Capillary phenomena in the theory of elasticity

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A complete system of equations describing the capillary deformation of solids in the presence of crystallite boundaries and other two-dimensional defects, free surfaces, or interfaces between different solids is derived. The coefficient of capillary reflection of sound from stacking faults and the energy of interaction between the point defects and the growth steps on a crystal surface are calculated.

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There occur in solids, in contrast to liquids, two different types of capillary phenomena,[1-4] corresponding to the presence in these bodies of two different types of particle motion. In the first case we have phenomena of the type of the establishment of the equilibrium shape of crystals, or the influence of interfaces on particle-number-related phase equilibrium. The decisive role in this case is played by the slow diffusion processes of reconstruction of the shape of the solids and by the value of the surface energy at a boundary.

The phenomena of the second type, which are the subject of the present paper, are connected with the possibility of elastic deformation associated with a given shape of a solid in the undeformed state. We have in mind the consideration, within the framework of the macroscopic elasticity theory, of capillary effects of the Laplace-pressure type in the presence of interfaces between different solids, crystallite boundaries, all kinds of two-dimensional defects, or, finally, free surfaces of solids. The main quantities that characterize a surface in the present case are the surface mass and the derivatives of the surface energy with respect to the elements of the strain (or stress) tensor, in particular, the surface elastic stress tensor introduced by Herring.[3] It is important to emphasize that the processes of reconstruction of the shape of a solid are extremely slow. If we consider the system during a significantly shorter period of time, i.e., a period during which it, in fact, behaves like a solid, then the problem of the computation of the capillary elastic strains makes sense for solids of arbitrary, and not just equilibrium, shapes.

Although capillary deformation is a relatively weak effect [at equilibrium its magnitude is of the order of the ratio of the interatomic distance to the characteristic dimensions of the sample (see Ref. 3)], it plays a decisive in a number of problems.[3,4] Capillary deformation is the dominant mechanism underlying the fairly long-range interaction between surface point or linear defects and impurities.[5-8] Capillary striction effects play an important role in two-dimensional phase transitions on crystal surfaces.[9,10]

The surface stress tensor is defined in Ref. 3 as made up of the derivatives of the surface energy with respect to the elements of the strain tensor, and has then in the general case five independent elements. Treating the surface strains as if they arose in some effective film on the surface, Marchenko and Parshin[8] arrived at the correct conclusion that the surface stress tensor has only three independent elements. But they, like Herring,[3] did not clarify the exact thermodynamic meaning of this tensor. In the present paper we give the exact definition of the surface stress tensor, derive a complete system of dynamic equations for the determination of the capillary strains, and consider several examples of their application.

1. SURFACE DYNAMICS

The problem of the determination of the effect of capillary phenomena on the elastic properties of solids amounts to the problem of the elucidation of the boundary conditions for the equations of volume elasticity theory at an interface between solids or at the surface corresponding to a two-dimensional lattice defect. The form of these conditions can be established on the basis of the momentum conservation law. Let ν be the mass of material on a unit surface area. This quantity can be positive or negative, depending on whether the defect in question is a region of compression or one of rarefaction. The time derivative of the surface momentum

$$\int dS \nu \ddot{u}_i, \tag{1}$$

where u_i is the displacement vector of the medium and the integral is evaluated over the surface in question, should, on account of the conservation of momentum, be equal to the sum of the momentum fluxes arriving at the surface from the contiguous media 1 and 2:

$$\int dS (\sigma_{in}^{(2)} - \sigma_{in}^{(1)}). \tag{2}$$

Here $\sigma_{ik}^{(1,2)} = \lambda_{iklm}^{(1,2)} u_{lm}^{(1,2)}$ is the volume stress tensor, which coincides up to its sign with the momentum flux tensor, $\lambda_{iklm}^{(1,2)}$ is the elasticity tensor, u_{ik} is the strain tensor, and $\sigma_{in} = \sigma_{ik} n_k$, n_i being the unit vector, directed from the medium 1 to the medium 2, along the normal to the surface.

