Formation of a step and interaction of defects on the surface of a crystal

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Equations describing capillary deformation of solids are used to consider the quasistatic problem of emergence of an edge dislocation parallel to the surface from the bulk onto the surface of a crystal. It is shown that the surface tension forces allow us to describe the resultant step as a dipole force center with a moment. The elastic interaction of point defects and dislocations with a planar lattice defect (such as a stacking fault) is also considered. It is shown that, because of the surface tension forces, the interaction of point defects and dislocations with a stacking fault in the plane of this fault does not generally have a fixed sign. The energy of the interaction with a point defect decreases in inverse proportion to the fourth power of the distance to the stacking fault plane, whereas the energy of the interaction with a dislocation parallel to this plane is inversely proportional to the first power of the distance.

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A complete system of dynamic equations describing deformation of solids subject to allowance for surface (capillary) phenomena is derived in Ref. 1, and several examples of application of such a system are given. In the present paper we shall determine more accurately the nature of changes in the boundary conditions of bulk dimensional equations of equilibrium on the surface of a solid resulting from capillary effects, and also the explicit dependence of the surface free energy on the strain. Further examples will be given of the application of the resultant equations to problems of formation of a step on the surface of a crystal as a result of quasistatic emergence of an edge dislocation from the bulk and of the elastic interaction of point defects and dislocations with the surface of a stacking fault.

DISCUSSION OF THE SURFACE ENERGY AND BOUNDARY CONDITIONS

It is shown in Ref. 1 that the density of the surface free energy α of an arbitrary two-dimensional defect (including a free surface of a crystal) separating media 1 and 2 obeys, at a given temperature, the following thermodynamic identity:

$$d\alpha=g_{\mu\nu}du_{\mu\nu}+\sigma_{in}d\Delta_i;\quad \mu,\ \nu=1,2;\quad i,\ k=1,\ 2,\ 3. \tag{1}$$

Here, u_{ik} is the strain tensor; σ_{ik} is the bulk stress tensor; $\sigma_{in}=\sigma_{ik}n_k$; $n_i=n_3$ is the unit vector along the normal to the interface directed from medium 1 to medium 2. The indices μ and ν label the coordinate axes in a plane tangential to the defect surface. In Eq. (1) the quantity $g_{\mu\nu}$ is the symmetric tensor of surface elastic stresses and $\Delta_i\equiv u_i^{(2)}-u_i^{(1)}$ is an abrupt change in the displacement vector u_i on the surface of a defect.

We shall describe $g_{\mu\nu}$ and Δ_i by the following linear expansions[1]:

$$\begin{aligned} g_{\mu\nu}&=g_{\mu\nu}^{(0)}-a_{i\mu\nu}\sigma_{in}+h_{\mu\nu\gamma\delta}u_{\gamma\delta},\\ \Delta_i&=a_{i\mu\nu}u_{\mu\nu}+c_{ik}\sigma_{kn}, \end{aligned} \tag{2}$$

where $g_{\mu\nu}^{(0)}$, $a_{i\mu\nu}$, c_{ik}, $h_{\mu\nu\gamma\delta}$ are independent parameters representing the elastic properties of the surface of a two-dimensional defect.

The thermodynamic relationship (1) and the expansion (2) allow us to find α as a function of its independent variables $u_{\mu\nu}$ and Δ_i:

$$\alpha(u_{\mu\nu},\Delta_i)=\frac{1}{2}g_{\mu\nu}^{(0)}\left(\frac{\partial u_\mu}{\partial x_\nu}+\frac{\partial u_\nu}{\partial x_\mu}+\frac{\partial u_l}{\partial x_\mu}\frac{\partial u_l}{\partial x_\nu}\right)$$
$$+\frac{1}{2}(h_{\mu\nu\gamma\delta}+c_{pq}^{-1}a_{p\mu\nu}a_{q\gamma\delta})u_{\mu\nu}u_{\gamma\delta}+\frac{1}{2}c_{ik}^{-1}\Delta_i\Delta_k-2c_{lm}^{-1}a_{l\mu\nu}u_{\mu\nu}\Delta_m, \tag{3}$$

where c_{ik}^{-1} is a tensor which is the reciprocal of the tensor c_{ik}. Equation (3) represents in fact an expansion of the surface energy of a two-dimensional defect in terms of independent invariants (scalars) composed of quadratic combinations of variables describing the state of the surface: $u_{\mu\nu}$ and Δ_i.

