y \;=\; U(x,y). \tag{3.6}$$

Then the equations may be presented as

$$\bar{\sigma} \;=\; \lambda\,\varepsilon \;-\; c\,(u \;-\; u^o), \qquad 0 \;=\; p\,sin(2\pi u) \;+\; c\,\varepsilon \tag{3.7}$$

Here $2\varepsilon \;=\; U_{y,x}$ and $\bar{\sigma} \;=\; \bar{\sigma}_{xy}$ -shear strain and stress, $c \;=\; c_{yyx}$. In the second equation (3.7) the additive $\hat{c}_{yyx}u_{y,x}$ is not presented due to tensor antisymmetry ($\hat{c}_{kij} \;=\; -\hat{c}_{ikj}$).

Let us analyze the expression for the effective stress tensor as a function of a strain only. Using the second equation in (3.7) one can present $\bar{\sigma}$ in such a way

$$\bar{\sigma} \;=\; (\lambda p/c)\,e \;-\; c\,arcsin\,e, \quad e \;=\; \varepsilon/\varepsilon_{b2},\; \varepsilon_{b2} \;=\; p/c. \tag{3.8}$$

This function is presented at the Figure 2 under the condition

$$\gamma \;=\; p\lambda/c^2 \;>\; 1 \tag{3.9}$$

The curve is a hysteresis loop. The upper branch corresponds to deformation of a primary structure. It reaches the limit of its stability

$$e_{b1}^2 \;=\; 1 \;-\; 1/\gamma^2 \tag{3.10}$$

The lower branch corresponds to unloading of the secondary structure. Between them there is some transient unstable structure due to state bifurcation. The second threshold $e \;\rightarrow\; 1$ means that $\varepsilon \;\rightarrow\; \varepsilon_{b2} \;=\; p/c$. Obviously, ε_{b2} is the limit of solidity of a lattice. A lattice cannot withstand the greater deformations. The square of the loop corresponds to latent energy reserved in the secondary structure - inelasticity effect of structure rearrangement takes place.

A process of unloading is completed when deformation reaches the value $e \;=\; e^p$. i.e. residual inelastic deformation. It is a macroscopic measure of the structure rearrangement. One finds a microscopic measure with the help of (3.7) if take into account there $\bar{\sigma} \;=\; 0 \;\rightarrow\; e \;=$

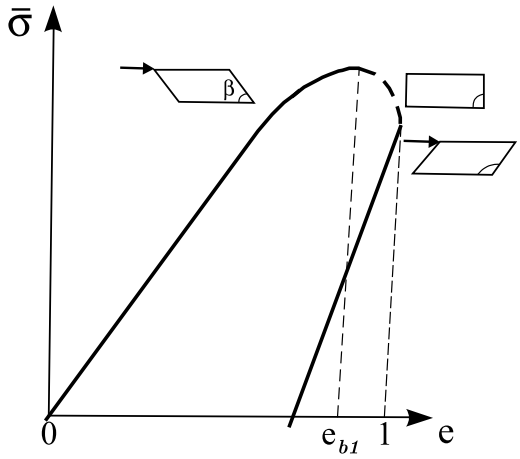

Figure 2:

$e^p, u = u^p$ by definition. Then $e^p = (c^2/p\lambda)(u^p - u^o)$, i.e. microscopic measure of rearrangement is local mutual translation of sublattices!

As an example of this structure transition may be twinning, i.e. transition of a crystal to a mirror-like state.

Structure bifurcations may be demonstrated due to effective pseudo elastic modulus

$$\Lambda = \partial\bar{\sigma}/\partial\varepsilon = \lambda - c(arcsin\, e)_{,e} = \lambda - +1/\sqrt{(}1 - e^2). \quad (3.11)$$

Here $()_{,e} \rightarrow \partial()/\partial e$. Two signs before radical correspond to two branches at the Fig. 2. At the Fig. 3 the both stable branches ($\Lambda > 0$) are presented by solid curves. A dashed curve is unstable transient part ($\Lambda < 0$). It corresponds to inelastic process.

The effective modulus Λ is an essential characteristic of dynamic processes too.