We shall denote by the symbols $A_{i'}, A_{i'k}$ the tangential parts of the vectors and tensors A_i, A_{ik}, i.e.,

$$A_{i'} = A_i - n_i n_l A_l, \qquad A_{i'k} = A_{ik} - n_i n_l A_{lk},$$

or the vectors and tensors $B_{i'}, B_{i'k}$, which by themselves satisfy the conditions $B_{i'} n_i = 0$, $B_{i'k} n_i = 0$. Then integrals of the type

$$\int dS \nabla_{i'} A_{i'k},$$

where $\nabla_i = \partial/\partial x_i - n_i n_i \partial/\partial x_l$, evaluated over an arbitrary surface, reduce to contour integrals with the boundary of the surface as the contour. It is therefore clear that,

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for the integrals (1) and (2) to be equal, it is necessary that the difference between the integrands be equal to some two-dimensional divergence:

$$\nu\ddot{u}_i+\sigma_{in}^{(1)}-\sigma_{in}^{(2)}=\nabla_{k'}g_{ik'}. \tag{3}$$

The tensor $g_{ik'}$ is the surface stress tensor, the element g_{ik} coinciding up to its sign with the flux of the i-th component of the momentum along the k-th direction on the surface. Kompaneets and one of us[11] have shown in connection with the problem of surface phenomena in superconducting liquids that the condition for the conservation of angular momentum (in the linear approximation under consideration here) imposes on the tensor $g_{ik'}$ the following limitations:

$$g_{nk'}=0, \quad g_{i'k'}=g_{k'i'}, \tag{4}$$

so that the tensor indeed has only three independent elements.

The quantities ν and $g_{ik'}$ entering into Eq. (3), like most surface quantities, are, generally speaking, arbitrary as a result of the ambiguity in the choice of the surface dividing the media under consideration. Let us suppose that the original interface shifts in the direction of the normal **n** through a small (of the order of the interatomic distance) distance ξ, and let us find how the quantities ν and $g_{ik'}$ then transform. The values of $\sigma_{in}^{(1,2)}$ on the new surface are equal to

$$\bar{\sigma}_{in}^{(1,2)}=\sigma_{in}^{(1,2)}+\frac{\partial\sigma_{in}^{(1,2)}}{\partial n}\xi. \tag{5}$$

Expressing the normal derivatives of $\sigma_{in}^{(1,2)}$ in terms of $\nabla_{k'}\sigma_{ik'}^{(1,2)}$ and $\ddot{u}_i$ with the aid of the volume equations $\rho\ddot{u}_i=\partial\sigma_{ik}/\partial x_k$, where ρ is the volume density, substituting the result into (5), and using (3), we find

$$\bar{\sigma}_{in}^{(1)}-\bar{\sigma}_{in}^{(2)}=\nabla_{k'}\bar{g}_{ik'}-\bar{\nu}\ddot{u}_i,$$

where

$$\bar{g}_{ik'}=g_{ik'}-\xi(\sigma_{ik}^{(1)}-\sigma_{ik}^{(2)}), \quad \bar{\nu}=\nu+(\rho^{(2)}-\rho^{(1)})\xi. \tag{6}$$

We can now neglect the small contribution of the surface, i.e., assume that the condition (3) with $\nu=g_{ik'}=0$ is fulfilled, when we substitute the stresses σ_{ik} into the first of the formulas (6). Then we find in accordance with (4) that

$$\bar{g}_{nk'}=g_{nk'}, \quad \bar{g}_{i'k'}=g_{i'k'}-\xi(\sigma_{in}^{(1)}-\rho_{ik}^{(2)}).$$

If the surface under consideration is a boundary between bodies with different densities, then we can choose ξ such that the surface mass is equal to zero. But in the case of crystallite boundaries or other plane defects in the crystal, the surface mass ν does not depend on the choice of the surface.

To elucidate the thermodynamic meaning of the tensor $g_{ik'}$, let us note that the expression $\nabla_{h'}g_{i'k'}-\sigma_{in}^{(1)}+\sigma_{in}^{(2)}$ is a force applied to a unit area of the surface. This force is determined by the variational derivative,

$$\delta E/\delta u_i=\sigma_{in}^{(1)}-\sigma_{in}^{(2)}-\nabla_{k'}g_{i'k'} \tag{7}$$

of the total energy of the system with respect to the components of the displacement vector at the boundary. Here the total energy is equal to the sum of the ordinary volume energy E_v and the surface energy

$$E_s=\int\alpha dS, \tag{8}$$

where α is the energy per unit surface area. By neglecting the effects of the thermal-expansion type, we do not, distinguish between energy and free energy. In contrast to Shuttleworth[2] and Herring,[3] we shall assume, as is usually done in the theory of elasticity, that the integration in the formula (8) is performed over a singular surface in the undeformed solid. Let us emphasize that, in the presence, as a result of capillary effects, of singular surfaces, the crystal is inhomogeneously deformed in its equilibrium state. The term "undeformed solid" implies the absence of this deformation as well.

