

It is known that plastic deformations of monocrystals are determined by the presence of dislocations in them. In solids the density of dislocations is usually rather high:  $10^6$ - $10^8$   $\text{cm}^{-2}$ . Therefore, if deviations of crystal deformation from the average value between dislocations are not taken into consideration, it is convenient to use the model of continuously distributed dislocations. In [1, 2] a transition to such a model was carried out by averaging the equations of linear theory of elasticity, in which single dislocations were considered. In that case the flows of linear defects remained undetermined. We believe that it is interesting to consider the given problem in terms of the general system of continuum mechanics equations and the concepts of thermodynamics of irreversible processes. First we consider the quantities which will help us to describe continuum deformation.

Considerable displacements of continuum components occur under deformation. In that case microscopic structure of a solid remains the same: atoms are in the sites of the lattice. As a result of short-range action of molecular forces, the stresses arise that are determined by the interaction between the nearest atoms, or, in other words, by the deformation of a crystal's unit cell. To describe the given deformation we may use a vector  $l^\alpha$  (here and further indices run the values of 1, 2, 3) which is a vector of elementary translations in undeformed crystal. The atoms that are connected by the vector  $l^\alpha$  are moving with the velocity of the medium at a given place. The equation for the "frozen in" vector  $l^\alpha$ , averaged over physically infinitesimal volume, has the form [3]

$$dl^\alpha/dt = (l^\alpha \nabla) v, \quad (1)$$

where  $v$  is the velocity of a substance at a given place and the parentheses denote a scalar product. Let us introduce a set of vectors  $W^\alpha$  connected with  $l^\alpha$  by the relations

$$(W^\beta l^\alpha) = \delta^{\beta\alpha} \quad (2)$$

( $\delta^{\beta\alpha}$  is the Kronecker symbol). From (1) and (2) for  $W^\alpha$  it follows that

$$dW^\alpha/dt = -(W^\alpha \nabla) v. \quad (3)$$

The symbol  $(W^\alpha \nabla)$  denotes the convolution  $W_k^\alpha \partial v_k / \partial x_i$ . Here and in what follows repeated latin indices imply summation. Equations (1) and (3) are valid in the absence of dissipative processes; (3) can be written as

$$\partial W^\alpha / \partial t = [v \text{ curl } W^\alpha] - \nabla (v W^\alpha). \quad (4)$$

If  $\text{curl } W^\alpha = 0$ , then  $W^\alpha$  can be represented in the form  $\nabla \Phi^\alpha$ . The functions  $\Phi^\alpha(x) = \text{const}$  are the equations for crystallographic planes in an undeformed crystal. A set of three functions  $\Phi^\alpha(x)$  determines the number of the atom located at a point  $x$ . Then with the appropriate normalizing of  $\Phi^\alpha$  the vector  $W^\alpha$  modulus is equal to the reverse distance between crystallographic planes at a given place and the vector  $W^\alpha$  is directed along the normal to them. The line integral along a closed contour is equal to zero:

$$\oint W^\alpha dx = 0. \quad (5)$$

When  $\text{rot } W^\alpha \neq 0$ ,  $W^\alpha$  can no longer be represented in the form of a gradient of certain scalar functions in the whole space, but locally the meaning of  $W^\alpha$  remains the same. In that case condition (5) is violated and the integral is equal to the number of singularities of the field  $W^\alpha(x)$ , which are covered by the contour. Using the Stokes theorem we write

$$\oint \mathbf{W}^\alpha dx = \int \text{rot } \mathbf{W}^\alpha dS$$

and introduce a new function  $\Omega^\alpha = \text{rot } \mathbf{W}^\alpha$ . The vector  $\Omega^\alpha$  describes the density of the type  $\alpha$  dislocations. If we consider separate dislocations, then  $\Omega^\alpha$  is the sum of two-dimensional  $\delta$ -functions, so that the direction of  $\Omega^\alpha$  coincides with the direction of the dislocation line at a given point. Here from (3) it follows that  $d(\oint \mathbf{W}^\alpha dx)/dt = 0$ , where  $d/dt$  implies

that the path of integration moves together with the substance. This means that the dislocations also move together with the substance, which is similar to conservation of velocity circulation in a liquid [4]. Taking the operation of curl in terms of (4), we obtain the law of conservation for  $\Omega^\alpha$ :

$$\partial \Omega^\alpha / \partial t = \text{curl}[\mathbf{v} \Omega^\alpha]. \quad (6)$$