The first term in the expansion (3) appears because on the surface of a crystal (or at an interface between two crystals) in equilibrium there are definite residual tangential stresses $g_{\mu\nu}^{(0)}=g_{\mu\nu}^{(0)}(T)$ independent of bulk strains[2] (T is the absolute temperature). In the expansion of the surface energy the surface strain tensor $g_{\mu\nu}^{(0)}$ obtained in the linear theory of elasticity corresponds to the invariant

$$g_{\mu\nu}^{(0)}u_{\mu\nu}=\frac{1}{2}g_{\mu\nu}^{(0)}\left(\frac{\partial u_\mu}{\partial x_\nu}+\frac{\partial u_\nu}{\partial x_\mu}+\frac{\partial u_l}{\partial x_\mu}\frac{\partial u_l}{\partial x_\nu}\right).$$

In terms quadratic in respect of the strain it is usual to assume that

$$u_{\mu\nu}=\frac{1}{2}\left(\frac{\partial u_\mu}{\partial x_\nu}+\frac{\partial u_\nu}{\partial x_\mu}\right).$$

The boundary conditions at an interface can be found by varying with respect to the displacement vector u_i the total bulk and surface free energy F. Application of the identity (1), of the definition of the vector Δ_i, and of the generally valid (in accordance with the above discussion) relationship for a surface

$$\delta u_{\mu\nu}=\frac{1}{2}\left(\frac{\partial\delta u_\mu}{\partial x_\nu}+\frac{\partial\delta u_\nu}{\partial x_\mu}+\frac{\partial u_l}{\partial x_\mu}\frac{\partial\delta u_l}{\partial x_\nu}+\frac{\partial u_l}{\partial x_\nu}\frac{\partial\delta u_l}{\partial x_\mu}\right),$$

yields the following boundary conditions:

$$-\left(\frac{\delta F}{\delta u_i}\right)_T=\nu\ddot{u}_i=\sigma_{in}^{(2)}-\sigma_{in}^{(1)}+\frac{\partial}{\partial x_\mu}g_{i\mu}^{*}. \tag{4}$$

Here, ν is the density of the excess surface mass and

$$g_{i\mu}^{*}=g_{\mu\nu}(\delta_{i\nu}+\partial u_i/\partial x_\nu).$$

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In the adopted approximation, we have

$$g_{i\mu}^{*}=g_{\mu\nu}\delta_{i\nu}+g_{\mu\nu}^{(0)}\,\partial u_i/\partial x_\nu. \qquad (5)$$

We shall now consider the boundary conditions on a plane free surface (ignoring the capillary phenomena so that $\sigma_{in}=0$). If a crystal surface is perpendicular to a sixfold symmetry axis (isotropic model), then the following relationships apply:

$$g_{\mu\nu}^{(0)}=g\delta_{\mu\nu};\quad c_{ik}=c_1\delta_{i\mu}\delta_{k\mu}+c_2n_in_k;$$
$$a_{i\mu\nu}=an_i\delta_{\mu\nu};\quad h_{\mu\nu\gamma\delta}=h_1\delta_{\mu\nu}\delta_{\gamma\delta}+h_2(\delta_{\mu\gamma}\delta_{\nu\delta}+\delta_{\mu\delta}\delta_{\gamma\nu}). \qquad (6)$$

If the z axis is directed along the outer normal to the undeformed surface $z=0$, then the static boundary conditions (4) subject to Eqs. (2), (5), and (16) assume the following form for a free surface:

$$\sigma_{zz}=g\frac{\partial^2u_z}{\partial x_\mu^2},\quad \sigma_{\mu z}=h_1\frac{\partial}{\partial x_\mu}u_{\nu\nu}+2h_2\frac{\partial}{\partial x_\nu}u_{\mu\nu}+g\frac{\partial^2u_\mu}{\partial x_\nu^2}. \qquad (7)$$

The components of the tensor $g_{i\mu}^*$ are subject to uncertainty typical of surface quantities: this uncertainty is due to the doubts about the correct selection of the position of the interface between two media. We shall assume that the initial free surface is displaced in the direction of the normal **n** by a small (of the order of the interatomic) distance ζ. We can show[1] that $g_{i\mu}^*$ is transformed in the following way to $\langle g_{i\mu}^*\rangle$ for the new surface:

$$\langle g_{i\mu}^*\rangle=g_{i\mu}^*-\zeta\sigma_{i\mu}. \qquad (8)$$

In the adopted principal (in respect of the surface parameters) approximation we can calculate $\sigma_{i\mu}$ in Eq. (8) on the assumption that $\sigma_{in}=0$.