4 Stationary waves of structure rearrangements

Let us consider one-component and one-dimensional motion

$$U_i \rightarrow U(x,t), \qquad u_i \rightarrow u(x,t). \quad (4.1)$$

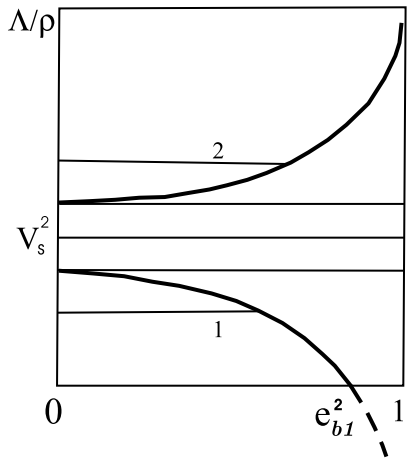

Figure 3:

Directions of vectors $\vec{U}, \vec{u}$ are arbitrary but fixed. Then ε may be considered as shear or stretch deformation. Then equations of motion (3.1), (3.2) may be rewritten as

$$\rho\ddot{U} \;=\; \lambda U_{,xx} \,+\, c\, u_{,x}, \tag{4.2}$$

$$0 \;=\; c\, U_{,x} \,+\, p\, sin(2\pi u). \tag{4.3}$$

After differentiating with respect to x and excluding u from the first one has

$$\rho\, \ddot{e} \;=\; [\lambda\, e \,-\, (c^2/p)\, arcsin\, e]_{,xx}, \tag{4.4}$$

$$0 \;=\; e \,+\, sin(2\pi u), \qquad e \,=\, \varepsilon/\varepsilon_{b2},\, \varepsilon_{b2} \,=\, p/c. \tag{4.5}$$

The first equation is quasi linear equation for deformation waves. The simplest solution is stationary wave $e(q)$ and q -its phase

$$q \,=\, k(x \,-\, Vt), \quad V > 0, \quad V < 0. \tag{4.6}$$

Two signs correspond to two waves running into opposite directions.

Due to (4.6) one has ordinary differential equation

$$[(V^2 - V_s^2)\, e \,+\, V_c^2\, arcsin\, e]_{,qq} \;=\; 0,$$
$$[]_{,qq} \to \partial^2[]/\partial q^2,\; V_s^2 = \lambda/\rho, \quad V_c^2 = c/\rho\varepsilon_{b2}. \tag{4.7}$$

After integrating one has the resolution

$$(V^2 - V_s^2)\, e \,+\, V_c^2\, arcsin\, e \,=\, V_c^2 q \,-\, \sigma/\rho, \quad q = k(x - Vt). \tag{4.8}$$

Here k and σ are the constants.

Now evidently that the profile of deformation wave depends on its speed V which is not equal to the sound speed V_s. Moreover, it is not material constant at all as in linear theory. Its amplitude is not arbitrary value but is equal to 1, i.e.to ε_{b2}. Therefore it is the wave of structure rearrangements.

If $V = V_s$, then the expression (4.8) may be reversed to

$$e \;=\; \varepsilon/\varepsilon_{b2} \;=\; sin(k_s t \,-\, \omega_s t \,-\, \sigma/\rho V_c^2), \quad \omega_s = k_s V_s. \tag{4.9}$$

This is a linear harmonic wave of fixed amplitude ε_{b2}.

If $V \,<\, V_s$ (subsound wave) then the sinusoidal profile becomes asymmetric. Under condition

$$V^2 \;\leq\; V_s^2 - V_c^2 \tag{4.10}$$

a tilting the wave back takes place (Fig. 4).

But a supersound wave ($V^2 > V_s^2$) is tilted forward when

$$V^2 \;\geq V_s^2 + V_c^2 \tag{4.11}$$

It is interesting that in the case $V = 0$ one has nontrivial solution

$$-V_s^2\, e_o \,+\, V_c^2\, arcsin\, e_o \;=\; k_s V_c^2\, x \,-\, \sigma/\rho. \tag{4.12}$$

Here σ- constant. It is clear that it is the static distribution of deformation $e_o(x)$. But $e_o(x) \neq e(x, 0)$. As it is easy seen from (4.8) that at $t = 0$ one has the following initial distribution of deformation

$$(V^2 - V_s^2)\, e(x,0) + V_c^2\, arcsin\, e(x,0) \;=\; V_c^2 kx \,-\, \sigma/\rho. \tag{4.13}$$

If it is so then one has the stationary wave evidently. At $x = 0$ static solution coincides with the hysteresis discussed early.

