Electron drag of elastic field sources and the conductivity of metals

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The relation between the short-wave asymptotic of the conductivity tensor of a metal and the electron component of the dragging of the plastic-deformation carriers in the crystal is established in the linear-response approximation. The short-wave ultrasound absorption coefficient and the phonon damping coefficient are also expressed in terms of the conductivity. It is shown that this relation makes possible in principle an experimental study of the deformation potential. Estimates of electron dragging of dislocation kinks and crowdions are obtained. The relative contribution to viscous energy losses during plastic deformation of the metal by electron drag of dislocations, kinks, and crowdions is elucidated. The temperature regions are indicated in which electron drag of dislocations, kinks, and crowdions exceeds phonon drag and limits viscous losses.

INTRODUCTION

At low temperatures in metals, when the phonon gas is frozen out, dynamic dragging of dislocations, kinks, crowdions, and other carriers of plastic deformation is limited by electron scattering from these deformations. In principle, the electronic component of the energy loss in plastic deformation is determined by the same dissipative processes in the electronic subsystem of the metal as the electric conductivity. Bearing this in mind, some authors (see, e.g.,[1,2]) attempted to connect the electron dragging of dislocations with the macroscopic electric conductivity of the metal. Such attempts turned out to be in error each time (as already indicated in the literature[3-6]), because, in final analysis, the main contribution to the energy dissipation is made by processes of electron scattering near the dislocations, processes that do not lend themselves to macroscopic description and require that the spatial dispersion of the electric conductivity be taken into account. The situation is similar here to the only recently explained problem of phonon dragging of dislocations.

We shall show below that the electron dragging of any source of elastic field in a metal can be expressed in explicit form in terms of the short-wave asymptotic expression for the dynamic electric conductivity. Establishment of a direct connection between these kinetic characteristics of the crystal makes it possible in principle to determine experimentally the deformation potential—the constant of the coupling between the electrons and the elastic field, concerning which only very scanty data are available at present[7-9].

FORMULATION OF THE PROBLEM

As a rule, plastic deformation in a crystal propagates at velocities much lower than that of sound, and the elastic field of the carriers of the deformation can be described in the quasistatic approximation. For a source moving with velocity v, we have

$$\varepsilon_{ij}(\mathbf{r}, t) = \varepsilon_{ij}(\mathbf{r} - \mathbf{v}t) = \sum_{\mathbf{k}} \varepsilon_{ij}^{\mathbf{k}} e^{i(\mathbf{kr} - \Omega_{\mathbf{k}} t)}, \quad \Omega_{\mathbf{k}} = \mathbf{kv}. \tag{1}$$

Here ϵ_{ij}^{k} is the Fourier transform of the deformation tensor of the static field of the source. In this language, the problem of pinning a moving source of elastic field reduces to an analysis of the damping of a certain packet of plane waves (1).

The Hamiltonian of the electronic subsystem of a crystal in an alternating elastic field (1) can be represented in the form of the sum

$$H = H_0 + H_{\text{int}}, \tag{2}$$

in which H_0 is the Hamiltonian of the electrons in the absence of deformation, and H_{int} is the Hamiltonian of the interaction of the electrons with the elastic field:

$$H_{\text{int}}(t) = \sum_{\mathbf{k}, \mathbf{p}} \lambda_{ij}^{\mathbf{p}} \varepsilon_{ij}^{\mathbf{k}} a_{\mathbf{p}-\mathbf{k}}^{+} a_{\mathbf{p}} e^{-i\Omega_{\mathbf{k}} t}. \tag{3}$$

Here λ_{ij}^{p} is the tensor of the deformation potential, a_p^+ and a_p are the creation and annihilation operators of an electron with momentum p (the spin variable has been omitted since it is of no importance for the present problem). For convenience, we shall henceforth assume a unit volume of the crystal and use a system of units in which Planck's constant is $\hbar = 1$.

