

Temperature dependence of the resistivity of a metal with dislocations

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(Submitted 1 August 1977)
Zh. Eksp. Teor. Fiz. **74**, 702–713 (February 1978)

The temperature dependence of the resistivity of a metal with dislocations is calculated. It is assumed that the dislocations are straight lines arranged in three mutually perpendicular directions. The dislocation is described as a local linear perturbation of the force constants of the matrix. These perturbations deform the phonon spectrum of the crystal, causing the temperature-dependent part of the resistivity to acquire an increment $\rho^d(T)$ proportional to the dislocation density and having a unique temperature dependence. The temperature-dependent part of the dislocation resistivity $\rho^d(T)$ and its dependence on the perturbation of the force constants as well as on the possible anisotropy of the dislocation orientation relative to the external electric field are investigated in detail. The calculation results are compared with the experimental data.

PACS numbers: 72.10.Fk

1. INTRODUCTION AND FORMULATION OF PROBLEM

By now, rather abundant experimental material has been accumulated concerning the resistivity of plastically deformed metals (see, e.g., ^[1,2]). The resistivity per dislocation, i.e., the cross section for electron scattering by dislocations, was measured for many metals (averaged, of course, over the configurations corresponding to the experimental dislocation structure). More subtle features have also been observed and thoroughly investigated, among which we shall note the unique temperature dependence of the dislocation resistivity, ^[2-5] which is of interest to us here. We recall the main characteristics of this effect.

Many metals (Cu, Ag, Au, Mo, Zn, Al) have revealed a sharp growth of the additional resistivity ρ^d due to the dislocations, in a rather narrow temperature interval (20–100 K), beyond which the slope of $\rho^d(T)$ decreases, flattening out in some cases and even showing a tendency to fall off. The effect is very strong: the values of the parameter $r_{\max} = \rho^d(T)_{\max} / \rho^d(0) - 1$ introduced in ^[4] reach 2 or 3 in some cases. The quantity r_{\max} is sensitive to the dislocation structure. Gantmakher and Kulesko ^[4] have advanced several suggestions concerning a possible interpretation of the effect; the data for aluminum ^[5] give grounds for preferring the suggestion that the electrons are scattered by phonon modes connected with the dislocation.

In this paper we consider the problem of resistivity of a metal with dislocations and take inelastic scattering into account. Before we proceed to formulate the problem, we mention that the theoretical calculations of the usual residual dislocation resistivity $\rho^d(0)$, performed by a number of workers, were not in satisfactory agreement with experiment: the calculated cross sections were smaller by one or two orders than the measured ones. ^[6] In the calculations the perturbation was chosen in some form of a deformation potential proportional to the tensor of the strain due to the dislocation. Such a perturbation should describe well the contribution from long-range lattice distortions, but is not suitable in regions close to the dislocation line itself. It is quite pos-

sible that the cause of so large a disparity between theory and experiment is indeed the underestimate of the role of the core, i.e., of that region where the displacements of the atoms from their positions in a perfect crystal are not small. Among other things, this strongly altered region distorts the electron spectrum and bound states of electrons can be produced. ^[7] We proceed from the assumption that the dislocation core makes the decisive contribution to the electron scattering. It is not our task to verify this assumption theoretically and to calculate rigorously the scattering by the core; we shall take the scattering properties of the core into account phenomenologically, by assigning to the atoms situated on the dislocation line pseudopotentials different from those of the atoms of a perfect crystal. The difference between the corresponding scattering amplitudes is a phenomenological parameter, whose value we shall obtain from the experimental residual dislocation resistivity $\rho^d(0)$. With the scattering problem so formulated, the influence of the dislocation as a singular line on the lattice-vibration spectrum is accounted for simultaneously in natural fashion.