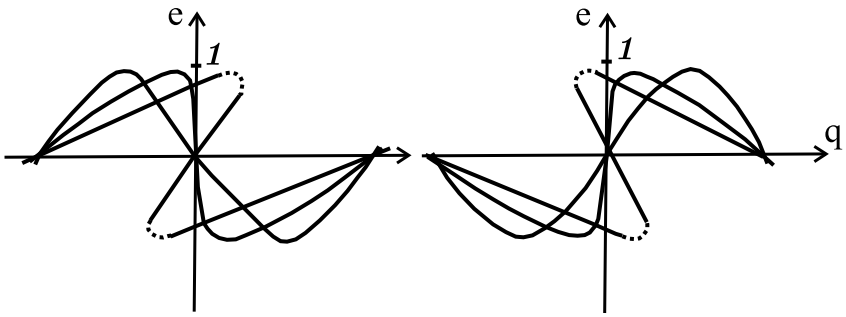

Figure 4:

5 Nonstationary bifurcation waves

If an initial distribution of deformation is differ from (4.13) then a wave with variable profile takes place. Then its speed is not constant. The interesting shock wave of bifurcation may run with the speed depending on a deformation as

$$V^2(e) = \Lambda/\rho = V_s^2 - V_c^2(arcsine)_{,e}, \quad ()_{,e} \to \partial()/\partial e. \tag{5.1}$$

Here Λ - effective pseudo elastic modulus was introduced early and demonstrated at the Fig. 3.

Correspondent solution of equation (4.4) is following

$$e = \epsilon(\xi), \qquad \xi = k[x - V(e)t]. \tag{5.2}$$

Here $\epsilon(\xi)$- an arbitrary function. As for $V(e) = +- \sqrt{\Lambda}/\rho$ it is presented by (5.1). Two signs correspond two waves running into opposite directions.

Different points of the wave profile have evidently different velocities. As a result it is distorted and very cardinally.

The function $\epsilon(\xi)$ is defined by initial conditions. It may be seen that $V(e) \to 0, t \to 0$. Then at initial moment of time

$$e(x, 0) = \epsilon(kx). \tag{5.3}$$

It is very interesting the case of sinusoidal initial space distribution of deformations

$$e(x, 0) = sin(kx) \tag{5.4}$$

Then evidently $\epsilon \to sin$ and nonstationary solution (5.2) is

$$e(x,t) \;=\; sin\xi, \quad \xi \;=\; k[x - V(e)t]. \tag{5.5}$$

or in converted form taking into account (5.1)

$$arcsine \;+\; kt[V_s^2 - +V_c^2(arcsine)_{,e}]^{1/2} \;=\; kx. \tag{5.6}$$

Two signs before radical correspond to two directions of wave spreading.

It is essentially that nonstationary wave (5.6) may reach the state of break wave, if at any moment of time $\check{t}$ the following condition is fulfilled

$$1 \;+\; kV_{,e}e_{,\xi}\check{t} \;=\; 0. \tag{5.7}$$

It means that the following derivatives are diverge, i.e.

$$e_{,x} \;=\; e_{,\xi}V/(1 + kV_{,e}e_{,\xi}\check{t}) \to \infty, \qquad e_{,t} \;=\; e_{,\xi}/(1 + kV_{,e}e_{,\xi}\check{t}) \to \infty. \tag{5.8}$$

In the first case so called gradient catastrophe and in the second kinematic one takes place.

