Electronic Component of Dislocation Drag in Metals

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The rate of energy dissipation resulting from the uniform motion of a dislocation through a free-electron gas is reevaluated. The analysis, which is based upon electron-transport theory, leads to a damping force upon the dislocation in agreement with that derived by Holstein using standard perturbation theory. The source of the discrepancy between the present result and that obtained from a previous treatment of the Boltzmann equation is elucidated.

AT the present time there are several conflicting results in the literature for the electronic component of the dislocation drag in metals. In an early theory, Mason[1] used an electron-gas viscosity model and found a drag force proportional to the electrical conductivity. This approach was criticized by Tittmann and Bömmel[2] on the grounds that the model is inappropriate for the rapidly varying strain-field components associated with a dislocation.[3,4] They analyzed their own experimental data in terms of a temperature-independent drag force obtained by Holstein[5] from standard perturbation theory and, independently, by Kravchenko[6] from a solution of the Boltzmann equation. Recently, however, Huffman and Louat[7–9] have reinvestigated the electron-transport-theory approach to the problem. They also obtain a drag force proportional to the conductivity,[8] even though the viscosity concept is not used. This is in open conflict[10] with the theory of Holstein, since the two methods are known to predict the same result for the electronic contribution to ordinary acoustic attenuation.[11] In view of this discrepancy we have reexamined the transport-theory approach to the problem, placing particular emphasis upon the relation to the treatment of attenuation in a standard text.[11] Our result is in agreement with Holstein's form of the drag force. The present paper contains an outline of this calculation and details the source of the error in the method used by Huffman and Louat (HL).

We begin by making connection with the standard theory of acoustic attenuation. If the displacement field of a stationary dislocation is $\mathbf{w}(\mathbf{r})$, then the corresponding form for a dislocation moving with uniform velocity $\mathbf{v}_D$ is $\mathbf{w}(\mathbf{r}-\mathbf{v}_D t)$, providing $\mathbf{v}_D$ is small compared with the sound velocity.[12] Hence, the local lattice velocity $\mathbf{u}(\mathbf{r},t)$ is

$$\mathbf{u}(\mathbf{r},t)=\sum_{\mathbf{q}} \mathbf{u}_{\mathbf{q}} \exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{v}_D t)], \tag{1}$$

where

$$\mathbf{u}_{\mathbf{q}}=\sum_{\lambda} -i\mathbf{q}\cdot\mathbf{v}_D \mathbf{e}_{\mathbf{q}\lambda} w_{\mathbf{q}\lambda}. \tag{2}$$

Here λ is an index specifying the normal mode with polarization vector $\mathbf{e}_{\mathbf{q}\lambda}$, and $w_{\mathbf{q}\lambda}$ is the Fourier amplitude of the displacement associated with that mode. Since the power dissipated by each component of Eq. (1)—say, $P_{\mathbf{q}}$—will, as a result of the motion, be of the form

$$P_{\mathbf{q}}=A_{\parallel}|\mathbf{u}_{\mathbf{q}\parallel}|^2+A_{\perp}|\mathbf{u}_{\mathbf{q}\perp}|^2, \tag{3}$$

where $\parallel$ and $\perp$ refer to longitudinal and transverse components, the effective drag force per unit length of dislocation Bv_D is given by

$$B=(Lv_D^2)^{-1}\sum_{\mathbf{q}} P_{\mathbf{q}}, \tag{4}$$

where L is the length of dislocation. Equation (4) is to be evaluated in the limit $L\to\infty$.

