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NON-LINEAR THEORY OF ELASTIC MICROSHEAR IN PERIODIC STRUCTURES. INSTABILITY OF HOMOGENEOUS DEFORMATION†

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A theory of a crystal lattice with substantially non-linear interaction between the atoms during arbitrary mutual displacements under conditions of elastic shear of a layer is proposed. The energy of two-dimensional deformations contains periodic and gradient terms. The equilibrium equation in the form of the sine-Helmholtz equation (with two characteristic coherence lengths) is solved accurately. It is shown that a shear virain homogeneous along the layer unstable and is stabilized by modulations. As a result, a superstructure with long periods arises, i.e. there is a change in the long-range translational order. Relations are obtained, linking the size and the amplitude of the displacement field, which provide the conditions for the superstructure to exist. A bifurcation transition from purely elastic deformation of the lattice to elastoplastic deformation is found. © 2000 Elsevier Science Ltd. All rights reserved.

Some results of the theoretical analysis were presented in a brief communication [1]. The present paper not only generalizes these results but also reveals the physical significance of the structural transitions and bifurcation points. The theory focuses mainly on the problem of the stability of elastic shear.

In continuum mechanics there is no fundamental difference between spatially homogeneous and inhomogeneous deformations. However, if the translational symmetry related to the periodic structure of the body is taken into account, it is clear *a priori* that the difference is substantial. The former deformations, unlike the latter, do not disrupt the long-range translational order. In continuum theory, account is taken of point but not of translational symmetry, and therefore some effects, including a change in the structure of the body, do not lend themselves to a description.

However, under large deformations, the structure of an actual body changes considerably. Not to mention the occurrence and activation of defects in the broadest sense of the word, the effects of loss of stability of homogeneous deformations become possible in the body, Thus, in bodies possessing a layered periodic structure (composites or smectic liquid crystals), undulations, or wavy distortions of plane layers, are observed during uniaxial stretching across the layers. The structure withstands homogeneous deformations (an increase in the interlayer distances) only up to a certain limit. Flexural deformations, i.e. inhomogeneous deformations, then become more favourable.

An analogous effect is probable in the case of high uniform shear, which may, after a certain instant of time, be accompanied by shear energy transfer to other degrees of freedom, generating inhomogeneous deformations. This may occur under large deformations which lower the interatomic potential barriers and weaken the internal crystal field maintaining the translational order in the system. As result of its disruption, the less energy-intensive inhomogeneous deformations become more preferable.

To predict structural instability of this kind, a theory taking account of the long-range translational order in the system and the possibility of it varying is of course required. The simplest model should take account of the competition of the interatomic potential (responsible for the maintenance of the periodic order) and gradient terms governing its breakdown. Bearing in mind the spatially smoothed description, there is no sense in proceeding on the basis of the paired interatomic potentials – this description has excessive detail. It is sufficient to introduce the potential interaction of atomic chains with each other as a periodic function of the mutual displacements and of the atoms of neighbouring chains. It would be possible to confine ourselves to this if the chains were unstretchable. Therefore, gradient terms should be present in the potential responsible for the final stretchability of the chains and for their non-uniform shear in the transverse direction.

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1. FUNDAMENTAL EQUATIONS

We will proceed on the basis of the simplest form of the overall potential E in relation to the model of a polyatomic layer of thickness H subjected to shear along the OY axis. The structure of the layer is a two-dimensional square lattice with period b. The energy E of the area of a layer of length $2B$ is taken in the form

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

where u is the microdisplacement (in units of b) along the layer (the OY axis), k_1 is the shear micromodulus, k_2 is the longitudinal tensile micromodulus of the lattice and p is the amplitude of the interparticle periodic potential, and also the amplitude (the greatest value) of the cohesion force.

The micromoduli are different, strictly speaking, from the corresponding moduli in the macroscopic theory of elasticity, which operates with macrodisplacements U (displacements of macroparticles with respect to their initial positions), i.e. with acoustic degrees of freedom. The microdisplacements u correspond, as it were, to optical modes of deformation, which are excited when the structure loses its stability.