Note that if  $\Omega^\alpha$  describes the edge dislocation, then  $(\mathbf{W}^\alpha \Omega^\alpha) = 0$ ; for the screw dislocation  $(\mathbf{W}^\alpha \Omega^\alpha) \neq 0$ . In that case from (3) we have  $d((\mathbf{W}^\alpha \Omega^\alpha)/\rho)/dt = 0$ . Dislocations are introduced in [5] with the help of curl  $\mathbf{W}^\alpha$  in somewhat another succession.

It is clear from (3) that in order to find displacements of the continuous points from  $\delta \mathbf{W}^\alpha$ , we must follow the development of the deformation process in time. For small deformations, however, we can write the connection  $\delta \mathbf{W}^\alpha$  with the displacements  $\mathbf{u}$ , introduced in the linear theory of elasticity. Displacements for a small period of time  $\delta t$  are expressed through velocity  $\mathbf{v}$  as  $\mathbf{u} = \mathbf{v} \delta t$ , then from (4) it follows

$$\delta \mathbf{W}^\alpha = [\mathbf{u} \text{rot } \mathbf{W}^\alpha] - \nabla(\mathbf{u} \mathbf{W}^\alpha).$$

For an undeformed lattice, i.e., when  $\mathbf{W}^\alpha = \overset{\circ}{\mathbf{W}}^\alpha$ , we have

$$\delta W_i^\alpha = - \overset{\circ}{W}_k^\alpha \partial u_k / \partial x_i. \quad (7)$$

In the general case, to describe the dynamics of continuum we use a standard set of hydrodynamic variables (density  $\rho$ , velocity  $\mathbf{v}$ , and entropy  $s$ ), for which the laws of conservation are valid:

$$\partial \rho / \partial t + \text{div } \rho \mathbf{v} = 0; \quad (8)$$

$$\rho dv_i / dt = \partial \sigma_{ik} / \partial x_k; \quad (9)$$

$$ds / dt = 0, \quad (10)$$

where  $\sigma_{ik}$  is the equilibrium stress tensor and Eq. (10) is written for the entropy by a gram. For  $\rho$  and  $\mathbf{W}^\alpha$  the connection  $\rho = m/v_a = m(\mathbf{W}^1, \mathbf{W}^2, \mathbf{W}^3)$  is valid ( $v_a = (\mathbf{W}^1, \mathbf{W}^2, \mathbf{W}^3)^{-1}$  is the volume of the crystal's unit cell). The expression  $(\mathbf{W}^1, \mathbf{W}^2, \mathbf{W}^3)$  indicates a mixed product. Here from (3) and (8) follows  $dm/dt = 0$ . If there are no defects in the medium, then  $m = \text{const}$  is simply a mass of atoms of a unit cell.

The energy must depend on combinations of  $\mathbf{W}^\alpha$ , which are invariant with respect to a rotation of a body as a whole. Such are  $G^{\alpha\beta} = (\mathbf{W}^\alpha \mathbf{W}^\beta)$ . A convolution with respect to indices  $\alpha$  and  $\beta$  can be performed with the help of the fundamental tensor  $\overset{\circ}{G}_{\alpha\beta} = (\overset{\circ}{i}_\alpha \overset{\circ}{i}_\beta)$ , where  $\overset{\circ}{i}_\alpha$  corresponds to an undisturbed crystal. Note that for elastic deformations to be significant ( $u_{ik} \sim 1$ ,  $u_{ik}$  is the deformation tensor [1]), the stresses  $\sigma_0 \approx \mu$  ( $\mu$  is the shear modulus) are necessary. From the experiment of [6] it is seen, however, that a stress relaxation due to plastic flow occurs at  $\sigma_T \approx 10^{-4} \sigma_0$ , which corresponds to sufficiently small deformations. Therefore, in writing down the elastic energy it is quite possible to use Hooke's law, i.e.,  $\delta \varepsilon \sim (\delta G^{\alpha\beta})^2$ . As an example let us write the expression for the energy in an isotropic case:

$$\varepsilon_{el} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left( \frac{\lambda}{2} (\overset{\circ}{G}_{\alpha\beta} \delta G^{\alpha\beta})^2 + \mu \overset{\circ}{G}_{\alpha\gamma} \overset{\circ}{G}_{\beta\delta} \delta G^{\alpha\beta} \delta G^{\gamma\delta} \right)$$