Since the tensor $g_{\mu\nu}^{(0)}$ is the zeroth term of the expansion of the tensor $g_{i\mu}^*$ in terms of strains, it cannot change as a result of the assumed displacement of the interface and, therefore, it is independent of the selection of the interface. In other words, the temsor $g_{\mu\nu}^{(0)}$ is a unique characteristic of the surface tension forces. For a planar problem ($u_y=\partial/\partial y=0$), we obtain

$$\langle g_{xx}^*\rangle=g+(g+h_1+2h_2)u_{xx}-\zeta\sigma_{xx},\quad \langle g_{zx}^*\rangle=g_{zx}^*.$$

Using Hooke's law subject to $u_{yy}=\sigma_{zz}=0$, we find that

$$\sigma_{xx}=\frac{E}{1-\sigma^2}u_{xx},$$

where σ is the Poisson ratio and E is the Young modulus. We can see that a suitable selection of the position of the interface (i.e., of ζ) can ensure that the coefficient in front of u_{xx} in the expansion for g_{xx}^* can vanish. We are then left with

$$\langle g_{xx}^*\rangle=g;\quad \langle g_{zx}^*\rangle=g\frac{\partial u_z}{\partial x}. \qquad (9)$$

Consequently, it is clear from Eqs. (7) and (9) that in a static planar problem in the theory of elasticity we can define a homogeneous boundary surface in such a way that it is free of tangential forces of capillary origin.

EMERGENCE OF AN EDGE DISLOCATION TO THE SURFACE

One of the main extended surface defects is a growth step frequently discussed in connection with the problem of crystallization. Recrystallization waves predicted in Ref. 3 and detected in Ref. 4 on the surface of a quantum

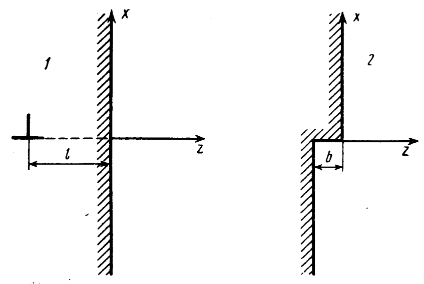

FIG. 1.

crystal have drawn special attention to growth steps as objects whose motion may be responsible for the motion of a crystallization–melting front. The special feature of the motion of discrete steps influences the dynamic properties of a vibrating surface and it makes a contribution to the dispersion law of recrystallization waves.[5]

However, a step on a crystal face may form not only in the process of crystallization but also because of emergence of an edge dislocation parallel to the surface (positions 1 and 2 in Fig. 1 illustrate the cases when a dislocation is in the bulk and on the surface). On the other hand, an edge dislocation can, in principle, be created in the bulk of a crystal by applying a load that suppresses a surface step. Therefore, there should be a definite correspondence between the properties of an edge dislocation and a surface step, both being sources of elastic stresses in a crystal. It is shown in Refs. 1 and 2 that, because of the surface tension forces, steps should create elastic stresses in the bulk. We shall demonstrate below that these stresses are governed by the properties of an edge dislocation that could create such a step by emerging on the surface.[12]

We shall seek the solution of the bulk equilibrium equations in the form

$$u_i=u_i^0+u_i^1,\quad \sigma_{ik}=\sigma_{ik}^0+\sigma_{ik}^1,$$

where u_i^0 and σ_{ik}^0 represent the solutions obtained without allowance for the capillary phenomena, i.e., the solutions obtained subject to the boundary condition $\sigma_{in}^0=0$. The fields u_i^1 and σ_{ik}^1 can be found by the method of successive approximations without exceeding the adopted degree of accuracy. In the case of a planar problem corresponding to $u_y=\partial/\partial y=0$ the boundary conditions (7) for σ_{ik}^1 subject to Eq. (9) assume the following form on a free surface ($z=0$):

$$\sigma_{zz}^1=g\frac{\partial^2u_z^0}{\partial x^2},\quad \sigma_{zx}^1=0. \qquad (10)$$