The first two terms in (1.1) correspond to microgradients. The third term in (1.1) corresponds to the energy of uniform shear of rigid monolayers (chains), while the first two terms take into account their compliance or the elasticity of the two-dimensional lattice under shear and tension along the OY coordinate axis. In the case of rigid monolayers, a simple condition where the microdisplacement field is constant denotes not the rigid displacement of the entire lattice as a whole but its uniform shear microstrain, which essentially is equal to the relative magnitude (in units of b) of the microdisplacement u. In the case of the rigid microshear of neighbouring chains by the magnitude of one interatomic distance in the crystal, a twinning deformation is produced.

Note that it is actually a three-dimensional lattice with two-dimensional displacement fields that is being examined. However, it is true that two-dimensional lattices have a specific feature in connection with fluctuations and correlation functions, but this is beyond the scope of the present theory.

The equilibrium equation corresponding to the minimum of the functional (1.1) has the form

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

This non-linear equation, well known as the sine-Helmholtz equation, obviously contains two characteristic coherence lengths of the lattice

$$l_1 = \sqrt{k_1/p}, \quad l_2 = \sqrt{k_2/p} \tag{1.3}$$

They determine the mesoscopic scales which appear in the given theory, unlike the theory of scaleless continuum theory. On scales smaller than the mesoscopic scales, the long-range translational order is broken down entirely by displacement gradients. The lattice retains a certain translational order only at long distances.

When $l_1 \to 0$ we arrive at the one-dimensional Frenkel–Kontorov model – an elastic chain of atoms interacting with a periodic substrate. In the model proposed, however, we consider a system of parallel chains interacting with each other (and not with the substrate), capable both of slip in relation to each other and of continuous deformation. The first two terms in equilibrium equation (1.2) correspond to continuous forces smoothed with respect to atomic scales, while the third non-linear term takes account of interatomic structural forces. On averaging with respect to sizes exceeding the mesoscopic scales, structural forces disappear and the model is converted to the continuum model. The case when the continuum forces vanish with zero gradients of microdisplacements is also not trivial. Then the structural forces are self-balanced if $u = \pm 1$, which follows directly from Eq. (1.2). Twin formation corresponds to this case.

If (1.2) corresponds to the minimum of functional (1.1), an equation with the opposite sign in front of the non-linear term corresponds to the maximum. Their solutions u_+ and u_- are obviously related to a transformation (changing the sign of the sine), i.e.

$$u_-(x,y) = u_+(x,y) - \tfrac{1}{2} \tag{1.4}$$

$$k_1(\partial^2 u_+/\partial x^2) + k_2(\partial^2 u_+/\partial y^2) + p\sin 2\pi u_+ = 0 \tag{1.5}$$

They differ by the translation of the structure by a lattice half-period (in units of b), in fact, in both directions. However, in (1.4) only one direction is specified, which is convenient for subsequent formulation of the boundary conditions. As a result of the transformation of (1.4), we change from a stable to an unstable lattice configuration, where some atoms are displaced from local minima to the apexes of potential barriers, while others are displaced from the apexes to the minima. It is clear that, for a shear by more than a half-period, the switching of interatomic bonds occurs with a change in the neighbours of particles – a situation that is impossible in a continuum model. In the present theory this is admissible (elastoplastic shears arise), but this case is not considered.

Here, we are interested only in elastic microde formations in the layer, where the maximum permissible (critical) shear at the boundaries $2u \leqslant 1$, while in the remaining volume the shear is less. Before proving the stability of inhomogeneous displacements modulated along the layer, we will return to an analysis of the accurate two-dimensional solution u of Eq. (1.2) for an infinite layer of thickness H, which will obey the boundary conditions of critical shear

$$u_-(0,y) = -\tfrac{1}{2}, \quad u_-(H,y) = +\tfrac{1}{2}, \quad u_-(x,y+2mB) = u_-(x,y), \quad m = \pm 1, 2, \ldots \tag{1.6}$$

In this case we are dealing with the mutual shear of neighbouring chains at boundaries $x = 0$ and $x = H$ by a half-period of the initial lattice, in both directions, when the atoms emerge at the apexes of the microrelief. The signs in the first two equalities can be replaced with the opposite signs in view of the equal shear to the left and right. Obviously, within a layer (of thickness H), these shears are of course less than half the interatomic distance. Such a deformation is correctly said to be purely elastic. The third condition in (1.6) is the condition of periodicity of deformations along the layer.