The quantity α depends on the state of the contiguous media, i.e., in our case on the values of $u_{ik}^{(1)}$ and $u_{ik}^{(2)}$. But these twelve parameters cannot, naturally, be considered to be independent arguments of the function $\alpha(u_{ik}^{(1)},u_{ik}^{(2)})$. The point is that, since the contribution of the surface to all phenomena is small, we should assume that α is defined only for those values of the variables $u_{ik}^{(1)}$ and $u_{ik}^{(2)}$ that can be realized when the surface effects are neglected. In the latter case, on account of the continuity of the displacement vector, we have $u_{i'k'}^{(1)}=u_{i'k'}^{(2)}=u_{i'k'}$, and, moreover, if in place of u_{in} we introduce the stresses σ_{in}, then $\sigma_{in}^{(1)}=\sigma_{in}^{(2)}=\sigma_{in}$. The variables $u_{i'k'}$ and σ_{in} can be considered to be independent.

The displacement vector is no longer continuous across the boundary when the surface effects are taken into consideration. The difference $\Delta_i=u_i^{(2)}-u_i^{(1)}$ is some function of the variables $u_{i'k'}$ and σ_{in}, and can, in the linear approximation, be written in the form

$$\Delta_i=a_{ik'l'}u_{k'l'}+b_{ik}\sigma_{kn}. \tag{9}$$

The coefficients $a_{ik'l'}$ and b_{ik} can be expressed in terms of the $u_{i'k'}$ and σ_{in} derivatives of the surface energy α. To find this relation, let us note that the surface energy α, considered as a function of the variables $u_{i'k'}$ and Δ_i, satisfies the obvious relation

$$\sigma_{in}=(\partial\alpha/\partial\Delta_i)_{u_{i'k'}}, \tag{10}$$

so that the following thermodynamic identity is valid:

$$d\alpha=g_{i'k'}du_{i'k'}+\sigma_{in}d\Delta_i.$$

The quantities $g_{i'k'}$, which are, by definition, equal to the $u_{i'k'}$ derivatives of α at constant Δ_i, coincide, as we shall show below, with the elements of the surface stress tensor. Let us introduce the new thermodynamic potential $\bar{\alpha}=\alpha-\sigma_{in}\Delta_i$, which satisfies the identity

$$d\tilde{\alpha}=g_{i'k'}du_{i'k'}-\Delta_i d\sigma_{in}.$$

From it we immediately obtain a formula of the form (9) with

$$a_{ik'l'}=-\left.\frac{\partial^2\tilde{\alpha}}{\partial\sigma_{in}\partial u_{k'l'}}\right|_0, \quad b_{ik}=-\left.\frac{\partial^2\tilde{\alpha}}{\partial\sigma_{in}\partial\sigma_{kn}}\right|_0, \tag{11}$$

where the index 0 indicates that the derivatives are evaluated at $\sigma_{in}=u_{i'k'}=0$. Since for $u_{i'k'}=0$ the surface energy α as a function of Δ_i should have a minimum at $\Delta_i=0$, the quantities b_{ik} satisfy the conditions for the quadratic form $b_{ik}\sigma_{in}\sigma_{kn}$ to be positive definite for all σ_{in}. Similarly, we obtain for $g_{i'k'}$ the expression

$$g_{i'k'}=g_{i'k'}^{(0)}-a_{li'k'}\sigma_{ln}+h_{i'k'l'm'}u_{l'm'}, \tag{12}$$

in which

$$g^{(0)}_{i'k'}=\frac{\partial\tilde{\alpha}}{\partial u_{i'k'}}\bigg|_0,\quad h_{i'k'l'm'}=\frac{\partial^2\tilde{\alpha}}{\partial u_{i'k'}\partial u_{l'm'}}\bigg|_0\,. \tag{13}$$

Using the given relations, we can proceed in the formulas (11) and (13) directly to the derivatives of α. We shall not, however, write out the corresponding obvious, but more unwieldy formulas.