This is easiest and simplest to do with the aid of the Lifshitz-Kosevich model, in which a linear defect is represented by a line of local changes of the force matrix of the crystal. ^[8] The electron-scattering probability $W_{\mathbf{k}\mathbf{k}'}$, which determines the resistivity, will be determined in the Born approximation using the free-electron model (\mathbf{k} and \mathbf{k}' are the wave vectors of the initial and final states). The perturbation is taken to be the combined pseudopotential of the metal with the dislocations; we confine ourselves to a cubic lattice of the perfect crystal and represent the dislocations as straight lines oriented along the cubic axes and disposed in random fashion. Simultaneously with accounting for the singular properties of the dislocation atoms as scatterers, we wish to take into account the role they play in the lattice vibrations, and particularly the influence of the corresponding changes of the force matrix on the phonon spectrum.

This purpose is well served by the calculation scheme used by Kagan and Zhernov. ^[9] In this scheme, $W_{\mathbf{k}\mathbf{k}'}$ is

expressed in terms of the Van Hove scattering correlation function $S(\mathbf{q}, \omega)$:

$$W_{\mathbf{k}\mathbf{k}'} = \frac{(2\pi)^2}{m^2 V_0} S, \quad S(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{n}\mathbf{n}'} a_{\mathbf{n}}(\mathbf{q}) a_{\mathbf{n}'}(\mathbf{q}) S_{\mathbf{n}\mathbf{n}'}(\mathbf{q}, \omega), \quad (1)$$

$$S_{\mathbf{n}\mathbf{n}'}(\mathbf{q}, \omega) = \langle \exp[-i\mathbf{q}\mathbf{R}_{\mathbf{n}}(t)] \exp[i\mathbf{q}\mathbf{R}_{\mathbf{n}'}(0)] \rangle_{\omega};$$

here

$$\mathbf{q} = \mathbf{k} - \mathbf{k}', \quad \omega = \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}, \quad \langle \dots \rangle_{\omega} = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \dots \rangle,$$

m is the effective mass of the electron, V_0 is the volume of the unit cell, N is the number of sites in the crystal, $a_{\mathbf{n}}(\mathbf{q})$ is the amplitude of the electron scattering by the n -th site ($a_{\mathbf{n}}(\mathbf{q}) = -(mV_0/2\pi)w_{\mathbf{n}}(\mathbf{q})$, where $w_{\mathbf{n}}(\mathbf{q})$ is the Fourier component of the pseudopotential), the radius vector of this site is $\mathbf{R}_{\mathbf{n}}(t) = \mathbf{R}_{\mathbf{n}}^0 + \mathbf{u}_{\mathbf{n}}(t)$, $\mathbf{u}_{\mathbf{n}}(t)$ is the operator of displacement from the equilibrium position in the Heisenberg representation, $\varepsilon_{\mathbf{k}}$ is the electron energy, and $\langle \dots \rangle$ denotes statistical averaging over the vibrational states. It suffices to retain in the correlation function $S_{\mathbf{n}\mathbf{n}'}(\mathbf{q}, \omega)$ the expansion terms quadratic in $\mathbf{u}_{\mathbf{n}}$, i.e.,

$$S_{\mathbf{n}\mathbf{n}'}(\mathbf{q}, \omega) = \exp[i\mathbf{q}(\mathbf{R}_{\mathbf{n}}^0 - \mathbf{R}_{\mathbf{n}'}^0)] \{ 2\pi\delta(\omega) (1 - \frac{1}{2}W_{\mathbf{n}} - \frac{1}{2}W_{\mathbf{n}'}) + \langle (\mathbf{q}\mathbf{u}_{\mathbf{n}}(t)) (\mathbf{q}\mathbf{u}_{\mathbf{n}'}(0)) \rangle_{\omega} \}, \quad (2)$$