We shall rewrite the right-hand side of the first condition (10) in terms of σ_{ik}^0. We note that in accordance with Hooke's law

$$\frac{\partial u_z}{\partial x}+\frac{\partial u_x}{\partial z}=2\frac{1+\sigma}{E}\sigma_{zx},$$

and therefore

$$\frac{\partial^2u_z}{\partial x^2}=2\frac{1+\sigma}{E}\frac{\partial\sigma_{zx}}{\partial x}-\frac{\partial u_{xx}}{\partial z}=2\frac{1+\sigma}{E}\frac{\partial\sigma_{zx}}{\partial x}-\frac{1-\sigma^2}{E}\frac{\partial\sigma_{xx}}{\partial z}+\frac{(1+\sigma)\sigma}{E}\frac{\partial\sigma_{zz}}{\partial z}$$

because for a planar problem we have

$$u_{xx}=\frac{1-\sigma^2}{E}\sigma_{xx}-\frac{(1+\sigma)\sigma}{E}\sigma_{zz}.$$

We shall now use the equilibrium equation

$$\frac{\partial\sigma_{zx}}{\partial x}+\frac{\partial\sigma_{zz}}{\partial z}=0$$

and the fact that on a free surface we have $\sigma^0_{zx}=0$ so that

$$\frac{\partial\sigma_{zx}{}^0}{\partial x}\Big|_{z=0}=\frac{\partial\sigma_{zz}{}^0}{\partial z}\Big|_{z=0}=0.$$

Consequently, on a free surface $z=0$, we have

$$\frac{\partial^2 u_z{}^0}{\partial x^2}=-\frac{1-\sigma^2}{E}\frac{\partial\sigma_{xx}{}^0}{\partial z}. \qquad (11)$$

We shall consider an edge dislocation parallel to a free surface $z=0$ located on the line $x=0$, $z=-l$ (Fig. 1) and characterized by a Burgers vector $\mathbf{b}(0,0,b)$ perpendicular to the surface. If an explicit expression for σ^0_{xx} is substituted in Eq. (11) (see, for example, Sec. 3–5 in Ref. 6), the first condition in Eq. (10) becomes

$$\sigma_{zz}{}^1=-gb\frac{8}{\pi}\frac{l^3x}{(l^2+x^2)^3}. \qquad (12)$$

We shall be interested in fields at distances r from a dislocation much greater than $l\,(r\gg l)$. This is equivalent to going to the limit $l\to 0$ in Eq. (12). In this limit the boundary condition (12) becomes

$$\sigma_{zz}{}^1=gb\frac{\partial}{\partial x}\delta(x),$$

where $\delta(x)$ is the Dirac δ function. The field σ^0_{ik} disappears in the limit $l=0$ and, therefore, the bulk elastic fields created by a newly formed step are subject to the following boundary conditions:

$$\sigma_{zz}|_{z=0}=gb\frac{\partial}{\partial x}\delta(x),\qquad \sigma_{zx}|_{z=0}=0. \qquad (13)$$

The density of the force normal to the surface $P_z=\sigma_{zz}$ under the conditions described by Eq. (13) is equal exactly to the density obtained earlier[1,2] for a step of height b. This force characterizes a step as a center of a dipole force with a moment. The problem of compensation of the moment of this force is eliminated by assuming that the emergence of a dislocation on the $x=z=0$ line is accompanied by the simultaneous emergence of a dislocation of the opposite sign on a surface at infinity $x=\infty, z=0$. Such a dislocation creating on that surface a center of a dipole force with a moment of opposite sign is associated with a second edge of an extraatomic layer carried to a given crystal face by an edge dislocation.

We shall study geometric changes in the surface in the limit $l\to 0$. When a dislocation emerges from a crystal, it gives rise to plastic deformation concentrated on its surface[7]:

$$\frac{\partial u_z{}^{\mathrm{pl}}}{\partial z}=b\delta(z)\theta(x),$$

where $\theta(x)$ is the Heaviside unit function.