Let us now write down the variation of the total surface energy:

$$\delta E_s=\int dS\{g_{i'k'}\nabla_{k'}\delta u_i+\sigma_{in}\delta\Delta_i\}=\int dS\{\sigma_{in}(\delta u_i^{(2)}-\delta u_i^{(1)})-\delta u_i(\nabla_{k'}g_{i'k'})\}. \tag{14}$$

The variation of the volume energy is equal to

$$\delta E_v=\int dS\{\sigma_{in}^{(1)}\delta u_i^{(1)}-\sigma_{in}^{(2)}\delta u_i^{(2)}\}\approx\int dS\{(\sigma_{in}^{(1)}-\sigma_{in}^{(2)})\delta u_i-\sigma_{in}(\delta u_i^{(2)}-\delta u_i^{(1)})\}. \tag{15}$$

The variational derivative of the sum E_v+E_s with respect to u_i coincides with the expression (7), which proves the above-stated assertion that the quantities (12) are equal to the elements of the surface stress tensor.

The Eqs. (3), (9), and (12) together with the volume equations of elasticity theory constitute a complete system of equations determining surface dynamics.

2. REFLECTION OF SOUND FROM STACKING FAULTS

The equations obtained can be used to compute the reflection and transformation of acoustic waves incident on a plane, two-dimensional lattice defect of the stacking-fault type. A characteristic of this case lies in the fact that the density and the elastic compliance coefficients have exactly equal values on the two sides of the singular surface, and therefore in the absence of capillary effects sound passes through the surface without any changes. Let

$$u_i=A_0e_ie^{i\mathbf{kr}-i\omega t} \tag{16}$$

be the displacement vector in the incident wave, where A_0 is the amplitude and e_i is unit polarization vector. Allowance for the capillary effects leads to the appearance in the expression (16) for the displacement a small correctional term. $\Delta\mathbf{u}$, that is, in order of magnitude, equal to the ratio of the interatomic distance to the wavelength of the sound. If the wave impinges on the surface from the medium 1, then $\Delta\mathbf{u}^{(1)}$ is a sum of three reflected waves. $\Delta\mathbf{u}^{(2)}$ is also a sum of three waves, one of which corresponds to the change in the coefficient A_0 in the transmitted wave and the other two correspond to the conversion of the incident wave into other types of acoustic waves. All the six waves have the same frequency ω and tangential wave-vector components $k_{i'}$ as the incident wave. The amplitudes of all the waves are determined by the six equations (3), (9) at the defect surface:

$$\begin{aligned}\Delta\sigma_{in}^{(1)}-\Delta\sigma_{in}^{(2)}&=(\nu\omega^2e_i+a_{li'k'}\lambda_{lnpq}k_{k'}k_pe_q-h_{i'k'l'm'}k_{k'}k_{l'}e_{m'})A_0e^{i\mathbf{kr}-i\omega t}\\ \Delta u_i^{(2)}-\Delta u_i^{(1)}&=i(a_{ik'l'}e_{k'}k_{l'}+b_{ik}\lambda_{knpq}k_pe_q)A_0e^{i\mathbf{kr}-i\omega t},\end{aligned} \tag{17}$$

where $\Delta\sigma_{in}^{(1,2)}=\lambda_{inlm}\partial\Delta u_l^{(1,2)}/\partial x_m$. Here we have taken into account the fact that the small $\Delta\mathbf{u}^{(1,2)}$ terms can be neglected when we substitute the displacement vector into those terms of Eqs. (3) and (9) which are connected with the contribution of the surface.

Let us give the solution to Eq. (17) for the simplest case in which the defect plane is perpendicular to a principal symmetry axis of the crystal, and the sound is normally incident on the surface. When the incident wave is a longitudinal wave, there arise, on account of the symmetry of the problem, only transmitted and reflected longitudinal waves. The amplitude A of the reflected wave is given by the formula

$$\frac{A}{A_0}=\frac{i\omega}{2\rho c_l}(\nu-\rho^2c_l^2b_{zz}), \tag{18}$$

where c_l is the velocity of the longitudinal wave and the z axis is oriented along the normal to the surface.