Let us consider the break condition (5.7). For the first time let us calculate an expression

$$(V^2)_{,e}e_{,\xi} \;=\; V_{,\xi}^2 \;=\; -V_c^2\sqrt{(}1 - cos^2\xi)/cos^2\xi. \tag{5.9}$$

Now rewrite (5.7) multiplying it by $2V$

$$2V \;+\; k(V^2)_{,e}e_{,\xi}\check{t} \;=\; 0. \tag{5.10}$$

Using here the first expression and formula (5.1) one has for catastrophic time $\check{t}$

$$\check{t}^2k^2V_s^2/4 \;=\; cos^3\xi\frac{cos\xi - \sqrt{(}1 - e_{b1}^2)}{1 - cos^2\xi} \tag{5.11}$$

This expression is valid for both branches of deformation. For the secondary one ($cos\xi < 0$) it is always positive. For the first branch ($cos\xi > 0$) when $cos^2 \geq e_{b1}^2$ the unstable structure starts. Then $\check{t}^2 < 0$.

If $e \to 0$,$cos\xi \to 1$ then $\check{t} \to \infty$ - no catastrophe for small deformations. On the contrary, $\check{t} \to 0$ when $e \to 1$ and when $e \to e_{b1}$. The other words, catastrophe take place immediately at the thresholds of structure stability.

The evolution of wave profile is presented at the Fig. 5. It is seen that at first moments of time some small damages of the profile at extremely points ($e^2 = 1$) are beginning. Each small zone of discontinuity is growing and its "shores" are diverging into opposite directions - kinematic catastrophe takes place. Separation of a sinusoidal profile into regions of the primary and the secondary structure or microphase separation is visible. All regions of the primary soft structure are moving with subsound speed $\sqrt{(}V_s^2 - V_c^2)$ but regions of the secondary (more hard) structure are moving in opposite direction with supersound speed $\sqrt{(}V_s^2 + V_c^2)$. At last the evolution is coming to a macroscopic separation of two phases in a space with an "empty" (undeformed) zone between them.

This break wave in solid is differ from shock wave in gases. The letter always is running in a single direction with raising of entropy. In our case there are two directions of spreading (two waves). They are running with decreasing of kinetic energy which is necessary for structure rearrangements. Indeed, the expression (5.9) has always negative left part - for both waves.

6 Inhomogeneous microdeformations in media with center of symmetry

Now let us consider a medium with center symmetry. As before we admit in the equations (1.9), (1.10) the following simple conditions

$$\hat{c}_{kij} = c_{kij} = O, \quad u_i = (o, u, o), \quad u = u(x, y), \qquad P_i(u_i) \to p\sin(2\pi u) \tag{6.1}$$

The first two conditions are due to symmetry of media but the other are limiting conditions. The high gradient members O_1, O_2 are omitted.