The part of the crystal surface above the glide plane of the dislocation $(x>0)$ experiences a residual plastic displacement by an amount equal to the Burgers vector:

$$u_z{}^{\mathrm{pl}}=\begin{cases} b, & z=0,\quad x>0;\\ 0, & z=0,\quad x<0.\end{cases}$$

The residual displacement alters the shape of the surface creating a characteristic step of height b.

We shall now consider the emergence of a dislocation whose Burgers vector is parallel to the surface. We shall assume that this dislocation is located as before and that its Burgers vector is $\mathbf{b}(b,0,0)$. The elastic stress field σ^0_{ik} in the half-space $z<0$ can be described by a superposition of three fields: the field of a dislocation located on the line $x=, z=-l$ in an infinite crystal, the field of an image dislocation on the $x=0, z=l$ line, and an additional field $\tilde{\sigma}_{ik}$ ensuring that the boundary conditions $\sigma^0_{in}=0$ are satisfied on the $z=0$ surface.

The stress function $\tilde{\psi}(x,z)$ describing the planar field $\tilde{\sigma}_{ik}$ can be described by the following expression:

$$\tilde{\psi}(x,z)=\frac{\mu bl}{\pi(1-\sigma)}\left\{\frac{z(l-z)}{x^2+(l-z)^2}+\frac{1}{2}\ln[x^2+(l-z)^2]\right\},$$

where μ is the shear modulus. A logarithmic divergence of $\tilde{\psi}$ at high values of z does not give rise to any physical inconsistencies, because real fields $\tilde{\sigma}_{ik}$ are governed by the second derivatives with respect to $\tilde{\psi}$, particularly

$$\tilde{\sigma}_{xx}=\partial^2\tilde{\psi}/\partial z^2.$$

If we now substitute σ^0_{xx} in Eq. (11), we find that the first condition of Eq. (10) becomes

$$\sigma_{zz}{}^1=P(x,l)\equiv gb\frac{2l^3(3x^2-l^2)}{\pi(x^2+l^2)^3}.$$

We shall consider the properties of the function $P(x,l)$ in the limit $l\to 0$, i.e., we shall find $P(x,0)$. We note that

$$P=0\ \text{for}\ l=0,\ x\neq 0,$$

$$\int_{-\infty}^{\infty}P(x,l)\,dx=0\quad\text{for}\quad l\neq 0.$$

Therefore, we should assume that $P(x,0)=0$. Therefore, both fields σ^0_{ik} and σ^1_{ik} vanish in the limit $l=0$. Hence, it follows that after emergence of a given dislocation on the surface there are no residual elastic stresses in a crystal.

This result is quite self-evident from the physical point of view. We shall consider plastic deformation which appears in a crystal as a result of emergence of such a dislocation on the surface. This plastic deformation can be assumed to be concentrated in the $x=0$ plane perpendicular to the free plane:

$$\frac{\partial u_x{}^{\mathrm{pl}}}{\partial x}=b\delta(x)[1-\theta(z+l)].$$

After the emergence of a dislocation on the surface $(l=0)$ half a crystal experiences a homogeneous residual displacement along the x axis by the vector $\mathbf{b}$. There is no change in the physical state of the crystal and there are no residual elastic stresses.

In view of the linearity of the theory, these results can be generalized to the case when a step is formed by emergence of an edge dislocation with a Burgers vector $\mathbf{b}$ making an arbitrary angle with the normal $\mathbf{n}$ to the surface. The elastic fields in the bulk of a crystal are subject to the following boundary conditions:

$$\sigma_{nn}=g\mathbf{bn}\frac{\partial}{\partial x}\delta(x),\qquad \sigma_{nx}=0.$$

Here the x axis is drawn on the surface at right-angles to the dislocation line in such a way that $\mathbf{b}\cdot\mathbf{n}>0$ and $b_x>0$ are satisfied simultaneously. Consequently, the resultant step with $\mathbf{b}\cdot\mathbf{n}>0$ can be called positive, whereas that with $\mathbf{b}\cdot\mathbf{n}<0$ may be called negative.