The system density matrix $\hat{\rho}$ is defined by the equation

$$\partial\hat{\rho} / \partial t + i[H, \hat{\rho}] = 0. \tag{4}$$

It is convenient to introduce the deviation of the matrix from the equilibrium value $\hat{\rho}_0$: $\Delta\hat{\rho} = \hat{\rho} - \hat{\rho}_0$, which determines the energy dissipation per unit time:

$$D = -\text{Sp}\,(\hat{\rho}\partial H / \partial t) = -\text{Sp}\,(\Delta\hat{\rho}\partial H_{\text{int}} / \partial t). \tag{5}$$

The solution of Eq. (4) with the initial condition $\hat{\rho}(-\infty) = \hat{\rho}_0$ in an approximation linear in the perturbation is[10]

$$\Delta\hat{\rho} = i\int_{-\infty}^{t} dt' e^{iH_0(t'-t)} [\hat{\rho}_0, H_{\text{int}}(t')] e^{-iH_0(t'-t)}. \tag{6}$$

Substituting (6) in (5) with allowance for (3) we obtain the following expression for the energy dissipation per unit time:

$$D = -i \sum_{\mathbf{k}} \sum_{\mathbf{p}, \mathbf{p}'} \Omega_{\mathbf{k}} (\lambda_{ij}^{\mathbf{p}} \varepsilon_{ij}^{\mathbf{k}}) (\lambda_{kl}^{\mathbf{p}'} \varepsilon_{kl}^{\mathbf{k}})^* G_{\mathbf{pp}'}(\mathbf{k}, \Omega_{\mathbf{k}}), \tag{7}$$

where $G_{pp'}(k, \omega)$ is the Fourier transform of the two-particle retarded Green's function:

$$G_{\mathbf{pp}'}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dx\, e^{i\omega x} \{-i\theta(x) \langle [e^{iH_0 x} a_{\mathbf{p}-\mathbf{k}}^{+} a_{\mathbf{p}} e^{-iH_0 x}, a_{\mathbf{p}'}^{+} a_{\mathbf{p}'-\mathbf{k}}] \rangle\},$$
$$\theta(x) = 1 \quad \text{if} \quad x \geqslant 0, \quad \theta(x) = 0 \quad \text{if} \quad x < 1. \tag{8}$$

The angle brackets $\langle \ldots \rangle$ denote averaging over the Gibbs grand canonical ensemble. We note that in our

approximation the energy dissipation is equal to the sum of the attenuation of the individual plane waves from the packet (1).

Retaining in (7) the first nonvanishing term of the expansion of D in the parameter v/v_F (v_F is the electron velocity on the Fermi surface), we obtain an expression for the viscous component of the dissipation:

$$D=-i\sum_{\mathbf{k}}\sum_{\mathbf{p},\mathbf{p}'}\Omega_{\mathbf{k}}^{2}(\lambda_{ij}{}^{p}\varepsilon_{ij}{}^{k})(\lambda_{kl}{}^{p}\varepsilon_{kl}{}^{k})^{*}\frac{\partial G_{\mathbf{pp}'}(\mathbf{k},\omega)}{\partial\omega}\Big|_{\omega=0}. \tag{9}$$

CONNECTION BETWEEN THE ELECTRONIC COMPONENT OF THE DAMPING OF A PACKET OF ELASTIC WAVE AND THE ELECTRIC CONDUCTIVITY OF A METAL

Thus, the problem of the damping of packet (1) reduces to a determination of a two-particle Green's function for the electrons in the unperturbed crystal. But the same function determines also the dynamic electric conductivity of the metal[11]:

$$\sigma_{\mu\nu}(\mathbf{k},\omega)=i\left(\frac{e}{m}\right)^{2}\sum_{\mathbf{p},\mathbf{p}'}\left(\mathbf{p}-\frac{\mathbf{k}}{2}\right)_{\mu}\frac{G_{\mathbf{pp}'}(\mathbf{k},\omega)-G_{\mathbf{pp}'}(\mathbf{k},0)}{\omega}\left(\mathbf{p}'-\frac{\mathbf{k}}{2}\right). \tag{10}$$