The main burden of the calculation is the determination of the proportionality factors $A_{\parallel}$ and $A_{\perp}$. Fortunately, their electronic components have already been calculated,[11,13] and we need only reiterate the pertinent results. They are obtained from the self-consistent solution of Maxwell's equations and the Boltzmann equation. In the latter, electron collisions are presumed to relax the electron distribution to a Fermi distribution centered on the local lattice velocity with a Fermi energy determined by the local electron density.[13] Thus, the electron distribution in phase space is $f(\mathbf{r},\mathbf{v},t)=f_0(\mathbf{v})+f_1(\mathbf{r},\mathbf{v},t)$, where $f_0(\mathbf{v})$ is the free-electron

[1] W. P. Mason, J. Appl. Phys. **35**, 2779 (1964).
[2] B. R. Tittmann and H. E. Bömmel, Phys. Rev. **151**, 178 (1966).
[3] The refutation of this criticism (see Ref. 4) appears to be invalid since the argument does not depend upon high dislocation velocities.
[4] W. P. Mason and A. Rosenberg, J. Appl. Phys. **38**, 1929 (1967).
[5] T. Holstein (see Appendix to Ref. 2).
[6] V. Ya. Kravchenko, Fiz. Tverd. Tela **8**, 927 (1966) [English transl.: Soviet Phys.—Solid State **8**, 740 (1966)].
[7] G. P. Huffman and N. P. Louat, Phys. Rev. Letters **19**, 518 (1967).
[8] G. P. Huffman and N. P. Louat, Phys. Rev. Letters **19**, 774(E) (1967).
[9] G. P. Huffman and N. P. Louat, Phys. Rev. **176**, 773 (1968). Their postulate of "perfect screening" as a means of obtaining a temperature-independent result is unjustified since it corresponds to the limit of an electron gas of infinite density.
[10] C. Elbaum and A. Hikata, Phys. Rev. Letters **20**, 264 (1968).
[11] C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), Chap. 17.
[12] For example, see A. D. Brailsford, Phys. Rev. **142**, 388 (1966).
[13] M. H. Cohen, M. J. Harrison, and W. A. Harrison, Phys. Rev. **117**, 937 (1960).

Fermi distribution and f_1 is the solution of

$$\frac{\partial f_1}{\partial t}+\mathbf{v}\cdot\nabla_r f_1+e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\epsilon}=-\frac{1}{\tau}\left[\left(m\mathbf{v}\cdot\mathbf{u}+\frac{2}{3}\frac{n_1}{n_0}\epsilon_F\right)\frac{\partial f_0}{\partial\epsilon}+f_1\right]. \quad (5)$$

Here n_1 is the deviation of the electron density from its equilibrium value n_0, $\epsilon=\frac{1}{2}mv^2$, ϵ_F is the Fermi energy, and $\mathbf{E}(\mathbf{r},t)$ is the self-consistent electric field in the metal produced by the moving dislocation. Solving (5) and Maxwell's equations by Fourier analysis as in Ref. 11, one finds that[14]

$$A_{11}=\frac{Vn_0m}{\tau}\mathrm{Re}\left[\frac{g(\sigma_0)}{|g(\sigma')|^2}\left(\frac{\sigma_0}{\sigma'^*}-1\right)\right], \quad (6)$$

where $g(x)=1-i\omega/4\pi x$, σ_0 is the dc conductivity, V the volume, n_0 and m the free-electron density and mass, respectively, and τ the relaxation time. Further, we have set $\mathbf{v}_D\cdot\mathbf{q}=\omega$ and

$$\sigma'=\sigma_{zz}(1+iqv_Fa\sigma_{zz}/3\sigma_0\omega)^{-1}, \quad (7)$$

where v_F is the Fermi velocity and $a=ql/(1-i\omega\tau)$. Here $l=v_F\tau$ is the electron mean free path and, finally,

$$\sigma_{zz}=\frac{\sigma_0}{1-i\omega\tau}\frac{3}{a^3}(a-\tan^{-1}a). \quad (8)$$