It is worth noting that an edge dislocation regarded as a lattice defect in the bulk does not carry to the surface a zero-moment dipole force, introduced phenomenologically in Refs. 1 and 2. This may be associated with a change in the dislocation core as a result of its transformation from a lattice into a surface defect,[8] and a calculation of such a force requires an appropriate microscopic analysis.

ELASTIC INTERACTION OF POINT DEFECTS AND DISLOCATIONS WITH THE SURFACE OF A STACKING FAULT

It is known that two-dimensional lattice defects exist in the bulk of real single crystals: these may be, for example, stacking faults with split partial dislocations as boundaries.[6,9] They include intrinsic stacking faults, extrinsic stacking faults, and associated thin twin layers. These defects can be generated by shear (this is true, for example, of close-packed {111} planes in fcc crystals) or by the conditions during growth of a real crystal. A general distinguishing feature of all the stacking faults is that a modification of the regular crystal structure is concentrated in a volume extending to several atomic layers near the plane of the defect and outside this region the atomic planes retain their regular sequence which is the same on both sides of the fault.

An excess surface energy is associated with the plane of a stacking fault. Moreover, since these faults retain a dense packing, it follows that they are generally characterized by a low surface energy compared with free surfaces or interfaces where the bonds with the nearest neighbors are deformed or broken (for example, in the case of grain boundaries of free surfaces). Planes with a low energy of a stacking fault usually coincide with glide planes of a crystal.

The special feature of the elastic interaction of point defects and dislocations with a stacking fault is that the density and elastic moduli on both sides of the fault plane are exactly the same. Therefore, this interaction vanishes in the absence of surface phenomena (when the edge defects can be neglected). A similar situation occurs also when sound is reflected from a stacking fault.[1] The energy of a stacking fault in an external elastic field can be found by expanding its surface energy (3) in terms of the components of the strain tensor of this field calculated in the absence of a stacking fault. The energy of the elastic interaction of a stacking fault with sources of an external field (point defects and dislocations) determines the direction of slow diffusion of the latter in the process of establishment of their equilibrium distribution near the stacking fault plane.

Since the surface energy contributes only a small correction to the bulk part of the total deformation energy of a crystal, the sign of Eq. (3) corresponding to arbitrary values of Δ_i and $u_{\mu\nu}$ is generally indeterminate [we can only say that for all values of σ_{in} there should be positive definite quadratic forms $c_{ik}\sigma_{in}\sigma_{kn}$ and $(c_{ik}+h_{\mu\nu\gamma\delta}c_{il}c_{km}a^{-1}_{l\mu\nu}a^{-1}_{m\gamma\delta})\sigma_{in}\sigma_{kn}$]. This means that the required total (bulk and surface) energy of a stacking fault in an external elastic field (see Ref. 1)

$$U=\frac{1}{2}\int\alpha(x_\mu,x_\nu)\,d^2x \tag{14}$$

can have either sign. The integral in Eq. (14) is taken over the undeformed surface of a stacking fault. The linear term

$$g^{(0)}_{\mu\nu}\left(\frac{\partial u_\mu}{\partial x_\nu}+\frac{\partial u_\nu}{\partial x_\mu}\right)$$

represents only a small contribution of the edges of the fault to this integral, because it represents the surface divergence. Hence, we may conclude that the elastic interaction of point defects and dislocations with a stacking fault generally does not have a definite sign: depending on the orientation of the fault plane relative to the crystallographic axis, we can expect attraction or repulsion from the object under investigation.

We can use Eq. (14) only if we know the surface energy density as a function of the coordinates on the surface of a stacking fault. Therefore, we shall transform Eq. (3) using the second relationship in Eq. (2). This gives

$$\alpha(x_\mu,x_\nu)=\frac{1}{2}g^{(0)}_{\mu\nu}\left(\frac{\partial u_\mu}{\partial x_\nu}+\frac{\partial u_\nu}{\partial x_\mu}+\frac{\partial u_l}{\partial x_\mu}\frac{\partial u_l}{\partial x_\nu}\right)$$
$$+\frac{1}{2}(h_{\mu\nu\gamma\delta}-2c^{-1}_{lm}a_{l\mu\nu}a_{m\gamma\delta})u_{\mu\nu}u_{\gamma\delta}+\frac{1}{2}c_{pq}\sigma_{pn}\sigma_{qn}-a_{l\mu\nu}u_{\mu\nu}\sigma_{ln}, \tag{15}$$

where $\sigma_{ik}=\lambda_{iklm}u_{lm}$, λ_{iklm} are the elastic moduli.