2. CONSTRUCTION OF THE SOLUTION

To find the solution of the problem in the form of (1.4) it is necessary to refer directly to Eq. (1.5). We will use Lamb's method [2] to separate the variables for the sine-Helmholtz equation (1.5), according to which the solution is found in the form

$$\operatorname{tg}(\pi u_+ / 2) = Q_1 / Q_2, \quad Q_1 = Q(x), \quad Q_2 = Q(y) \tag{2.1}$$

Using this representation, the initial equation (1.5) is divided into two ordinary non-linear differential equations in the partial functions Q_1 and Q_2

$$(\partial Q_1 / \partial x)^2 = a^2(Q_1^2 + B_1)(Q_1^2 + C_1) \tag{2.2}$$
$$(\partial Q_2 / \partial y)^2 = a^2(Q_2^2 - B_2)(C_2 - Q_2^2)$$

In the original book [2], on the right-hand side of these equations there are three arbitrary integration constants which were selected in advance so that the initial equation was satisfied. It is best, as in [3], to write the binomials on the right-hand side in terms of five constants (a, B_1, B_2, C_1 and C_2) and to obtain [by substituting expressions (2.2) into (1.2)], in explicit form, two additional relations that these constants obey

$$B_1 C_1 = B_2 C_2, \quad a^2(B_1 + C_1) - a^2(B_2 + C_2) = 1 \tag{2.3}$$

Equations (2.2) have a solutions in elliptic functions. The introduction, at the intermediate stage, of surplus integration constants provides greater scope for selecting particular elliptic functions, guided by the specified boundary conditions. This selection is later checked using relations (2.3), which are the conditions for a solution to exist.

The procedure for constructing the solution of interest to us was described in detail in [4, 5]. It has the form of a doubly periodic function

$$\operatorname{tg}(\pi u_+ / 2) = \pm \operatorname{tn}(q_1 x) / (A \operatorname{sn}(q_2 y)) \tag{2.4}$$
$$A^2 = \nu_2 / \sqrt{1 - \nu_1^2}, \quad q_1 = K_1 / H, \quad q_2 = K_2 / B$$

where q_1 and q_2 are spatial elliptic frequencies. H and $2B$ are the half-periods of the Jacobi elliptic tangent tn and sine sn, respectively, and K_1 and K_2 are complete elliptic integrals of the first kind, depending

in a known way on their arguments – moduli ν_1 and ν_2 [6]. The latter are defined in the range from 0 to 1.

The following asymptotic forms hold [6]

$$K \to \infty, \quad \text{tn} \to \sinh, \quad \text{sn} \to \text{th}, \quad \nu \to 1$$
$$K \to \pi/2, \quad \text{tn} \to \text{tg}, \quad \text{sn} \to \sin, \quad \nu \to 0 \tag{2.5}$$

In particular, they show that moduli ν_1, ν_2 and K_1, K_2 determine the degree of ellipticity of the corresponding functions and their degree of localization along the corresponding axes, and with it the magnitudes of the displacement gradients. The latter can theoretically also be infinitely large with limited periods $2H$ and $4B$ or spatial frequencies of the displacement field.

Expression (2.4) is an unstable solution since it satisfies Eq. (1.5). However, it enables us to construct a stable solution of Eq. (1.2) in the form of (1.4), satisfying the necessary boundary conditions (1.6), which can be easily checked. To proceed directly from Eq. (1.2), however, would be difficult.

The solution is periodic along the OY axis (with a period of $4B$) by virtue of the periodicity of the function sn. Since it is sign-variable, all cross-sections of the layer are characterized by a complex displacement profile. It is clear that expression (2.4) is also a periodic solution along OX axis with a period of $2H$, but the filed of microdisplacements itself can increase in the positive direction along the OX axis. The solution obtained [(1.4),(2.4)] indicates that, in the deformed state, when the conditions of critical shear are achieved along certain lines, a translational order is also possible, which is realized in the form of a domain superstructure.

3. DISPERSION RELATIONS

Continuing the analysis of the elastic configuration (2.4), (1.4), (1.6), we will examine the criteria for its existence. We will initially consider the fact that, after satisfying the boundary conditions, solution (2.4) contains two arbitrary integration constants ν_1 and ν_2. Theoretically they are found from (2.3), which must be referred to as dispersion relations, since constraints are imposed on the spatial frequencies q_1 and q_2. They can be expressed in terms of the constants indicated as follows:

$$(2-\nu_1^2)k_1q_1^2 - (1+\nu_2^2)k_2q_2^2 + p = 0 \tag{3.1}$$

$$k_1q_1^2 = A^2k_2q_2^2, \quad p \geqslant 0 \tag{3.3}$$

The first of these is a prototype of Eq. (1.5) itself and is obtained by substituting expressions (2.4) into it. Note that, based on the stable solution (1.4), it must be substituted into Eq. (1.2). Of course, we will obtain the same relation (3.1).