These results hold for general values of the parameters. However, for realistic dislocation velocities it is to be expected that $|a|\gg1$ (for $ql\gg1$) and $\sigma_0\gg\omega$. Then (6) reduces to

$$A_{11}\simeq(Vn_0m/\tau)[1+(q/q_{\mathrm{TF}})^2]^{-2}\tfrac{1}{6}\pi ql, \quad (9)$$

which is independent of the relaxation time (q_{TF} is the reciprocal of the Thomas-Fermi screening length; $q_{\mathrm{TF}}=\sqrt{3}\omega_p/v_F$, where $\omega_p=4\pi n_0e^2/m$ is the plasma frequency). Hence, when we combine (2)–(4) and (9), the longitudinal-wave contribution B_l to B is

$$B_l\simeq\frac{n_0mv_F\pi V}{6Lv_D^2}\sum_{\mathbf{q}}\frac{(\mathbf{q}\cdot\mathbf{v}_D)^2|\Delta_{\mathbf{q}}|^2}{q[1+(q/q_{\mathrm{TF}})^2]^2}, \quad (10)$$

where $\Delta_{\mathbf{q}}=iqw_{\mathbf{q},1}$ is the Fourier component of the dilatation (we have taken $\lambda=1$ as the longitudinal mode).

For a straight-screw dislocation we get $B_l=0$, since the dilatation vanishes. For a straight-edge dislocation lying along the x axis, say, with $z=0$ being the slip plane,[15]

$$\Delta_{\mathbf{q}}=\frac{2b}{V}\left(\frac{1-2\nu}{1-\nu}\right)\frac{q_z}{q_y^2+q_z^2}\frac{\sin(\frac{1}{2}q_xL)}{iq_x}. \quad (11)$$

Combining this with (10) and integrating over a Debye sphere of radius q_D, we find that

$$B_l=\left(\frac{1-2\nu}{1-\nu}\right)^2\frac{n_0mv_Fb^2q_D}{96}\phi\left(\frac{q_D}{q_{\mathrm{TF}}}\right), \quad (12)$$

where

$$\phi(x)=\tfrac{1}{2}[(1+x^2)^{-1}+x^{-1}\tan^{-1}x]. \quad (13)$$

Apart from numerical factors,[16] the form (12) agrees with the result of Holstein, as indeed it must since (10) can be obtained directly from perturbation theory if one uses the static Thomas-Fermi dielectric function to determine the screened electron-lattice interaction.[16] Thus, transport theory leads to a temperature-independent electronic contribution to the drag force.[6]

It will be noted that (12) is based upon the large ql limit of A_{11} for all modes of the Debye spectrum. For $ql\ll1$, on the other hand, one finds

$$A_{11}\simeq(4/15)Vn_0mv_F^2\tau q^2. \quad (14)$$

Were this valid for all modes, one would then obtain a form for B_l of the type given by the electron viscosity model. However, as Tittmann and Bömmel[2] point out, the number of modes for which (14) is applicable is negligibly small. Consequently (12) is the appropriate form of the damping force.

A similar calculation can be carried through to determine the shear-wave contribution to B. However, since we have found that $A_\perp\sim(ql)^{-1}A_{11}$ for $ql>1$, such a contribution is negligible and the details will not be given. This conclusion is in agreement with that stated in Ref. 9.

As we have stated earlier, the result for the longitudinal contribution to B disagrees with that given by HL. The source of the discrepancy lies in their treatment of the path-integral solution for the distribution function $f_1(\mathbf{r},\mathbf{v},t)$. Although not given explicitly, the Boltzmann equation satisfied by their f_1 is

$$\frac{\partial f_1}{\partial t}+\mathbf{v}\cdot\nabla_r f_1+(e\mathbf{E}'-\nabla V_D)\cdot\mathbf{v}\frac{\partial f_0}{\partial\epsilon}=-\frac{1}{\tau}\left((m\mathbf{v}\cdot\mathbf{u}-V_D)\frac{\partial f_0}{\partial\epsilon}+f_1\right), \quad (15)$$

[14] The "phonon drag" contributed to A_{11} can be shown to be small. It has been omitted in the interest of brevity.

[15] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Clarendon Press, Oxford, 1961), p. 40.