A similar formula gives the corresponding ratio for transverse waves:

$$\frac{A}{A_0}=\frac{i\omega}{2\rho c_t}(\nu-\rho^2c_t^2b_{xx}), \tag{19}$$

where c_t is the velocity of the transverse wave.

3. INTERACTION BETWEEN SURFACE POINT DEFECTS

The presence on the crystal surface of point defects (surface vacancies, additional and impurity atoms) changes the surface energy and, thereby, the surface stress tensor. As a result, there arises in the interior of the crystal a strain that effects a long-range interaction between the point defects. To compute the interaction energy, let us assume that two types of point defects are distributed over the free surface of a crystal of arbitrary shape. Their contribution $\delta\alpha$ to the energy per unit surface area is equal to $\delta\alpha=\varepsilon^{(a)}n_a$, where $a=1,2$, $\varepsilon^{(a)}$ is the energy of the defect of the type a, and n_a is the number of defects per unit surface area. The corresponding change in the surface stress tensor is given by the formula

$$\delta g_{i'k'}=\varepsilon^{(a)}_{i'k'}n_a\,, \tag{20}$$

where $\varepsilon^{(a)}_{ik'}=(\partial\varepsilon/\partial u_{i'k'})\sigma_{in}$. On the free surface, the quantities $u_{i'k'}$ at fixed zero stresses σ_{in} constitute a complete set of variables on which the surface energy depends.

Let δu_i be the change that occurs in the displacement vector as a result of the presence of the defects. The corresponding change in the total surface energy E_s is, on account of (14), equal to

$$-\oint dS\delta u_i\nabla_{k'}g_{i'k'},$$

where the integration is performed over the closed surface of the crystal. The defect-defect interaction energy is given by the quadratic—in n_a—part of the total energy. Separating these quadratic terms from the last expression, we obtain the surface part of the interaction energy

$$\delta E_s=-\oint dS\delta u_i\nabla_{k'}\delta g_{i'k'}. \tag{21}$$

The quadratic—in n_a—part of the volume energy is given by the relation

$$\delta E_v=\frac{1}{2}\oint dS\delta u_i\delta\sigma_{in}, \tag{22}$$

where the $\delta\sigma_{in}$ are the stresses corresponding to the displacement δu_i. Since, on account of the Eqs. (3), the quantities $\delta\sigma_{in}$ and $\delta g_{i'k'}$ are connected in the present case by the formula

$$\delta\sigma_{in}=\nabla_{k'}\delta g_{i'k'}, \tag{23}$$

the total interaction energy, which is equal to the sum of the expressions (21) and (22), can be written in the form

$$\delta E=-\frac{1}{2}\oint dS\delta u_i\delta\sigma_{in}. \tag{24}$$

Let us introduce the Green tensor $G_{ik}(\mathbf{r},\mathbf{r}')$ that determines the solution to the volume equations of elasticity theory for a crystal of a fixed shape corresponding to prescribed forces applied to the surface. Then the quantities δu_i and $\delta\sigma_{in}$ are connected by the relation

$$\delta u_i(\mathbf{r})=\oint dSG_{ik}(\mathbf{r},\mathbf{r}')\delta\sigma_{kn}(\mathbf{r}'),$$

whose substitution into (24) yields, after simple transformations with the use of (23) and (20), the formula

$$\delta E=-\frac{1}{2}\oint dS\oint dS' n_a(\mathbf{r})n_b(\mathbf{r}')\varepsilon^{(a)}_{i'l'}(\mathbf{r})\varepsilon^{(b)}_{k'm'}(\mathbf{r}')\nabla_{l'}\nabla_{m'}{}'G_{ik}(\mathbf{r},\mathbf{r}'). \tag{25}$$

The Green tensor increases in inverse proportion to $|\mathbf{r}-\mathbf{r}'|$ as $\mathbf{r}'\to\mathbf{r}'$. Therefore, the integral (25) diverges at small $\mathbf{r}-\mathbf{r}'$. This divergence is, however, quite unimportant for the problem, of interest to us here, of determining the defect–defect interaction energy for large $|\mathbf{r}-\mathbf{r}'|$.

