Effect of electrons on the motion of dislocations in metals

A. M. Roshchupkin, V. E. Miloshenko, and V. E. Kalinin
Voronezh Polytechnic Institute

(Submitted March 18, 1979)

Pis'ma Zh. Eksp. Teor. Fiz. **29**, No. 8, 479–482 (20 April 1979)

We calculated the total force acting on a unit length of a moving linear screw dislocation from the conduction electrons of the metal. It is shown that a "lifting effect" analogous to that in aerodynamics of the wing occurs because of asymmetry in the scattering of electrons.

PACS numbers: 61.70.Ga, 72.10.Fk

The dynamic damping of different kinds of dislocations by quasiparticles is usually determined by the energy dissipation in the crystal.[1–3] This makes it possible to calculate only the parallel force component to the direction of motion, which affects the dislocation. Since the scattering of quasiparticles by dislocations is generally asymmetric relative to the glide plane of the latter, we suspect that there is also a perpendicular force component to this plane.

To prove this fact, let us examine, for example, the response of the electron subsystem of the metal, whose Hamiltonian is denoted by H_0, to the perturbation described by the operator

$$H_{int}(t) = \int \lambda_{in} u_{in}(\mathbf{r} - \mathbf{v}t)\, n(\mathbf{r}) dv. \tag{1}$$

Here λ_{in}'s are the constants of the strain potential of the order of the width of the electron band, $u_{in}(r - vt)$ is the strain tensor produced by the dislocation moving at a velocity v and $n(r)$ is the electron density operator. Differentiating (1) with respect to the moving dislocation coordinate, we write the following expression for the force operator, which affects it via the electrons

$$F(t) = \int \lambda_{in} \vec{\nabla} u_{in}(\mathbf{r} - \mathbf{v}t) n(\mathbf{r})\, dv. \tag{2}$$

We now take into account that the deviation of the electron density matrix from its equilibrium value ρ_0 in the linear approximation with respect to the perturbation is determined by the formula[4]

$$\Delta\rho(t) = \frac{i}{\hbar} \int_{-\infty}^{t} e^{-iH_0(t-t')/\hbar} [\rho_0, H_{int}(t')] e^{iH_0(t-t')/\hbar} dt'.$$

Thus, for the linear reaction of magnitude (2) we have

$$\begin{aligned} \mathbf{F} &= \mathrm{Sp}(\mathbf{F}\Delta\rho) \\ &= -\int_{-\infty}^{t} dt \iint dv dv' \lambda_{in} \vec{\nabla} u_{in}(\mathbf{r} - \mathbf{v}t) \lambda_{km} u_{km}(\mathbf{r}' - \mathbf{v}t') \Pi(\mathbf{r} - \mathbf{r}'; t - t'). \end{aligned} \tag{3}$$

Here

$$\Pi(\mathbf{r} - \mathbf{r}', t - t') = \frac{i}{\hbar} < [n(\mathbf{r}, t), n(\mathbf{r}', t')] > \theta(t - t')$$

is the polarization operator of the electron gas, the angle brackets $\langle ... \rangle$ denote averaging over the large canonical Gibbs ensemble,

$$n(\mathbf{r}, t) = e^{iH_0 t/\hbar} n(\mathbf{r}) e^{-iH_0 t/\hbar}$$

is the Heisenberg electron-density operator, and $\theta(t - t')$ is a step function equal to zero at $t < t'$ and to unity at $t > t'$. Representing in Eq. (3) the polarization operator by the Fourier integral

$$\Pi(\mathbf{r} - \mathbf{r}', t - t') = \int \Pi(\mathbf{q}, \omega)\, e^{i[\mathbf{q}(\mathbf{r} - \mathbf{r}') - \omega(t - t')]} \frac{d^3q\, d\omega}{(2\pi)^4}$$

and performing simple transformations, we obtain

$$\mathbf{F} = -\int \mathbf{q}\, |\lambda_{in} u_{in}(\mathbf{q})|^2 \operatorname{Im}\Pi(\mathbf{q}, \mathbf{q}\mathbf{v}) \frac{d^3q}{(2\pi)^3}. \tag{4}$$