In the isotropic case, Eq. (15) becomes

$$\alpha(x_\mu,x_\nu)=g\left[\frac{\partial u_\mu}{\partial x_\mu}+\frac{1}{2}\left(\frac{\partial u_i}{\partial x_\mu}\right)^2\right]$$
$$+\frac{1}{2}\left(h_1-2\frac{a^2}{c_2}\right)u_{\mu\mu}^2+h_2u_{\mu\nu}^2+\frac{c_1}{2}\sigma_{\mu n}^2+\frac{c_2}{2}\sigma_{nn}^2-a\sigma_{nn}u_{\mu\mu}. \tag{16}$$

Substituting Eq. (15) or (16) into Eq. (14), we find the required energy of the elastic interaction of a stacking fault with a source of the field u_i.

Since our aim is to demonstrate a certain phenomenon, we shall confine ourselves to an isotropic solid. In the isotropic model a point defect (interstice or vacancy) is a dilatation center which creates an elastic displacement field of the following type[10] (it is assumed that the defect is located at the coordinate origin):

$$\mathbf{u}(\mathbf{r})=-\frac{\Omega_0}{12\pi}\frac{1+\sigma}{1-\sigma}\,\mathrm{grad}\,\frac{1}{r}. \tag{17}$$

Here, Ω_0 is the increase in the volume of a crystal caused by the presence of a point defect.

Let us assume that the stacking fault plane is $z=l$. Using Eqs. (16) and (17), we can show that the energy of $U=U(l)$ representing the interaction of a stacking fault with a dilatation center is

$$U(l)=\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\alpha(x,y,l)\,dx\,dy=A/l^4,$$
$$A=\frac{3\pi}{16}\left(\frac{\Omega_0}{12\pi}\frac{1+\sigma}{1-\sigma}\right)^2\left[h_1+4\mu a-\frac{2a^2}{c_2}+h_2+2g+4\mu^2(c_1+c_2)\right]. \tag{18}$$

It is clear from Eq. (18) that the interaction parameter A is independent of the sign Ω_0 (it is the same for an interstice or a vacancy), because the interaction itself is essentially of polaron origin. It is clear that the interaction law $U(l) \propto 1/l^4$ of Eq. (18) applies also to an arbitrary point defect in an anisotropic medium described by a bulk density of forces[10]:

$$f_i(\mathbf{r}) = -K\Omega_{ik}\frac{\partial}{\partial x_k}\delta(\mathbf{r}),$$

where K is the bulk modulus and Ω_{ik} is a symmetric tensor representing the strength of a point defect (for a dilatation center we have $\Omega_{ik} = \Omega_0\delta_{ik}$). In this case the required interaction energy should be calculated by utilizing in Eq. (15) not Eq. (17) but the following expression[10]:

$$u_i(\mathbf{r}) = -K\Omega_{kl}\frac{\partial}{\partial x_l}G_{ik}(\mathbf{r}),$$

where $G_{ik}(\mathbf{r})$ is the static Green tensor of an ideal (defect-free) unbounded anisotropic crystal.

Let us assume that a distribution of point defects forms a dilute solution in a crystal. Then, the equilibrium concentration c of point defects near the plane of a stacking fault is related to the concentration c_0 far from the fault:

$$c = c_0 \exp\left\{-\frac{U}{T}\right\} = c_0 \exp\left\{-\frac{A}{Tl^4}\right\}. \tag{19}$$

Near the planes of those stacking faults for which $A < 0$ (attraction case), we find from Eq. (19) that there is a region where the distribution of point defects is denser and the width of this region is $d = 2(|A|/T)^{1/4}$. However, if $A > 0$ (repulsion) then near the plane of such a stacking fault there is a region where the density of point defects is less (its width is of the order of d). In terms of the Gibbs adsorption isotherm this means that if $A < 0$ then $(\partial\alpha/\partial\mu_2)_T < 0$ (μ_2 is the chemical potential of an impurity atom) and impurities are adsorbed on a stacking fault, whereas for $A > 0$ we have $(\partial\alpha/\partial\mu_2)_T > 0$ and desorption occurs.