( $\lambda$  and  $\mu$  are the Lamé coefficients). In that case if we use connection (7), we obtain a conventional expression for elastic energy, determined through  $u_{ik}$  [1].

We use the following method for calculating the stresses. For the density of the full energy  $U$  the following law of conservation is valid:

$$\partial U / \partial t + \text{div } \Pi = 0 \quad (11)$$

( $\Pi$  is the energy flux density). Writing  $U = \rho \varepsilon + \rho v^2 / 2$  and using (8) and (9), we see that in order for (11) to be true, we must take

$$\rho d\varepsilon / dt = \sigma_{ik} \partial v_i / \partial x_k + \text{div}(\Pi - \dot{q}) \quad (12)$$

where  $\dot{q}_i = \rho(\varepsilon + v^2/2)v_i + \sigma_{ik}v_k$ . In the general case internal energy will depend on, besides  $W^\alpha$ , the derivatives of  $W^\alpha$  (for example,  $\Omega^\alpha$ , which corresponds to the dislocation core energy). Then for  $d\varepsilon$  we write

$$d\varepsilon = Tds + \sum_{\alpha} w_i^{\alpha} dW_i^{\alpha} + \sum_{\alpha} \omega_i^{\alpha} d\Omega_i^{\alpha} \quad (13)$$

Here  $w_i^{\alpha} = \partial \varepsilon / \partial W_i^{\alpha}$ ;  $\omega_i^{\alpha} = \partial \varepsilon / \partial \Omega_i^{\alpha}$ . Substituting (3), (6), (10), and (13) into (12), we obtain the expression

$$\sigma_{ik} = - \sum_{\alpha} W_i^{\alpha} D\varepsilon / DW_k^{\alpha} \quad (14)$$

where  $D\varepsilon / DW^{\alpha} = \rho w^{\alpha} + \text{curl } \rho w^{\alpha}$  is the variational derivative. Other quantities, which may determine the energy, are taken into account in a similar manner. For example, for the volume concentration of point defects

$$\partial c / \partial t + \text{div } cv = 0 \quad (15)$$

is valid. For the concentration per gram we have  $n = c/\rho$  and respectively

$$dn/dt = 0 \quad (16)$$

In (13)  $\zeta dn$  ( $\zeta$  is the chemical potential of point defects) must be added. For simplicity let us consider defects of one kind. It follows from (12) and (16) that point defects do not contribute to stresses.

In (4) and (6) the vector  $\Omega^\alpha$  is the sum of  $\delta$ -functions corresponding to separate dislocations. In this sense Eqs. (4) and (6) are "microscopic." Passing to "macroscopic" equations, we must average  $\Omega^\alpha$  over physically infinitesimal volume. The volume is selected with respect to a specific configuration of dislocation lines, distance between them, and scales  $L$ , on which a characteristic change in physical quantities occurs (see [2]). In the simplest case  $\langle \Omega^\alpha \rangle$  can be represented in the form

$$\langle \Omega^\alpha \rangle = \Omega^\alpha + \text{curl } m^\alpha$$

where  $\Omega^\alpha$  is the density of slightly curved dislocation lines, so that  $|\nabla \Omega / |\Omega||^{-1} \gg L \gg \lambda$  ( $\lambda$  is the distance between the dislocations) and  $m^\alpha$  is the dislocation moment's density vector, which describes the loops of radius  $r$ , so that  $r \ll L$ . The vector  $m^\alpha$  is equal to zero outside a solid and is expressed through an average dislocation moment of the loop  $s^\alpha$  and density of the loops  $n^\alpha$  in the following manner:

$$m^\alpha = s^\alpha n^\alpha \quad (17)$$

The following equation is valid for the density of dislocation loops:

$$\partial n^\alpha / \partial t + \text{div } n^\alpha v = 0 \quad (18)$$

The vector of dislocation moment  $s^\alpha$  corresponds to a plate stretched over the vectors "frozen in" into a substance and, then, satisfies the equation following from (1):

$$ds^\alpha / dt = - (s^\alpha \nabla v) + s^\alpha \text{div } v \quad (19)$$

Finally, from (17)-(19) we obtain the equation for the moment's density

$$dm^\alpha/dt = -(m^\alpha \nabla v), \quad (20)$$

which coincides with the equation for  $W^\alpha$ .

The general scheme for introducing dissipative processes into hydrodynamics equations is as follows: dissipative flows and sources are introduced into the equations for different hydrodynamic quantities. Determining in terms of these equations the law of variation for entropy, we obtain a dissipative function. In case of small flows, they can be expressed through generalized thermodynamic forces according to the Onsager relations [7].

In the elasticity theory problems the presence of the dissipation, connected with the dislocations movement, means that the dislocations move with a velocity different from that of the continuum. Let us introduce into (6) the velocity of "slipping"  $V^\alpha$ :

$$\partial \Omega^\alpha / \partial t = \text{rot}[(v + V^\alpha) \Omega^\alpha].$$

For the latter equation to be compatible with the equation for  $W^\alpha$ , a corresponding term must be included in (3):

$$dW^\alpha/dt = -(W^\alpha \nabla v) + [V^\alpha \text{rot} W^\alpha]. \quad (21)$$

Equation (1) for  $I^\alpha$  must be changed according to (2) and (21). In that case macroscopic deformation will be determined not by an averaged deformation of a unit cell (i.e.,  $W^\alpha$  or  $I^\alpha$ ), but by a hydrodynamic velocity  $v$  of the substance. In the general case two types of movement relative to a crystal lattice are possible for dislocations, namely, slipping and creeping over. While creeping over, the dislocation is the source (discharge) of point defects. Therefore, besides an ordinary dissipative flow  $i$ , it is necessary to introduce the source  $Q$  into (15):

$$\partial c / \partial t + \text{div}(cv + i) = Q.$$

The relation between  $Q$  and movement of dislocations is purely geometrical:

$$Q = \sum_{\alpha} (I^\alpha, V^\alpha, \Omega^\alpha) / v_{\alpha}.$$

Similarly we must introduce the flow  $j$  into the equation for the energy. Finally for the dissipative function  $R$  we obtain

$$-TR = j \nabla T + i \nabla \zeta + \sum_{\alpha} [V^\alpha \Omega^\alpha] (D\varepsilon / DW^\alpha + \zeta I^\alpha / v_{\alpha}),$$

where  $D\varepsilon / DW^\alpha$  is the same variational derivative as stands in (14) for  $\sigma_{ijk}$ . The relation between generalized flows and generalized forces can be written in the form [4]

$$\begin{vmatrix} i \\ j \\ V^\alpha \end{vmatrix} = \hat{A} \begin{vmatrix} \nabla \zeta \\ \nabla T \\ [N^\alpha F^\alpha] \end{vmatrix}. \quad (22)$$

Here  $N^\alpha = \Omega^\alpha / |\Omega^\alpha|$ ;  $F^\alpha = D\varepsilon / DW^\alpha + \zeta I^\alpha / v_{\alpha}$ . The matrix  $\hat{A}$  is the matrix of kinetic coefficients.

Formally we must take into account the introduction of dissipative processes into the stress tensor. To this end, into the equations for pulse (9) we must add  $\tau_{ijk}$ , corresponding to a nonequilibrium part of the stress tensor. From the form of dissipative function we obtain that to the given generalized flow  $\tau_{ijk}$  there corresponds the generalized force of the form  $\partial v_i / \partial x_k$ . If there is no any "built-in" vector in the medium, it seems impossible to connect a tensor quantity  $\partial v_i / \partial x_k$  with vector quantities  $i, j, V^\alpha$  in a linear, with respect to  $\partial v_i / \partial x_k$ , approximation. In the given case we have only one vector quantity  $N^\alpha = \Omega^\alpha / |\Omega^\alpha|$ , which is a pseudovector. Therefore, the generalized flows  $i, j, V^\alpha$  are determined only by  $\nabla \zeta, \nabla T, [N^\alpha F^\alpha]$ . In its turn,  $F^\alpha$  is determined by the equilibrium part of the stress tensor  $\sigma_{ijk}$ , which is just considered here. The nonequilibrium part of the stress tensor will influence the crystal's dynamics only through Eq. (9). We ignore these processes, considering viscosity of solids and velocity gradients to be rather small. And in the general case the flow  $V^\alpha$  will depend on all three generalized forces, which stand in the right-hand column of (22).