$$W_{\mathbf{n}} = \langle (\mathbf{q}\mathbf{u}_{\mathbf{n}}(0))^2 \rangle.$$

In accord with the foregoing, we ascribe to the dislocation line itself all the changes in the electron scattering, and assume that the atoms situated on this line have a scattering amplitude $a_1(\mathbf{q})$ different from the scattering amplitude $a_0(\mathbf{q})$ of the other atoms.¹⁾ To select the sites on the dislocation lines we label the directions of the latter by the index α of the coordinate axis congruent with this line. In the atomic plane perpendicular to the axis α , the coordinates of the atoms are labeled by a two-dimensional index $n_{\xi_{\alpha}}, \xi_{\alpha} \perp \alpha$, with $n = (n_{\alpha}, n_{\xi_{\alpha}})$; we introduce a function $c_{\alpha}^{\xi}(\mathbf{r}_{\xi_{\alpha}})$ equal to unity if $n_{\xi_{\alpha}}$ falls on a dislocation site and to zero in all other places. We can now use for $a_{\mathbf{n}}$ in (1) the expression

$$a_{\mathbf{n}} = a_0 + \sum_{\alpha=x, y, z} \Delta_{\alpha} c^{\alpha}(n_{\xi_{\alpha}}), \quad \Delta_{\alpha} = a_1 - a_0. \quad (3)$$

We neglect the contribution from the intersection of dislocation lines, since it is quadratic in the dislocation density.

The influence of the dislocation manifests itself, further, in the expressions for the correlators in (2). The equations for the oscillations can be written in the Lifshitz-Kosevich model in the form

$$\ddot{\mathbf{u}}_{\mathbf{n}} + \frac{1}{M} \sum_{\mathbf{n}'} A(\mathbf{n} - \mathbf{n}') \mathbf{u}_{\mathbf{n}'} = - \sum_{\alpha} \sum_{n_{\xi_{\alpha}}, n'_{\xi_{\alpha}}} c^{\alpha}(n_{\xi_{\alpha}}) \delta(n_{\xi_{\alpha}}, n'_{\xi_{\alpha}}) U(n_{\alpha} - n'_{\alpha}) \mathbf{u}_{\mathbf{n}'}. \quad (4)$$

Here M is the mass of the atom, $A(\mathbf{n} - \mathbf{n}')$ is the unperturbed force matrix, and the right-hand side describes its local perturbation. The force matrices in (4) are taken

in a form diagonal in the vibration polarization indices; this simplification, which exerts no fundamental effect on the results, allows us to use henceforward the scalar value of the displacement and obviates the need for writing down the polarization indices.

We introduce in the usual manner the lattice Green's function ($\hbar = 1$)

$$G(\mathbf{n}, \mathbf{n}'; t) = -iM \begin{cases} \langle [u_{\mathbf{n}}(t), u_{\mathbf{n}'}(0)] \rangle, & t > 0 \\ \langle [u_{\mathbf{n}'}(0), u_{\mathbf{n}}(t)] \rangle, & t < 0 \end{cases} \quad (5)$$

It is easy to obtain for its frequency Fourier component, with the aid of (4), the Dyson equation

$$G(\mathbf{n}, \mathbf{n}'; \omega) = G^0(\mathbf{n} - \mathbf{n}'; \omega) + \sum_{\alpha, \mathbf{n}_1, \mathbf{n}_2} c^{\alpha}(\mathbf{n}_{1\xi_{\alpha}}) \delta(\mathbf{n}_{1\xi_{\alpha}}, \mathbf{n}_{2\xi_{\alpha}}) \times G^0(\mathbf{n} - \mathbf{n}_1; \omega) U(n_{1\alpha} - n_{2\alpha}) G(\mathbf{n}_2, \mathbf{n}'; \omega) \quad (6)$$

(G^0 is the Green's function of the ideal lattice). After determining $G(\mathbf{n}, \mathbf{n}'; \omega)$ from (6), we obtain the Fourier components of the correlators in (2), using the known relation

$$\langle u_{\mathbf{n}}(t) u_{\mathbf{n}'}(0) \rangle_{\omega} = -2M^{-1} (n_{\alpha} + 1) \text{Im} G(\mathbf{n}, \mathbf{n}'; \omega + i\delta), \quad (7)$$