This effect simulates the Suzuki effect[11] of the interaction between split dislocations with impurities and atoms in a solid solution by their adsorption on a stacking fault. The parameter d is the effective width of a split dislocation in the process of adsorption of impurity atoms when the latter form a dilute solution.

We shall now consider an edge dislocation parallel to the defect plane $z = l$. We shall assume that the dislocation is located on the $x = z = 0$ line and has the Burgers vector $\mathbf{b}(0, 0, b)$ perpendicular to the stacking fault plane. Using the familiar expressions for the elastic field of an edge dislocation, we can show that the required interaction energy per unit length of the dislocation is

$$U(l) = \frac{1}{2}\int_{-\infty}^{\infty}\alpha(x, l)\,dx = \frac{B}{l},$$

$$B = \frac{b^2}{256\pi(1-\sigma)^2}\left\{\left(h_1 + 2h_2 - \frac{2a^2}{c_2}\right)(8\sigma^2 - 4\sigma + 1) + 2g(8\sigma^2 - 12\sigma + 7) + 4\mu^2(c_1 + 5c_2) + 4\mu a(6\sigma - 1)\right\}. \tag{20}$$

Clearly, the interaction law $U(l) \propto 1/l$ given by Eq. (20) is retained for an arbitrary rectilinear dislocation (both edge and screw) parallel to the stacking fault plane. The parameter B for an anisotropic medium depends on the orientation of the dislocation line in the stacking fault plane.

The results obtained can be applied to the motion of a dislocation near the stacking fault plane provided we bear in mind that the interaction of point defects with a dislocation decreases with distance much more slowly than the interaction with the stacking fault plane (the corresponding laws are $1/r$ and $1/l^4$). Therefore, formation of an atmosphere of Cottrell and Snoek point defects near a dislocation line and of a Suzuki atmosphere near the stacking fault plane are two independent processes. We can thus investigate independently the influence of these atmospheres on the drag experienced by a dislocation near the stacking fault plane.

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[1]A. F. Andreev and Yu. A. Kosevich, Zh. Eksp. Teor. Fiz. **81**, 1435 (1981) [Sov. Phys. JETP **54**, in press (1981)].
[2]V. I. Marchenko and A. Ya. Parshin, Zh. Eksp. Teor. Fiz. **79**, 257 (1980) [Sov. Phys. JETP **52**, 129 (1980)].
[3]A. F. Andreev and A. Ya. Parshin, Zh. Eksp. Teor. Fiz. **75**, 1511 (1978) [Sov. Phys. JETP **48**, 763 (1978)].
[4]K. O. Keshishev, A. Ya. Parshin, and A. V. Babkin, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 63 (1979) [JETP Lett. **30**, 56 (1979)].
[5]A. M. Kosevich and Yu. A. Kosevich, Fiz. Nizk. Temp. **7**, 809 (1981) [Sov. J. Low. Temp. Phys. **7**, in press (1981)].
[6]J. P. Hirth and J. Lothe, Theory of Dislocations, McGraw-Hill, New York, 1968 (Russ. Transl., Atomizdat, M., 1972).
[7]A. M. Kosevich, Dislokatsii v teorii uprugosti (Dislocations in the Theory of Elasticity), Naukova Dumka, Kiev, 1978.
[8]M. J. Marcinkowski, Phys. Status Solidi A **38**, 223 (1976).
[9]N. W. Ashcroft and N. D. Mermin, Solid State Physics, Holt, Rinehart and Winston, New York, 1976 (Russ. Transl., Mir, M., 1979).
[10]A. M. Kosevich, Osnovy mekhaniki kristallicheskoĭ reshetki (Fundamentals of Crystal Lattice Mechanics), Nauka, M., 1972.
[11]H. Suzuki, Sci. Rep. Res. Inst. Tohoku Univ. Ser. A **4**, 455 (1952); J. Phys. Soc. Jpn. **17**, 322 (1962).
[12]A. M. Kosevich and Yu. A. Kosevich, Fiz. Nizk. Temp. **7**, 1347 (1981) [Sov. J. Low. Temp. Phys. **7**, in press (1981)].

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