The second term in (3.1) corresponds to the gradients of displacements along the layer that are responsible for the inhomogeneous elongation of chains. It is significant that the sign in front of it is negative, unlike the first term. This means that competition occurs between the corresponding forces in establishing equilibrium. Whereas the longitudinal elongations (compressions) create forces directed against the structural forces, maintaining the order, the transverse gradients act in the same direction as the structural forces. The arrangement of the signs in (3.1) already indicates that, for it to be satisfied (the emergence of stable elastic deformations), the longitudinal gradients must predominate over the transverse gradients. If this is not the case, equality in (3.1) is impossible. The longitudinal gradients obviously stabilize large shear, which becomes unstable when there are no longitudinal modulations.

The relation between the gradients is specified by the second dispersion relation (3.2) depending on the value of the parameter A, which was initially defined in (2.4). However, relation (3.2) gives this parameter the simple meaning of the ratio of the characteristic energies of microshear and microelongation. It plays a decisive role in problems of the stability of these deformations. Its critical value may be determined more precisely after elementary transformation of relations (3.1) and (3.2) into the following two conditions

$$-S = A^2P_1 = P_2 \tag{3.3}$$

where

$$S = (A^2 - 1)(1 - \nu_2^2 / A^2); \quad P_1 = p/(k_1 q_1^2), \quad P_2 = p/(k_2 q_2^2) \tag{3.4}$$

Note that separation of the dispersion relations with respect to the spatial elliptic frequencies q_1 and q_2 is actually obtained in (3.3). In non-linear theory, the frequencies are not only expressed in terms of the material constants but also depend on the parameter A. Note also that the effective relative potentials P_1 and P_2 reintroduced into (3.4) stand for certain collective characteristics of the interaction not of the individual atoms but of chain sections of length $4B$ and $2H$ in the superstructure. Like the lattice potential p of the underformed structure, they are positive.

The latter is extremely important, since it requires the inequality $A < 1$, for which $S < 0$, and dispersion relations in the form of (3.3), i.e. the conditions for a stable solution to exist are satisfied. As pointed out earlier, an unstable elastic lattice configuration and negative values of the effective barriers P_1 and P_2 correspond to values of A greater than unity, when transverse gradients begin to predominate. As shown in [1], stabilization is also possible in the region of values of A greater than unity on account of plastic shear. It is then possible to construct a stable solution, but with new boundary conditions, transition to which occurs via the point $A = 1$.

For this reason, it is interesting to examine the point of structural transition $A = 1$ from other viewpoints. As follows from (3.3), the condition for making the potential barrier vanish $p = 0$, say, on account of temperature, also corresponds to this point. Here, the structural forces disappear – disappearance of translational order also occurs as a result of loss of resistance of the sublattices to shear. Then the model degenerates into two independent structureless continua related only by the boundary conditions. In fact, both fields (micro-and macrodisplacements) now obey identical equations of the classical theory of elasticity. It is clear that the branching point of the solution of Eq. (1.2) corresponds the condition $S = 0$ or $A = 1$, and A has the meaning of a bifurcation parameter (Fig. 1).

In fact, it is not necessary to suppose that the potential barrier p vanishes when the temperature of the body increases. This would lead to a basic change in the initial model itself. The point $S = 0$ can be approached, although it is true only asymptotically, by allowing the effective potential barriers P_1 and P_2 defined in (3.4) to tend to zero. The role of the lattice potential is suppressed by the increase in the deformation gradients, disrupting the translational order. As a result, as in the case when $p = 0$, there is a change in the sign of S, and the parameter A passes through unity. Here, the transverse and longitudinal gradients swap roles.

This transition means that the resistance to shear of the deformed sublattices (superstructure) is lost, and considerable rearrangement of the distorted translational order of the deformed configuration occurs. Therefore, the effective potentials, which are relative quantities, can be regarded as parameters of the distorted translational order in the deformed crystal.

Thus, regions of purely elastic deformation ($A < 1$) and elastoplastic deformation ($A > 1$) are separated by the bifurcation point $A = 1$, at which transition is accompanied by slip at the boundary, into half-periods of the initial lattice.