Kravchenko[3] and Kaganov and Natsik[12] have shown, for the case of dislocations, that the main contribution to the dissipation is connected with the shortest partial waves of the packet (1), for which $kl \gg 1$ (l is the electron mean free path)[1)]. This conclusion remains in force also for other carriers of plastic deformation with sufficiently rapid fall-off of the elastic field. We confine ourselves therefore to a study of the damping of short elastic waves with wave vectors $k \gg l^{-1}$, when, according to[11], the Green's function $G_{\mathbf{pp}'}(\mathbf{k},\omega)$ can be regarded as diagonal in p and p′:

$$G_{\mathbf{pp}'}=\delta_{\mathbf{pp}'}G_{\mathbf{p}}. \tag{11}$$

Since the principal role in scattering processes are played by electrons with energies $\epsilon_{\mathbf{p}}$ and $\epsilon_{\mathbf{p}-\mathbf{k}}$ close to the Fermi energy ϵ_F, the decisive contribution in expressions (9) and (10) are made by the vectors p, which move along a certain contour $\mathscr{L}$ corresponding to the line of intersection of the surfaces $\epsilon_{\mathbf{p}}=\epsilon_F$ and $\epsilon_{\mathbf{p}-\mathbf{k}}=\epsilon_F$. Assuming that the contour $\mathscr{L}$ belongs to a Fermi-surface section that can be described by the quadratic formula

$$\varepsilon_F={}^{1}/_{2}m_{\alpha\beta}^{-1}p_{\alpha}p_{\beta}, \tag{12}$$

it is easy to obtain from (10), with allowance for (11)

$$m_{\alpha\beta}^{-1}\sigma_{\alpha\beta}(\mathbf{k},0)=2i\left(\frac{e}{m}\right)^{2}\left(\varepsilon_F-\frac{1}{8}m_{\alpha\beta}^{-1}k_{\alpha}k_{\beta}\right)\sum_{\mathbf{p},\mathbf{p}'}\frac{\partial G_{\mathbf{pp}'}(\mathbf{k},\omega)}{\partial\omega}\Big|_{\omega=0}. \tag{13}$$

Taking outside the summation sign in (9) a certain value averaged on the contour $\mathscr{L}$

$$\overline{|\lambda_{ij}{}^{p}|^{2}}=|\Lambda_{ij}{}^{k}|^{2}$$

and eliminating with the aid of (9) and (13) the Green's function $G_{\mathbf{pp}'}(\mathbf{k},\omega)$, we obtain an expression that establishes a connection between the electronic component of the damping of the packet (1) and the short-wave asymptotic form of the electric-conductivity tensor:

$$D=-\frac{1}{2}\left(\frac{m}{e}\right)^{2}\sum_{\mathbf{k}}\Omega_{\mathbf{k}}^{2}|\Lambda_{ij}{}^{k}\varepsilon_{ij}{}^{k}|^{2}\frac{m_{\alpha\beta}^{-1}\sigma_{\alpha\beta}(\mathbf{k},0)}{\varepsilon_F-{}^{1}/_{8}m_{\alpha\beta}^{-1}k_{\alpha}k_{\beta}}. \tag{14}$$

A direct consequence of formula (14) is the simple connection between the absorption coefficient Γ of the short-wave ($kl \gg 1$) ultrasound and the electric conductivity of the metal:

$$\Gamma=-\frac{1}{2}\left(\frac{m}{e}\right)^{2}\frac{|\Lambda_{ij}{}^{k}\omega_{\mathbf{k}}|^{2}}{C_{ij}\varepsilon_F}m_{\alpha\beta}^{-1}\sigma_{\alpha\beta}(\mathbf{k},0). \tag{15}$$

Here $\omega_{\mathbf{k}}$ is the ultrasound frequency, C_{ij} is the corresponding component of the elastic-modulus tensor of the crystal. Equation (15) takes into account the fact that the inequality $k \ll p_F$, where $p_F=(2m\epsilon_F)^{1/2}$ is the Fermi momentum, certainly holds true for any ultrasound. In this case the contour $\mathscr{L}$ is the intersection of the Fermi surface with the plane $\mathbf{p}\cdot\mathbf{k}=0$.