Let us discuss the case, where  $\zeta = \nabla\zeta = \nabla T = 0$ , i.e., the movement of dislocations is determined by the stresses existing in the medium. In that case the expression for the velocity of dislocation flow has a simple form

$$V_i^\alpha = b^\alpha e_{ijk} N_j^\alpha D\varepsilon / DW_k^\alpha \quad (23)$$

( $b^\alpha$  is the component of the matrix  $\hat{A}$ , corresponding to the mobility of dislocations). Taking into account the expression for the stresses (14) and connection (2), we find  $D\varepsilon / DW_i^\alpha = \sigma_{ik}^\alpha l_k^\alpha$ . Substituting in such form  $D\varepsilon / DW^\alpha$  into (23), we obtain  $V_i^\alpha = b^\alpha f_i^\alpha$ , where  $f_i^\alpha = e_{ijk} \sigma_{kl}^\alpha l_j^\alpha N_k^\alpha$ , which exactly corresponds to the expression for the Pich-Keller force, if we put  $l^\alpha$  equal to Burgers vector [1].

According to the fact that in a crystal a dislocation can move in strictly defined directions, for mobility we should write the tensor  $b_{ik}^\alpha = b_c^\alpha n_i^\alpha n_k^\alpha + b_\Pi^\alpha (\delta_{ik} - n_i^\alpha n_k^\alpha)$  ( $b_c^\alpha$ ,  $b_\Pi^\alpha$  are the coefficients of mobility in the plane of slipping and creeping over, and  $n_i^\alpha = l_i^\alpha / |l^\alpha|$ ). Let us consider the dissipative processes associated with the motion of dislocation loops. If the centers of the loops can move relative to the substance, this corresponds to the introduction into (18) of the dissipative flow  $j^\alpha$ :

$$\partial n^\alpha / \partial t + \text{div}(n^\alpha v + j^\alpha) = 0.$$

For dislocation moment we add to (19) the source  $\xi^\alpha$ , which corresponds to a turn of the loop and/or change in its size:

$$ds^\alpha / dt = -(s^\alpha \nabla v) + s^\alpha \text{div} v + \xi^\alpha.$$

Finally instead of (20) we obtain

$$dm^\alpha / dt = -(m^\alpha \nabla v) - s^\alpha \text{div} j^\alpha + n^\alpha \xi^\alpha.$$

Here growth (collapse) of dislocation loops takes place due to a variation in concentration of point defects; therefore, the corresponding source should be introduced into (15)

$$\partial c / \partial t + \text{div} cv = \sum_\alpha n^\alpha (\xi^\alpha l^\alpha) / v_\alpha.$$

For compatibility of the obtained equations with the equation for  $W^\alpha$ , instead of (3) we have

$$dW^\alpha / dt = -(W^\alpha \nabla v) - s^\alpha \text{div} j^\alpha + n^\alpha \xi^\alpha.$$

We calculate the dissipative function

$$TR = \sum_\alpha \{ (j^\alpha \nabla) (w^\alpha s^\alpha) + n^\alpha \xi^\alpha (w^\alpha + \xi l^\alpha / v_\alpha) \}.$$

In the simplest cases we can write

$$j^\alpha \sim \nabla (w^\alpha s^\alpha), \quad n^\alpha \xi^\alpha \sim (w^\alpha + \xi l^\alpha / v_\alpha).$$

The relation  $w_i^\alpha = \sigma_{ik}^\alpha l_k^\alpha$  yields

$$n^\alpha \xi_i^\alpha \sim (\sigma_{ik} + \xi \delta_{ik} / v_\alpha) l_k^\alpha.$$

Here the second term in the right-hand side is responsible for the growth (collapse) of the loops due to a nonequilibrium concentration of point defects. The same role is played by a normal component  $\sigma_{ik}^\alpha l_k^\alpha$ . The tangential part leads to a turn of loops (to the appearance of screw component of the loop's dislocation line).