As can be seen from the formula (25), the interaction energy U_{12} for two point defects of the types 1 and 2 located respectively at the points $\mathbf{r}$ and $\mathbf{r}'$ on the surface is equal to

$$U_{12}(\mathbf{r},\mathbf{r}')=-{}^1\!/_2\varepsilon_{i'l'}\varepsilon_{k'm'}\nabla_{l'}\nabla_{m'}{}'[G_{ik}(\mathbf{r},\mathbf{r}')+G_{ki}(\mathbf{r}',\mathbf{r})]. \tag{26}$$

If the distance between the defects is not too great, then the crystal surface can be considered to be plane. Then in the elastically isotropic case we can use for the tangential—with respect to the surface—components of the Green tensor the well-known (see Ref. 12, § 9) expression

$$G_{\mu\nu}(R)=\frac{1+\sigma}{\pi ER}\left\{(1-\sigma)\delta_{\mu\nu}+\sigma\frac{R_\mu R_\nu}{R^2}\right\},$$

where $\mathbf{R}=\mathbf{r}-\mathbf{r}'$, μ and ν each assumes two values in the plane of the boundary, E is Young's modulus, and σ is Poisson's ratio. Furthermore, we can set $\varepsilon^{(1,2)}_{i'k'}=\varepsilon^{(1,2)}_{xx}\times\delta_{i'k'}$. As a result, the interaction energy (26) assumes the following simple form:

$$U_{12}(R)=\varepsilon^{(1)}_{xx}\varepsilon^{(2)}_{xx}(1-\sigma^2)/\pi ER^3. \tag{27}$$

As in the case of volume point defects (see Refs. 13, §3), the interaction is inversely proportional to the cube of the distance, and identical defects repel each other.

4. INTERACTION BETWEEN THE GROWTH STEPS

We can similarly compute the energy of interaction between parallel straight-line growth steps on a plane atomically-smooth, free basal plane of a crystal. If the original crystal surface coincided with the plane $z=0$, then the new equation for the undeformed surface in the presence of steps parallel to the y axis has the form $z=\zeta(x)$, where the function $\zeta(x)$ satisfies the condition $\partial\zeta/\partial x=l(n_+n_-)$, l being the step height and $n_+(n_-)$ the number of positive (negative) steps per unit length along the x axis. Since the energy ε per unit length of the steps does not depend on the sign, the change in the energy per unit surface area is equal to $\delta\alpha=\varepsilon(n_++n_-)$. The nonzero elements of the step-related part $\delta g_{i'k'}$ of the surface stress tensor have the form

$$\delta g_{z'x'}=g_{xx}\partial\zeta/\partial x=g_{xx}l(n_+-n_-),\quad \delta g_{x'x'}=\varepsilon_{xx}(n_++n_-), \tag{28}$$

where g_{xx} is the surface stress at the original plane crystal face and $\varepsilon_{xx}=\partial\varepsilon/\partial u_{xx}$.

Equations (3) assume in the present case the form

$$\delta\sigma_{iz}=\partial\delta g_{i'x'}/\partial x, \tag{29}$$

where the subscript i takes on the values x and z.

As in the preceding section, the defect–defect interaction energy is given by the formula

$$\delta E=-\frac{L}{2}\int dx\delta u_i\delta\sigma_{iz}, \tag{30}$$

in which L is the step length along the y axis and δu_i is the lattice displacement vector due to the presence of the steps. It can, in principle, be found by solving the volume equilibrium equations for fixed $\delta\sigma_{in}$. The result for the case of an elastically isotropic crystal is given in Landau and Lifshitz's book (Ref. 12, § 8):

$$\begin{aligned}\delta u_x(x)&=\frac{1+\sigma}{2\pi E}\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dx'\left\{(1-2\sigma)\frac{x-x'}{(x-x')^2+y^2}\delta\sigma_{zz}(x')\right.\\&\left.+\left\{\frac{2(1-\sigma)}{[(x-x')^2+y^2]^{1/2}}+\frac{2\sigma(x-x')^2}{[(x-x')^2+y^2]^{3/2}}\right\}\delta\sigma_{xz}(x')\right\},\\ \delta u_z(x)&=\frac{1+\sigma}{2\pi E}\int_{-\infty}^{\infty}dy\int_{-\infty}dx'\left\{\frac{2(1-\sigma)}{[(x-x')^2+y^2]^{1/2}}\delta\sigma_{zz}(x')\right.\\&\left.-\frac{(1-2\sigma)(x-x')}{(x-x')^2+y^2}\delta\sigma_{xz}(x')\right\}.\end{aligned} \tag{31}$$

These formulas contain integrals that diverge in y. The divergence, however, disappears when we differentiate the equality (31) with respect to x. As a result, we obtain

$$\frac{\partial}{\partial x}\delta u_i=-\frac{2(1-\sigma^2)}{\pi E}\int_{-\infty}^{\infty}\frac{dx'}{x-x'}\delta\sigma_{iz}(x')+\text{loc}, \tag{32}$$

where loc denotes quantities locally connected with the stresses $\delta\sigma_{in}$ at the point x, and of no interest to us.