It is possible, in perfect analogy, to express with the aid of (14) the phonon damping coefficient

$$\Gamma_{\lambda}(\mathbf{k})=-\frac{1}{2}\left(\frac{m}{e}\right)^{2}\overline{|M|^{2}}\omega_{\lambda}(\mathbf{k})\frac{m_{\alpha\beta}^{-1}\sigma_{\alpha\beta}(\mathbf{k},0)}{\varepsilon_F-{}^{1}/_{8}m_{\alpha\beta}^{-1}k_{\alpha}k_{\beta}} \tag{16}$$

in terms of the electric conductivity, where $\omega_{\lambda}(\mathbf{k})$ is the frequency of a phonon with wave vector k and polarization λ, $\overline{|M|^{2}}$ is the square, averaged over the contour $\mathscr{L}$, of the matrix element characterizing the value of the electron-phonon coupling. In the long-wave limit we have

$$\overline{|M|^{2}}\sim|\Lambda_{ij}{}^{k}k_{i}l_{\mathbf{k}\lambda}{}^{j}|^{2}/\rho\omega_{\lambda}(\mathbf{k})$$

(ρ is the density of the crystal and $l_{\mathbf{k}\lambda}$ is the phonon polarization vector), and expression (16) goes over into (15).

It can be shown that formulas (14)—(16) remain in force in the general case when the contour $\mathscr{L}$ cannot be described by the quadratic formula (12). The tensor $m_{\alpha\beta}^{-1}$ should then be replaced everywhere by

$$m_{\alpha\beta}^{-1}=2\delta_{\alpha\beta}\varepsilon_F\int_{0}^{2\pi}\frac{d\varphi}{p^{2}|K(\varphi)|}\Big/\int_{0}^{2\pi}\frac{d\varphi}{|K(\varphi)|}.$$

Here $K(\varphi)$ is the Gaussian curvature of the Fermi surface, and the integration is carried out along the contour $\mathscr{L}$.

Returning to the problem of the pinning of moving sources of internal stresses, we note that the problem calculating the energy dissipation consists merely of substituting in (14) the explicit expression for the tensor ϵ_{ij}^{k} and summing over all the wave vectors k. We consider here the three most important examples of sources: a linear dislocation, a dislocation kink, and a crowdion.

DRAGGING OF A LINEAR DISLOCATION

As a first check on relation (14), we estimate with its aid the damping constant for a dislocation in the approximation where the Fermi surface is spherical, $m_{\alpha\beta}^{-1}=\delta_{\alpha\beta}/m$, and compare the result with the known estimate obtained from direct calculations[3,15]. Following Éliashberg[11], it is easy to obtain an expression for the short-wave asymptotic electric-conductivity coefficient:

$$\sigma_{\mu\nu}(\mathbf{k},\omega)=i\left(\frac{e}{m}\right)^{2}\sum_{\mathbf{p}}\frac{p_{\mu}p_{\nu}}{\omega-\mathbf{v}_{e}\mathbf{k}+2i/\tau}\frac{\partial n(\varepsilon_{\mathbf{p}+\mathbf{k}/2})}{\partial\varepsilon_{\mathbf{p}+\mathbf{k}/2}}. \tag{17}$$

Here

$$n(\varepsilon_{\mathbf{p}})=\left[\exp\left(\frac{\varepsilon_{\mathbf{p}}-\varepsilon_F}{T}\right)+1\right]^{-1},\quad \varepsilon_{\mathbf{p}}\doteq\frac{p^{2}}{2m},\quad \mathbf{v}_{e}=\frac{\mathbf{p}}{m},\quad \tau=\frac{l}{v_F}, \tag{18}$$

and T is the temperature in energy units.

Taking into account the smallness of the parameters $T/\epsilon_{\mathbf{p}}$ and $(kl)^{-1}$, we have a simple estimate for the trace of the tensor $\sigma_{\mu\nu}$:

$$\sigma_{\mu\mu}(\mathbf{k},0)=-\frac{e^{2}}{m}\left(p_F{}^{2}-\frac{k^{2}}{4}\right)\int\frac{d\mathbf{p}}{(2\pi)^{2}}\delta(\varepsilon_{\mathbf{p}+\mathbf{k}/2}-\varepsilon_F)\delta(\mathbf{pk})$$

$$= -\frac{e^2}{2\pi}\frac{p_F^2 - k^2/4}{k}\theta\left(p_F - \frac{k}{2}\right). \quad (19)$$