For the motion of the center of the loops we have

$$j_i^\alpha \sim \partial (\sigma_{kl} l_l^\alpha s_k^\alpha) / \partial x_i.$$

The part proportional to the  $\partial \sigma_{kl} / \partial x_i$  coincides completely with the force acting on the loop from [1]. The term proportional to  $\sigma_{kl} l_l^\alpha \partial s_k^\alpha / \partial x_i$  is also of interest. It corresponds to the

fact that at constant stresses there exists a flow of loop determined by the gradient from the dimensions. In the general case the introduced dissipative flows and generalized forces must be inserted in relation (22).

As an illustration of the described system of equations let us consider the deformation of a crystal, uniformly filled by immobile straight edge dislocations of one kind. Let a sample have a rectangular section in the plane  $(x, y)$  and be extended along the  $z$ -axis. We assume the problem to be two-dimensional and consider the deformations  $W^1$  and  $W^2$ :  $\text{curl } W^1 = \Omega^1$ ,  $\text{curl } W^2 = 0$ . The dislocations are directed along the  $z$ -axis  $Oz$  ( $\Omega^1 = (0, 0, \Omega)$ ) and are distributed with a constant density ( $\Omega = \text{const}$ ). In the case of stationary deformations we have the equilibrium equation  $\partial \sigma_{ik} / \partial x_k = 0$ . The equality to zero of the forces applied at the boundary yields the boundary condition  $\sigma_{ik} n_k |_{\Gamma} = 0$ , where  $n_k$  is the normal vector. We select the vectors  $W^\alpha$  for an undistorted sample in the form  $\dot{W}^1 = (1/a, 0)$ ,  $\dot{W}^2 = (0, 1/a)$  ( $a$  is the lattice parameter). Then for  $\delta W^\alpha = W^\alpha - \dot{W}^\alpha$  we obtain  $\delta W^1 = (0, -\Omega x/2)$ ,  $\delta W^2 = (\Omega x/2, 0)$ . Here we note that for the given deformations the stresses in the whole crystal are equal to zero:  $\sigma_{ik} = 0$ . The given type of deformations corresponds to the presence of "extra" crystallographic half planes, and the lines of the edge of these half planes are edge dislocations.

As the second example let us consider a stationary flow of a crystal with dislocations under the action of the applied shear stresses. The sample arrangement and dislocations configuration are the same as in the previous example. A shear  $\sigma_{xy} |_{\Gamma} = F$  is applied to the crystal surface, which is perpendicular to the  $y$ -axis. We will assume that the dislocations density is sufficiently small, so that the deformations due to the applied stresses are much larger than the deformations caused by dislocations:  $\Omega L \ll F/\mu a$  ( $L$  is the system's dimension along the  $x$ -axis). Finding  $\delta W^\alpha$  from the equilibrium equation, and, consequently,  $\sigma_{ik}$ , we determine  $V^1$  from (23). The velocity of the medium is found from the stationary equation (21), which is previously linearized with respect to  $\delta W^\alpha$ :

$$(\dot{W}^\alpha v_V) = [V^\alpha \Omega^\alpha].$$

An expression for the velocity has the form  $v_x = b\Omega a^2 F y$  ( $b$  is the coefficient of the dislocation mobility). Note that the dislocations move with the velocity  $V = bFa$ , whence the substance velocity can be expressed in terms of  $V$ :  $v_x = V\Omega a y$ , which corresponds to the conventional formula for the plastic deformation velocity  $\dot{\epsilon} = BNv_d$  (see [2]), where  $B$  is the Burgers vector,  $N$  is the dislocation density, and  $v_d$  is their velocity. Such plastic flow of the sample corresponds formally to the flow of viscous liquid with the viscosity coefficient  $\eta_* = (b\Omega a^2)^{-1}$ .

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