We find from the formulas (28)–(30) and (32) by means of simple transformations the following expression for the nonlocal part of the interaction energy:

$$\begin{aligned}\delta E&=L\frac{1-\sigma^2}{\pi E}\int dx\int dx'\frac{\delta g_{i'x'}(x)\delta g_{i'x'}(x')}{(x-x')^2}\\&=L\frac{1-\sigma^2}{\pi E}\int\frac{dxdx'}{(x-x')^2}[\varepsilon_{xx}^2(n_++n_-)(n_+'+n_-')+g_{xx}^2l^2(n_+-n_-)(n_+'-n_-')].\end{aligned}$$

The corresponding interaction energy for two steps located at a distance x from each other is, depending on the signs of the steps, given by the formulas

$$\begin{aligned}U_{++}(x)=U_{--}(x)&=\frac{2L}{\pi}\frac{1-\sigma^2}{Ex^2}(\varepsilon_{xx}^2+l^2g_{xx}^2),\\ U_{+-}(x)&=\frac{2L}{\pi}\frac{1-\sigma^2}{Ex^2}(\varepsilon_{xx}^2-l^2g_{xx}^2).\end{aligned} \tag{33}$$

That part of the interaction energy $U(x)$ which is proportional to ε_{xx}^2 can be obtained through a simple integration of the result (27) of the preceding section if we treat a step as a set of point defects located along a straight line. The terms proportional to l^2 describe a specific interaction that distinguishes steps from simple line defects. As can be seen from (33), and as has been pointed out by Marchenko and Parshin,[8] this interaction is responsible for the fact that the interaction between steps of opposite signs does not have a fixed sign.

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[1] J. W. Gibbs, Collected Works, Vol. 1, New York, 1928, p. 55.
[2] R. Shuttleworth, Proc. Phys. Soc. London Sect. A **63**, 444 (1950).
[3] C. Herring, in: Structure and Properties of Solid Surfaces (ed. R. Gomer and C. S. Smith), University of Chicago Press, Chicago, 1953, p. 5.
[4] A. J. Shaler, in: Structure and Properties of Solid Surfaces (ed. R. Gomer and C. S. Smith), University of Chicago Press, Chicago, 1953, p. 120.
[5] K. H. Lau and W. Kohn, Surf. Sci. **65**, 607 (1977).
[6] A. M. Stoneham, Solid State Commun. **24**, 425 (1977).
[7] W. Kappus, Z. Phys. B **29**, 239 (1978); **38**, 263 (1980).
[8] V. I. Marchenko and A. Ya. Parshin, Zh. Eksp. Teor. Fiz. **79**, 257 (1980) [Sov. Phys. JETP **52**, 129 (1980)].
[9] A. F. Andreev, Pis'ma Zh. Eksp. Teor. Fiz. **32**, 654 (1980) [JETP Lett. **32**, 640 (1980)]; Zh. Eksp. Teor. Fiz. **80**, 2042 (1981) [Sov. Phys. JETP **53**, 1063 (1981)].
[10] V. I. Marchenko, Pis'ma Zh. Eksp. Teor. Fiz. **33**, 397 (1981) [JETP Lett. **33**, 381 (1981)].
[11] A. F. Andreev and D. A. Kompaneets, Zh. Eksp. Teor. Fiz. **61**, 2459 (1971) [Sov. Phys. JETP **34**, 1316 (1972)].
[12] L. D. Landau and E. M. Lifshitz, Teoriya uprugosti (Theory of Elasticity), Nauka, Moscow, 1965, §8 (Eng. Transl., Pergamon Press, Oxford, 1970).
[13] A. M. Kosevich, Osnovy mekhaniki kristallicheskoǐ reshetki (Principles of the Mechanics of the Crystal Lattice), Nauka, Moscow, 1972, §13.

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