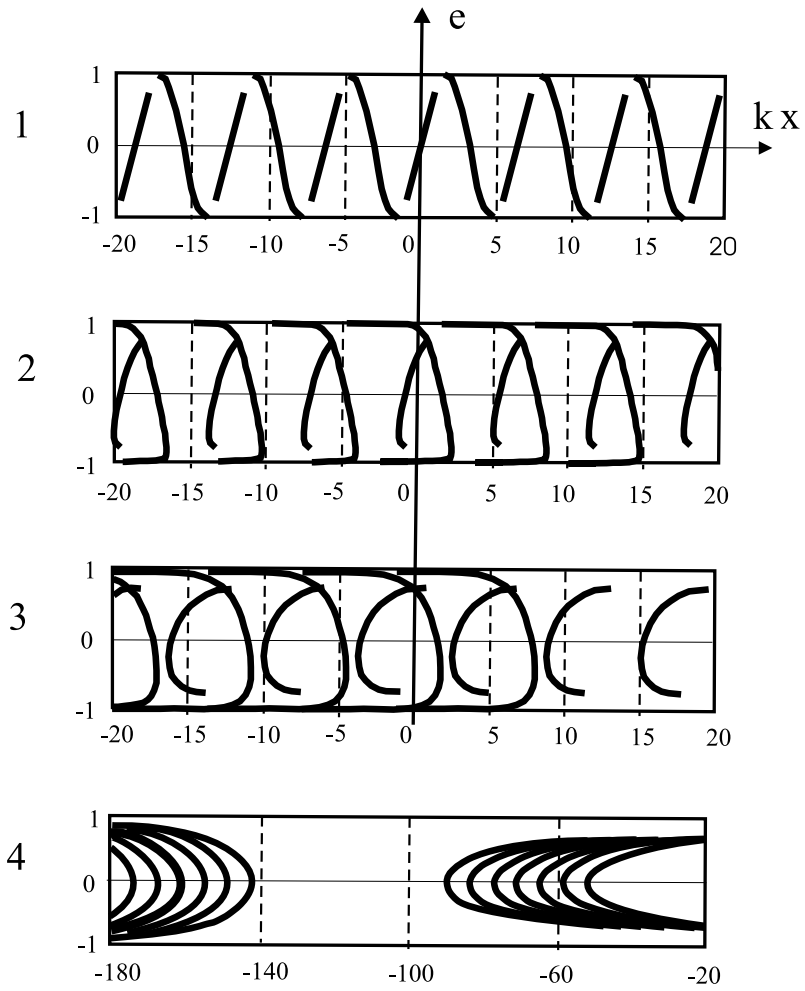

Figure 5:

For the high symmetry crystals excluding triclinic and monoclinic systems one has the following representation (taking into account one-dimensional motion)

$$k_{ikjm}u_{k,jm} \rightarrow k_1 u_{,xx} + k_2 u_{,yy} \tag{6.2}$$

A coma in subscript indexes indicates the space derivatives. As a result one has two equations of low frequency motion

$$\rho\ddot{U}_i \;=\; \lambda_{ikjm}U_{k,jm}, \tag{6.3}$$

$$0 \;=\; -\,p\,\sin(2\pi u) \;+\; k_1 u_{,xx} \;+\; k_2 u_{,yy}. \tag{6.4}$$

Here crossed members are absent - no local mode interaction due to media symmetry. But it is possible if unlocal members O_1,O_2 (see (1.12), (1.13)) are taken into account. Unfortunately direct consideration this problem is not effective. In the last section a mesoscopic theory will be presented.

Let us return to an analysis of the equation of microdisplacements (6.4). It corresponds to a minima of the energy functional

$$E = (1/2)\int_{-H}^{H}\int_{-2B}^{2B}[k_1(u_{,x})^2 + k_2(u_{,y})^2 + 2p(1-\cos 2\pi u)]\,dxdy. \tag{6.5}$$

The limits of integration will be clear up. Let to call the coefficients k_1 k_2 as stretch and shear micro modulus. Their dimensions are differ from ones of macroscopic modulus.

The positive value p is an amplitude of periodic atomic potential. It is a maximal atomic force. Note then it has a dimension of volume energy density.

Essentially that potential (6.5) is realized in cubic, hecsagonal, rhombohedric, tetrahonal and rhombic crystals but when ($\vec{u} \to (0, u_y, 0)$) only!. The third, periodic member in (6.5) presents the shear energy of hard indeformable sublattices (in long wave approximation) but the first two are responsible for their deformability. As a result one has inhomogeneous field of microdeformations and scale effects The potential (6.5) was used in [4] as heuristic one but the equation (6.4) was derived due to a variation principle. Some solutions was analyzed in [5,6]. In this section we will analyze elasto plastic microshear and discuss the problem of its stability in the field of macroscopic deformations.

7 Fragmentation of a lattice

The equation of microdeformations (6.4) has no homogeneous solutions except of trivial - integer number when sublattices are translated to

equivalent positions, i.e. when $u = 1, 2, ...$ Special interest presents double periodic solutions with finite scales.

This equation (of sine-Helmholtz type) includes two material scales (coherent distances)

$$l_1 = \sqrt{k_1/p}, \qquad l_2 = \sqrt{k_2/p}. \tag{7.1}$$

They define some mesoscopic volumes. Inside them mutual distortions of sublattices are small enough and only hard shear take place. The other words, they are coherent or simply-homogeneous. In one dimension case one has Frenkel- Kontorova s circuit with misfit dislocation (soliton).