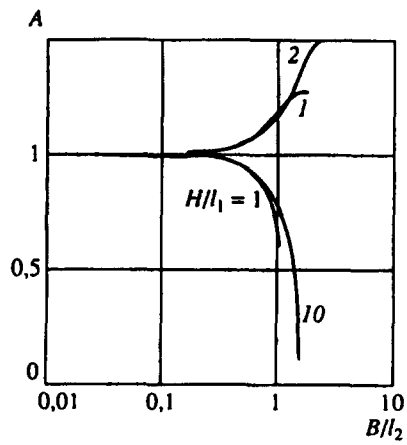

Fig. 1.

4. CRITERIA OF LOCAL STABILITY OF THE DEFORMED CONFIGURATION

Along with the inequality $A < 1$, additional constraints are imposed on the region of existence of stable elastic shear. They likewise follow from the dispersion relations. To determine them it is necessary to eliminated the integration constants ν_1 and ν_2 from relations (3.1) and (3.2). Having defined these constants from (3.2) and (3.1) in terms of H and B, we obtain A as a function of the same quantities.

Figure 1 shows how, A depends on the scale of the longitudinal modulations B (in units of l_2) for different thicknesses. The branching of the solutions is obvious. The case examined here of elastic deformations $A < 1$ is presented as a family of lower curves, each of which corresponds to a certain value of the thickness: $H/l_1 = 1, 10$. It is clear that a solution exists only for fairly short-wave modulations $B/l_2 < \pi/2$, while there are simply no homogeneous deformations along the layer. Elastoplastic shear corresponds to the upper family $A > 1$ [1].

A more detailed analysis of the local stability of solutions is possible. For this it is necessary to show the relation between the three quantities A, B and H as a system of curves of H against B for various values of the bifurcation parameter A (Fig. 2). Curves of existence of the solution (1.4), (2.4) are then obtained.

In the case examined of $A < 1$, each curve in the (HB) plane for a specified value of A has $B = B_i$ along one asymptote and arrives at the final point H_c, B_c without reaching the origin of coordinates, so that the inequalities

$$H \geqslant H_c, \quad H \leqslant \infty, \quad B_c \leqslant B \leqslant B_i \tag{4.1}$$

are satisfied. The values of these limits are as follows:

$$H_c = \pi l_1(1-A^2)/(2A), \quad B_c = l_2(1-A^2)K_{22}, \quad K_{22} = K_2(\nu_2 = A^2)$$
$$B_2 = \pi l_2\sqrt{1-A^2}\,/2 \tag{4.2}$$

It is clear that not all values of the parameters H and B are admissible – obvious constraints follow from (4.1). The region of large longitudinal scales of the superstructure is entirely eliminated. In fact, the value of B does not exceed the coherence length with a factor depending on A that can be extremely small as $A \to 1$. Thus, only short-wave modulation structures are possible, and elastic shear that is uniform along the layer does not occur along the layer. However, if the size of the superlattice cell is even smaller than the admissible H_c and B_c, then such a small-scale superstructure is also unstable.

It is clear that, of the entire range of admissible sizes, only the structures of lowest energy occur as equilibrium structures. In Fig. 2, the segment of the horizontal line that at the level $H = H_c$ intersects the equilibrium curves from left to right reaches the final point B_c, beyond which there is no solution – locally there are no stable states. This point also determines the most stable configuration since, for an appropriate layer thickness H_c, this is the least deformed structure – with the greatest value of the modulation period B_c. For any thickness, such a limiting point and the corresponding most favourable modulated superstructive (with a modulation length B_c) exist.

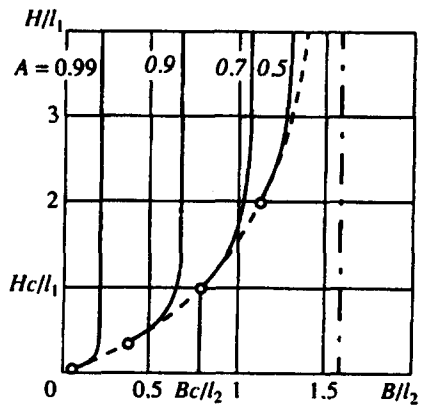

Fig. 2.