It can be shown[13] that for a linear dislocation of length L we have

$$|\varepsilon_{ij}^{k}|^2 \approx 2\pi b^2 L \frac{\delta(\mathbf{kn})}{k^2}\Phi\left(\frac{\mathbf{k}}{k}\right), \quad (20)$$

where $\Phi(\mathbf{k}/k)$ is function of the directions and is of the order of unity, b is the Burgers vector, and n is a unit vector along the dislocation. Using (19) and (20), and assuming, in order of magnitude, that $\Lambda_{ij}^{k} \sim \epsilon_F$, we obtain from (14) an estimate of the damping constant $B = D/v^2L$, which agrees with the results of direct calculations[2]:

$$B \sim \frac{1}{2\pi} b^2 q_m \frac{N\varepsilon_F}{v_F}. \quad (21)$$

Here $q_m = \min\{2p_F, r_0^{-1}\}$, r_0 is the radius of the dislocation kernel ($r_0 \sim b$), and $N = p_F^3/3\pi^2$ is the density of the number of conduction electrons.

Plastic deformation reduces to a uniform motion of linear dislocations in only rare cases. However, taking into account the smallness of the characteristic dislocation velocities in comparison with the average electron velocity, it is easily understood that the electrons follow practically the instantaneous dislocation velocity, and the limitation on the non-uniformity of the motion cannot be significant. On the other hand, since the main contribution to the effect is made by processes near the dislocation, the bending of the dislocation needs to be taken into account only in exceptional cases, when the radius of curvature is comparable with the lattice parameters. A similar situation is realized, however, in the cases of practical importance, those of a kink on a dislocation and of a crowdion.

DRAGGING OF DISLOCATION KINK

In crystals having a high Peierls relief, the dislocations are arranged along the valleys of the relief and are displaced by an amount equal to the lattice parameter into the neighboring valley by the mechanism of ejection and lateral spread of the kinks. The kink width w is determined by the shape and height of the relief and can be of the order of one or several interatomic distances. The electronic dragging of the kink cannot be analyzed in this case by means of formula (21), and the calculation must be carried out anew.

The components of the tensor ϵ_{ij}^{k} for a kink on a screw dislocation oriented along the z axis and located in the slip plane XZ have been written out in explicit form by Seeger and Engelke[16]. It is easy to verify that the main contribution to the dissipation is connected with components of the form

$$\varepsilon_{ij}^{k} \sim ab\frac{\sin(\mathbf{kd}/2)}{k_z(kd/2)}\varphi\left(\frac{\mathbf{k}}{k}\right). \quad (22)$$

Here $\mathbf{d} = \{a, 0, w\}$, $\varphi(\mathbf{k}/k)$ is the direction function, has no singularities, and is of the order of unity. Substituting (22) and (19) in (14) and changing over from the dissipation D to the dragging coefficient $\eta_k = D/v^2$, we obtain

$$\eta_k \sim \frac{1}{2\pi}\frac{N\varepsilon_F}{v_F}\frac{a^2b^2q_m}{d}F\left(\frac{q_m d}{2}\right) \approx B\frac{a^2}{d}F\left(\frac{q_m d}{2}\right), \quad (23)$$

$$F(x) = \frac{2}{\pi x}\int_0^1 dz\,\frac{\sin^2 xz}{z^2}(1-z^2)^{1/2}.$$

For wide kinks ($w \gg a$), when $F(x) \approx 1$, our estimate (23) can be obtained from formula (21) by taking into account the obvious connection between the velocity of the kink and the normal component of the velocity of the moving section of the dislocation, $v_n = avd^{-1}$. For narrow kinks, the dragging coefficient η_k depends on the width of the kink in a more complicated manner.