Let us begin to solve equation (6.4). It is possible to construct private but exact and interesting solution which describe some fragmentation of a body or rising of a domain superstructure due to defects formation. Let microfield $u(x, y)$ obey to following boundary conditions

$$u(H, y) = +1, \quad u(0, y) = 0, \quad u(-H, y) = -1, \quad (0 < y < 2B)$$

$$u(H, y) = -1, \quad u(0, y) = 0, \quad u(-H, y) = +1, \quad (-2B < y < 0). \tag{7.2}$$

These conditions must be repeated along horizontal axe OX with a period $2H$ and along vertical OY- with a period $4B$. These conditions means that sign alternating sliding along OX takes place on one interatomic distance. i.e. sliding into opposite directions - fig.6. Maximum of sliding ($|u| = 1$) takes place on "boundaries" $x = nH$. Between them it is less. If $|u| \leq 1/2$ no inter atomic barriers are not overcome and elastic reversible deformations take place. But if $1 < |u| < 1$ then there are inelastic rearrangements and cardinal variations of structure (local topology).

An exact solution of (6.4) obeying to these conditions may be constructed due to Lamb method of separating of variables [7]. As a result we derived[5,6] such an expression

$$tg(\pi u/2) \; = \; + - \, tn(xK_1/H) \, / Asn(yK_2/B), \tag{7.3}$$

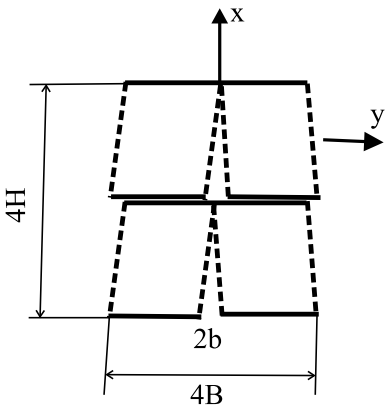

Figure 6:

$$A^{-2} = \sqrt{1-\nu_1^2}/\nu_2. \tag{7.4}$$

Here A^{-1} - an amplitude characteristics of microdisplacements. Two signs at right response for two directions of microshear. Next, the relative lengths $2H$ and $4B$ are the periods of elliptic tangent (tn) and elliptic sine (sn). Best of all, the values K_1 K_2 are complete elliptic integral of the first kind, depending on its modules $0 \leq \nu_1$, $\nu_2 \leq 1$ [8]. If one takes into account that $tn0 = 0$ $tnK \to \infty$, then it is clear that the solution (7.3) obeys to the boundary conditions (7.2).

As a result one has double periodic deformed structure. Initial translating symmetry is disordered but only partly! Scale roughening takes splace- from b to H, B. Cells of superstructure (domains) are divided by sliding lines and singular (topological) defects. The letter are specific elements of solutions of sine-Helmholtz equation.

Indeed, let us consider the vicinity of the point $x = y = 0$. Here elliptic functions $tn()$ and $sn()$ may be presented by linear members only and then the solution (7.3) may be presented by the approximation

$$tg(\pi u/2) \approx (xk_1/yk_2) = +- (k_1/k_2)tg\phi \tag{7.5}$$

Here ϕ - an angle of local polar coordinate system. Obviously a microdisplacement field in vicinity of coordinate origin is multivalent function depending on number of going around it. Then one has

$\pi u/2 = arctg(k_1\phi/k_2)$, i.e. topology defect of the field u with positive (negative) charge. If it is equal to 1 (due to ratio k_1/k_2) then one has a complete edge dislocation or simply, dislocation. and partial dislocation if the charge less than unity.

These defects (charges) there are in each point, where $tn() = 0$, i.e. $x = 0, 2H, 4H, ...$, and $sn() = 0$ simultaneously ($y = 0, 2B, 4B, ...$). As for the signs it is clear that one has alternating series only along OY but not along OX. Therefore topology defects are formed regular net.

These defects are connected with fragmentation - sliding $u = +-1$ (in limited scales $2B$) into opposite directions. As a result one has pairs of solid vortexes of opposite signs.

It is worthwhile to note that on vertical boundaries $y = (2r + 1)B$, $r = +0, 1, 2, ...$, when the right part of (7.3) is infty one has vertical series of Frenkel-Kontorova s solitons or misfit dislocations.

Thus, this theory is able to predict forming of defects -dislocations, lines of sliding etc.

We demonstrated only one private solution of the equation (6.4). The other ones are differ from this by configuration and nature of defects. It depends on external (macroscopic) field of stresses and strains. Therefore some researches of stability of superstructure are actual of cause.