[16] The deformation-potential approach of Ref. 5 corresponds to the formal limit $q_{\mathrm{TF}}\to\infty$ in (11), when $\phi\to1$. In this limit, (11) is Holstein's result for B_l multiplied by the factor $[(1-2\nu)/(1-\nu)]^2/2\pi$ if one takes his parameters $C=\frac{2}{3}E_F$ and (his) $K=\frac{1}{4}$. The factor of 2π difference can be traced to an error in writing the equation where K was introduced. The remaining discrepancy arises because of Holstein's incomplete expression for $\Delta_{\mathbf{q}}$.

where V_D, the deformation potential of the moving dislocation, is assumed to have a Fourier transform $V_{Dq,\omega}=-4\pi n_0 e^2 q u_{q\parallel}/[\omega q^2\epsilon(q)]$, $\epsilon(q)$ being the static dielectric function of the electron gas. Now a comparison of the inhomogeneous term on the left-hand sides of (15) and (5) indicates the origin of the unusual result of HL, for they interpret $\mathbf{E}'$ in (15) as the total electric field in the metal in their subsequent treatment of Maxwell's equations. This is not correct. The deformation potential in metals is an electrostatic potential. Thus the total electric field is really $\mathbf{E}'-\nabla V_D/e$ in their formulation; the whole term (and not just $\mathbf{E}'$) must be inserted in the *in vacuo* form of Maxwell's equations to determine the relation between the current and the electric field. In fact, one finds from the solution of (5) and from Maxwell's equations that in the limits $\omega\tau\ll 1$ and $ql\gg 1$ the result for the longitudinal electric field is $\mathbf{E}=-e^{-1}\nabla V_D$, so that the screening charge effectively moves bodily with the dislocation. The quantity $\mathbf{E}'$ in (15), which is really the excess electric field, is zero. Fundamentally it is for this reason that the transport-theory result and time-dependent perturbation theory yield the same B. In addition, in the above limits one can show also that $V_D=-(2n_1\epsilon_F/3n_0)$. Hence with $\mathbf{E}'=0$ Eqs. (5) and (15) become identical. Questions of perfect or imperfect screening raised by HL are automatically resolved by the self-consistency of the calculation and do not depend upon invoking different forms for $\epsilon(q)$. The latter is derived implicitly by this method, at least within the accuracy of Boltzmann transport theory.[17]

In further contrast with HL we mention briefly the effect of a finite dislocation width λ upon the form of B. Inclusion of this factor in the displacement field tends to give greater relative weight to the low-q contributions to the attenuation.[9] This can only enhance the relative importance of those modes for which (14) is applicable in our treatment. But since we have realistically $\lambda\ll l$, the effect of such a factor is negligible. In any event the *tendency* would be just the opposite of HL, namely, to introduce a slight temperature dependence where there otherwise is none instead of suppressing a temperature dependence already present.

At first sight it is disquieting that we find essentially no (electronic) damping on screw dislocations. However, it should be borne in mind first that our estimates are based upon free-electron theory as opposed to that appropriate for real Bloch electrons and secondly that the calculation implies that dislocations move like rigid rods. It is now more customary to discuss dislocation dynamics in terms of the motion of kinks.[18] In real crystals these entities always have dilatational strains associated with them. We anticipate, therefore, that the effective electronic damping force for all dislocation motion in real crystals will be given approximately by (12).

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[17] In this regard it should be noted that the proof that $\mathbf{E}'=0$ follows from (15) and Maxwell's equations only if one uses $\epsilon(q)=1+(q_{TF}/q)^2$. This form of $\epsilon(q)$ is derived from (5) and Poisson's equation if $\mathbf{E}$ is here treated as the self-consistent field due to some external static potential plus the screening charge, $\mathbf{u}$ is set equal to zero, and the condition of zero current is imposed. We realize that this dielectric function is less accurate than the Lindhard form, but in a phenomenon such as acoustic attenuation, which depends upon the competition between diffusion and convective currents, it is important to maintain consistency by calculating the real and imaginary parts of the complex dielectric function within the same formalism. Since the Boltzmann equation is used to calculate the imaginary part (i.e., the conductivity), the form for $\epsilon(q)$ given above should be used for the real part.

[18] J. Lothe and J. P. Hirth, Phys. Rev. **115**, 543 (1959).