In the case of a linear screw dislocation with the Burgers vector b parallel to the z axis, the nonvanishing components of the strain tensor are the $u_{\alpha z}$ components ($\alpha = 1, 2$)[5]

$$u_{\alpha z} = -\frac{b}{2\pi} e_{\alpha\beta z} \frac{x_\beta}{x_\gamma^2}.$$

Calculating the Fourier transforms corresponding to them, we find

$$|\lambda_{in} u_{in}(\mathbf{q})|^2 = 2\pi L \delta(q_z) \frac{b^2}{q_\gamma^2} (\lambda_{xz}^2 \sin^2\phi + \lambda_{yz}^2 \cos^2\phi - \lambda_{xz}\lambda_{yz} \sin 2\phi), \tag{5}$$

where L is the dislocation length $\phi = \text{arc} \tan(q_y/q_x)$. Note that the last term in the expression, in contrast to the first two terms, changes its sign as a result of changing the sign of ϕ. The aforementioned asymmetry in the scattering of electrons is attributable to this fact.

Further analysis requires knowledge of the imaginary part of the polarization operator. According to Lindhard's calculations when the condition $|\omega| \ll q v_F$ is satisfied (quasistatic reaction), the following equality holds[6]

$$\operatorname{Im}\Pi(\mathbf{q}, \omega) = \begin{cases} \dfrac{m^2\omega}{2\pi\hbar^3 q}, & 0 \leqslant q \leqslant 2k_F \\ 0, & q > 2k_F \end{cases}. \tag{6}$$

Here, as usual, k_F is the Fermi wave vector, v_F is the velocity of the electron at the Fermi surface, and m is its mass. Substituting Eqs. (5) and (6) into Eq. (4) and performing simple transformations, we obtain

$$\frac{F_\alpha}{L} = -B_{\alpha\beta} V_\beta, \tag{7}$$

where the two-dimensional symmetric tensor $B_{\alpha\beta}$ has the form

$$B_{\alpha\beta} = \frac{\pi k_F m^2 b^2}{2(2\pi\hbar)^3} (3\delta_{\alpha\beta}\lambda_{\gamma z}^2 - 2\lambda_{\alpha z}\lambda_{\beta z}).$$

The "lifting" force directed perpendicularly to the dislocation glide plane follows directly from the tensor nature of Eq. (7). This force, as can easily be shown, is missing only when the dislocation moves in the direction of the major axes of the $B_{\alpha\beta}$ tensor. Note that one of these directions is given by the unit vector $\lambda_{\alpha z}/\sqrt{\lambda_{\gamma z}^2}$ and the other is perpendicular to it.

The presence of a temperature-dependent gap Δ in the energy spectrum of elementary excitations of a superconductor, as is well known,[1] decreases the electron damping of the dislocations. It seems that this also applies to the "lifting" force. This can be verified by substituting in Eq. (4) rather than in Eq. (6) the expression for

ImΠ (q,ω) corresponding to the superconducting state.[7] Thus, for example, when the rate of motion of the dislocation is low $V \ll T/2\hbar k_F$, the $\Delta(T)/2\hbar k_F$ modification of Eq. (7) simply amounts to a reduction of all the components of the $B_{\alpha\beta}$ tensor by a factor of $\frac{1}{2}(1+\exp[\Delta/T])$. Specifically, such a reduction indicates that the screw dislocations, which move under the influence of external strain, will change not only the velocity but also the direction of their motion as a result of a superconducting transition. This may contribute additionally to the softening of superconductors.[8]

1. M.I. Kaganov, V. Ya. Kravchenko, and V.D. Natsik, Usp. Fiz. Nauk **111**, 655 (1973) [Sov. Phys. Usp. **16**, 878 (1974)].
2. V.I. Al'shitz and V.L. Indenbom, Usp. Fiz. Nauk **115**, 3 (1975) [Sov. Phys. Usp. **18**, 1 (1975)].
3. V.G. Bar'yakhtar and E.I. Druinskiĭ, Zh. Eksp. Teor. Fiz. **72**, 218 (1977) [Sov. Phys. JETP **45**, 114 (1977)].
4. D.N. Zubarev, Neravnovesnaya statisticheskaya termodynamika (Non-equilibrim Statistical Thermodynamics), Nauka, M., 1971.
5. L.L. Landau and E.M. Lifshitz, Teoriya uprugosti (Theory of Elasticity), Nauka, M., 1965.
6. D. Païne and F. Noz'er, Teoriya kvantovykh zhidkosteĭ (Theory of Quantum Liquids), Mir, M., 1967.
7. V.L. Pokrovskiĭ, Zh. Eksp. Teor. Fiz. **40**, 143 (1961) [Sov. Phys. JETP **13**, 100 (1961)].
8. V.I. Startsev, Kristall und Technik **12**, 329 (199).