8 Local stability of microdeformations

Periods of domain structure H and B are not arbitrary. They depends on physical properties of a solid, micro and macro deformations. The latter will be analyzed. Now let us consider the role of the first two factors. They may be taking into account due to so called dispersion expressions.

Let us substitute the solution (7.3) to the equation (6.4). It will be satisfied indeed if the following conditions will be realized

$$(2 - \nu_1^2)k_1q_1^2 - (1 + \nu_2^2)k_2q_2^2 - p = 0, \tag{8.1}$$

$$k_1q_1^2 = A^2k_2q_2^2, \qquad q_1 = K_1/H,\ q_2 = K_2/B, \quad p > 0. \tag{8.2}$$

Using here a definition of A (7.4), one can derive that

$$(k_1 q_1^2/A^2 + k_2 q_2^2)S \, - \, 2p \, = \, 0, \qquad S = (A^2 - 1)(1 - \nu_2^2/A^2), \quad (8.3)$$

In a linear theory such expression connects space and time frequencies with material constants. In this nonlinear theory this includes an amplitude factor A. It define a region of existence of the solution.

First of all, it is easy to see from (8.3 that $A > 1$ if $p > 0$. It is a criteria of elasto plastic fragmentation described by the solution (7.3). The other restrictions may be clear up if exclude from (8.1), (8.2) and (7.4) integration constants ν_1, nu_2. Then one come to an expression that connects three values - H, B and A. As a result one has a family of hyperbola-like curves with a parameter A. They have two asymptote $B = B_t$, $H = H_t$ for each A

$$H_t < H < \infty, \qquad B \to B_t (B < \infty) \quad (8.4)$$

$$H_t = l_1(1 - A^{-2})K_{11}, \qquad B_t \, = \, \pi l_2 \sqrt{(}A^2 - 1)/2 \quad (8.5)$$

Here $K_{11} = K_1(\nu_1)$ when $\nu_1 = \sqrt{(}1 - 1/A^4)$.

These curves presents spectrums of domain scales. Obviously its dimensions are limited- too small domains are impossible or the other words -too sharp

inhomogeneities are not advantage. Let us consider a problem of stability of superstructure. It is local stable because the equation (6.4) is the condition of minima of energy integral (6.5) but when its limits H, B are fixed! It means that a global stability of superstructure must be clear up yet. It is necessary to research extremes of function $E = E(H, B)$. Optimal dimensions H, B are reached in external field of macroscopic deformations of net shear - see the next section.

We considered before the case of elasto plastic microdeformations ($A > 1$) due to conditions (7.2) of great slidings ($1/2 < u < 1$). But if $u \leq 1/2$, then atomic barriers are not overcome and there are elastic effects. New solution of (6.4) is

$$u_+(x, y) \, = \, u(x, y) - 1/2. \quad (8.6)$$

Here $u(x,y)$ is may be presented by the expression (7.3) but when $A < 1$. New solution $u_+(x,y)$ being introduced into (6.4) give us dispersion expressions which are differ from (8.1),(8.2) only by a sign before the member p, i.e.

$$(2-\nu_1^2)k_1q_1^2 - (1+\nu_2^2)k_2q_2^2 + p = 0, \tag{8.7}$$

$$k_1q_1^2 = A^2k_2q_2^2, \qquad p \geq 0. \tag{8.8}$$

If one writes the expression analogical to (8.3), then inverse sign before p means that $A < 1$. Each curve on the plane (HB) has one asymptote $B \to B_i$ and outcome from one point $H = H_c, B = B_c$, i.e.

$$H \geq H_c, \qquad H < \infty, \quad B_c \leq B \leq B_i \tag{8.9}$$

$$\begin{gathered} H_c = \pi l_1(1-A^2)/2A, \qquad B_c = l_2(1-A^2)K_{22}, \\ B_i = \pi l_2\sqrt{(}1-A^2)/2 \end{gathered} \tag{8.10}$$

Here $K_{22} = K_2(\nu_2)$ at $\nu_2 = A^2$. Some limits of elastic spectra take place too as it follows from the above inequalities. There are only short domains evidently. Detail analysis is developed in [5,6].