Of course, there still remains a wide range of possible structures. In fact, eliminating the parameter A from the expressions for H_c and B_c in (4.2), we obtain the curve of equilibrium structures $B_c(H_c)$ (the dashed curve in Fig. 2). This is the lower boundary of the region of existence, passing through the initial points of the curves and having a vertical asymptote (the dash-dot line). The latter intersects the abscissa axis at the point $B_i l_2 = \pi/2$.

The problem of a unique real superstructure must then be solved by selecting the layer thickness, which will be addressed below.

Inequalities (4.1) can be presented as the energy conditions for the realization of stable critical shear, after the corresponding values have been revealed according to (4.2). We then obtain

$$p \geqslant k_1(\pi/2H)^2(1-A^2)^2/A^2, \quad (1-A^2)^2/A^2 \leqslant P_1 \leqslant (1/A^2-1) \tag{4.3}$$

$$k_2(\pi/2B)^2(1-A^2) \geqslant p \geqslant (k_2/B^2)(1-A^2)^2K_{22}^2, \quad (1-A^2)^2 \leqslant P_2 \leqslant (1-A^2) \tag{4.4}$$

The constraint on the potential barrier, not only from below but also from above, is important. In order to understand this, we will once again consider dispersion relation (3.1), from which it follows that, for the stability of elastic shear, the longitudinal gradients should predominate. The domains of the superstructure must not be too short – they should at least exceed the interatomic distances considerably. For this reason, potential barriers of the lattice that are too great cannot be surmounted under these conditions. Thus, purely elastic critical arises at the fork of the values of p and B or the gradients, as presented in relations (4.4).

Purely elastic but large microdeformation and their gradients are possible, as is now clear, without plastic relief by virtue of the specific mechanism of discharge. It is realized by the compensating (stabilizing) forces generated by the microdeformation gradients along the layer.

The fact is that extension (contraction) of chains along the layer prevents the particles from rolling into potential pits since this would lead to additional elongation extension (contraction). In other words, the neighbouring chains acquire a mismatch of structures. As a result, instead of plastic deformations, large longitudinal gradients arise, drawing off the excess energy of shear deformation. Such a redistribution of energy between the microdeformation modes occurs in a small-scale (along the layer) modulated structure, such as that which occurs when $A < 1$.

The mismatch in the structure of the neighbouring chains is only favourable for stability up to a certain limit. For long chain lengths $2B$, the energy of transverse shear is compensated insufficiently to ensure stability. Therefore, there is a constraint on the chain lengths of purely elastic structures in accordance with (4.1).

5. DISCUSSION OF THE RESULTS

Strictly speaking, locally stable shear deformations satisfying the condition of a minimum of the functional (1.1) have been examined so far. At the boundary of the region of existence, the smoothest long-wave modulations occur, already assumed to be energetically preferable and therefore more stable. In fact, the minima of the integral energy of microdeformations $E/(pHB)$ correspond to them. A series of curves is obtained, indicating a drop in energy towards an increase in the length of modulation B for different thicknesses H. Each curve, sloping down, ends at the final point B_m. A subsequent rise on each curve is not revealed – this goes beyond the region of existence of a solution. Thus, we are dealing with a minimization of the energy at the boundary of the region of existence of solutions.

The relation between the minimizing values B_m and H_m forms a curve of energetically preferable superstructures, which coincides with the boundary of the region of existence of solutions (the dashed curve in Fig. 2). This means that $B_m = B_c$ and $H_m = H_c$. The latter are given by the first two formulae of (4.2).

It is clear that the energetically preferable superstructures also form an entire spectrum, i.e. are non-equivalent. However, it is not advisable to compare them with respect to the energy of microdeformation. In order to find the globally stable superstructure possessing the lowest shear energy, it is necessary to extend the analysis so that it also includes the energy of the macroscopic field of shear deformation ε.

The fact is that, unlike longitudinal modulations, the transverse microdeformations are established not arbitrarily but under the action of shear microdeformations ε which act as an external field. On reaching some threshold, a superstructure with domains of a certain thickness H_m, depending on ε, suddenly arises. By equating H_m to H_c from (4.2), it is possible to find the specific value of the parameter

A, and also the scale of modulation B_c. Then, using these values in the arguments of the elliptic functions in (2.4), we obtain solution (1.4) in its final form, describing the unique superstructure that arises in the macroscopic field of shear deformations.

The problem of global stability and generation of microdeformations in the macroscopic field merits a special consideration.

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