DRAGGING OF CROWDION

Data have been recently published concerning the significant role of the crowdion mechanism of plastic deformation these data have stimulated both theoretical and experimental studies of crowdion dynamics. Electron dragging of crowdions can be estimated from the formula of[14]. The elastic field of a crowdion is equivalent to the field of a small prismatic loop of radius R on the order of the lattice parameter, and can be calculated with the formulas indicated by one of the authors[20]. The components of the corresponding Fourier transform ϵ_{ij}^{k} have the following structure:

$$\varepsilon_{ij}^{k} \sim \Omega\left[\frac{\sin kR}{kR} - \mathrm{ci}(kR)\right], \quad (24)$$

where Ω is a quantity on the order of the atomic volume and ci(x) is the integral cosine.

Combining formulas (14), (19), and (24) we can obtain, just as in the case of a kink, an estimate of the dragging coefficient of a crowdion:

$$\eta_c \sim \frac{1}{2\pi}\frac{N\varepsilon_F}{v_F}\left(\frac{\Omega}{R^2}\right)^2 f(q_m R), \quad f(x) = \int_0^x dt\,t^3\left[\frac{\sin t}{t} - \mathrm{ci}(t)\right]^2. \quad (25)$$

As expected, formula (25), generally speaking, does not reduce to the estimate (21), although when recalculated "per unit length" the dissipation level is of the same order in both cases: $\eta_c/2\pi R \sim B$. Comparison of the dragging of a crowdion and of a kink shows that in order of magnitude we have $\eta_k \sim \eta_c a/l$.

DISCUSSION

1. The connection obtained by us between macroscopically measurable kinetic characteristics of crystals in terms of little-investigated microscopic constants makes it possible to investigate these constants experimentally and in this sense can be of fundamental interest. The needed short-wave asymptotic expression for the electric-conductivity tensor can be obtained from experiments (say on the anomalous skin effect[21]). On the other hand, there exist at present reliable methods of measuring both the dynamic dragging of defects in crystals, and the absorption of short-wave ultrasound and phonon damping. All this gives ground for hoping to be able to carry out an all-inclusive investigation of the deformation potential and of the electron-phonon coupling constant in different metals.

Another aspect of the problem is the prediction of the plastic properties of metals from known singularities of the electric conductivity and of the deformation potential. Thus, according to Nowak and Lee[9], there is a strong anisotropy of the deformation potential in copper near the "neck" on the Fermi surface. One can therefore expect a corresponding anisotropy of the dynamic plastic properties of copper to appear at low temperatures.

2. Dynamic dragging of the carriers of plastic deformation is usually attributed to phonon mechanisms of energy dissipation. It is of interest, on the basis of the estimates (21), (23) and (25) given in the paper, and also on the basis of known data on phonon dragging of

dislocations[13,22], and kinks[16] and the estimate obtained by analogy for the phonon dragging of crowdions, to ascertain the temperature starting with which the phonons in metals are frozen out to such a degree that the predominant dissipation mechanism is the temperature-independent electron scattering. Such a comparison, at reasonable values of the parameters for the normal metal, can show that the critical temperatures below which electron dragging predominates are different for dislocations (T_d), kinks (T_k), and crowdions (T_c), and are of the order of

$$T_d \approx (2-3)T_c \sim 10^{-1}\Theta, \quad T_k \sim 10^{-1}(a/w)\Theta, \tag{26}$$

where Θ is the Debye temperature. The difference between the characteristic temperatures T_d, T_k, and T_c may be useful when it comes to revealing the mechanisms that limit viscous energy losses in plastic deformation under various conditions.

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[1)]In the region $kl < 1$ it is necessary, when $G_{pp'}(k, \omega)$ is calculated, to take relaxational processes into account; this analysis is not trivial, owing to the presence of singular diagrams, summation of which is equivalent to the solution of the kinetic equation [11]. As applied to to the problem of phonon dragging of dislocations, an analogous Green's function for phonons was investigated in [13] both in the short wave ($kl > 1$) and in the long wave ($kl < 1$) region, which made it possible to estimate the relative role of the relaxation processes in the phonon subsystem. Unfortunately, in our case there is no need for such an analysis, since the corresponding kinetic problem for the electrons was solved earlier in a well known paper by Akhiezer [14]. Its results have indeed the basis of the conclusion that the region $kl < 1$ plays no significant role in dislocation pinning [3,12].

[2)]Substitution of (19) in (15), naturally, also leads to the result known from the direct calculations [14].

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