9 Global stability of superstructure in external field

Let us discuss, just a little bit, a problem of optimization of a domain structure with respect to domain dimensions H, B. Detail consideration is presented in [9]. In above developed theory it was impossible because in a medium with a center symmetry macroscopic and microscopic modes do not interact in long wave approximation. Crossed members in the equations (6.3), (6.4) may appear only due to high gradients. It means that their interaction may be realized only in finite volume elements. Then it is necessary to average microfield and to introduce an interaction between mean field and macroscopic deformations. Fortunately averaging procedure may be realized easy if one

consider a domain as an element for averaging. Then the values $1/H$ and $1/B$ are the mean microgradients simply.

Then one can develop mesoscopic theory introducing a total energy of interacting modes- macroscopic deformations and mean microscopic gradients

$$\check{E}/8pBH = \eta_1\varepsilon_1^2/2 + \eta_1\varepsilon_2^2/2 + \eta_2\varepsilon_1\varepsilon_2 - L + D, \qquad (9.1)$$

$$\eta_1 = \lambda_1/p, \quad \eta_2 = \lambda_2/p, \qquad \varepsilon_1 = \partial U_x/\partial x, \quad \varepsilon_2 = \partial U_y/\partial y. \qquad (9.2)$$

The first two members present the energy of macroscopic deformations of net shear for rhombohedric, tetrahonal, hecsahonal and cubic crystals. In addition, D- the density of microscopic energy (6.5) as a function of H, B

$$D = E/8pBH \qquad (9.3)$$

A crossed member L in the total energy $\check{E}$ can be constructed as the following expression

$$L = \chi_1\varepsilon_1/H + \chi_2\varepsilon_2/B. \qquad (9.4)$$

Here χ_1, χ_2 - positive coefficients.

If $L > 0$ then a minimum of the total energy (9.1) is possible and optimal finite dimensions of domains may be calculated. It is necessary for it to calculate the integral in (6.5) and to deal with function $E(B, H)$. Detail theory is published in [9]. The main result is as following.

The total energy $\check{E}(B, H)$ is a saddle-like potential. But there are two minima at its boundaries when $B > H$ and when $B < H$. Two branches of domain are exist- elongated along OX and along OY axes. Their dimensions depend on macroscopic deformations ε_1 and ε_2. There are thresholds for a superstructure formation. Before them no microdisplacements and domain structure are formed- classic theory of elasticity is correct. Essentially nonlinear theory is necessary.

10 Conclusion

A lot of inelastic phenomena are connected with structure rearrangements. Now many famous mechanics pay attention to a phenomenological theory in which these effects would be presented adequately [9]. In this work we try to begin with microscopic, atomistic model. The main attention is payed to variable local topology of continua and diffeomorphic principle when catastrophic deformations are taking into account. Are they compatible? It is so in the frame of double pseudo continuum model which is prototipe of complex lattice consisting of two or more sublattices. We try also to illustrate the possibilties of the theory by very simple but not trivial examples. If it is correct, in what connection with phenomenological theories is it?

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Esencijalno nelinearna teorija mikrodeformacija periodične sredine

UDK 531.01, 539.374

Prikazana je esencijalno nelinearna teorija mikro i makrodeformacija neke sredine sa kardinalnom preraspodelom periodične strukture korišćenjem dvostrukog kontinuuma sa promenljivom lokalnom topologijom. Unutar predloženog modela postoje dva deformaciona moda (makroscopski i mikroscopski) kada se dostigne neka granica. Zatime se razmatraju neki problemi kao: prenosi bliznačenja, katastrofalni deformacioni talasi, udarni i tilt-bifurkacioni talasi. Konstruiše se jedno ekgzaktno rešenje koje opisuje elasto-plastičnu fragmentaciju sredine takodje i kada se formiraju dvostruke preiodične superstrukture domena. Tada se izmedju njih nalaze čvrsti rotoni suprotnih znakova sa singularnim defektima. Oni se pojavljuju u kritičnom polju makroskopskih deformacija čistog smicanja. Kada se ova bifurkaciona tačka predje, tada se dimenzije domena stabilizuju zavisno od vrednosti makroscopske deformacije. Uspostavljen je jedan kriterijum globalne stabilnosti.