$$n_{\omega} = [e^{n_{\alpha}/T} - 1]^{-1}.$$

Finally, we obtain the resistivity from the formula

$$\rho = \frac{1}{2Tj^2} \int dk dk' (\varphi_{\mathbf{k}} - \varphi_{\mathbf{k}'})^2 f_{\mathbf{k}}^0 (1 - f_{\mathbf{k}'})^0 W_{\mathbf{k}\mathbf{k}'}, \quad (8)$$

$$j = e \int dk v_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}}.$$

Here $\varphi_{\mathbf{k}} \partial f_{\mathbf{k}}^0 / \partial \varepsilon_{\mathbf{k}}$ is the nonequilibrium increment to the Fermi distribution function $f_{\mathbf{k}}^0$. Of course, it is necessary to average in (8) over the dislocation configurations.

2. CALCULATION OF THE RESISTIVITY

We choose $\varphi_{\mathbf{k}}$ in the form customary in the free-electron model:

$$\varphi_{\mathbf{k}} = \mathbf{k}\mathbf{E}, \quad (9)$$

where \mathbf{E} is the electric field. It is then necessary to average over the configurations only the structure factor S that enters in (1). Taking (2) and (7) into account and using (3), we obtain for that part of S which corresponds to elastic scattering, in the approximation linear in the dislocation density,

$$\langle S_{\alpha} \rangle_c = (2\pi)^2 \delta(\omega) \sum_{\alpha} c_{\alpha} \delta(q_{\alpha} b) [(\Delta a)^2 - W_1 (\Delta a)^2 - (W_1 - W_0) a_0 \Delta a]. \quad (10)$$

Here W_0 and W_1 are the Debye-Waller factors (2) for sites outside the dislocation and on the dislocation, respectively, b is the lattice constant, $c_{\alpha} = D_{\alpha} b^2$, and D_{α} is the density of the dislocations parallel to the α axis. In inelastic scattering the structure factor reduces to the expression

$$\langle S_{inel} \rangle_c = -\frac{2q^2}{M}(n_\omega + 1) \left\langle \frac{1}{N} \sum_{n, n'} \exp[iq(n-n)b] \right. \\ \times \left\{ a_0^2 + a_0 \Delta a \sum_{\alpha} [c^2(n_{\alpha}) + c^2(n_{\alpha}')] \right\} \\ \left. + (\Delta a)^2 \sum_{\alpha, \beta} c^2(n_{\alpha}) c^2(n_{\beta}) \operatorname{Im} G(n, n'; \omega + i\delta) \right\rangle_c. \quad (11)$$

The averaging of all three terms of (11) over the configurations in the approximation linear in c_α can be carried out by a method which is a certain generalization of the method used by Elliott and Taylor.^[10] We shall not give the calculations here, but present the final expressions for the averaged Green's functions encountered in (11). The term with a_0^2 contains a Green's function with arbitrary lattice indices, and we have for it

$$\langle G(n, n'; \omega) \rangle_c = \frac{1}{N} \sum_{\alpha} G_{\alpha}^{\circ}(\omega) \exp[iq(n-n')b] \\ \times \left[1 - \sum_{\alpha} c_{\alpha} \chi_{\alpha}(q_{\alpha}, \omega) G_{\alpha}^{\circ}(\omega) \right]^{-1}, \quad (12)$$

where

$$\chi_{\alpha}(q_{\alpha}, \omega) = U_{q_{\alpha}} / [1 - U_{q_{\alpha}} G_{\alpha}^{\circ}(0; \omega)] = \chi_{\alpha}(\omega); \quad (13)$$

$U_{q_{\alpha}}$, $G_{\alpha}^{\circ}(\omega)$, and $G_{\alpha}^{\circ}(n_{\alpha}; \omega)$ are the spatial Fourier components of the local potential U from (4) and of the Green's function of a perfect crystal:

$$U_{q_{\alpha}} = \sum_{n_{\alpha}} U(n_{\alpha}) \exp(-iq_{\alpha} n_{\alpha} b), \\ G_{\alpha}^{\circ}(\omega) = \sum_{n_{\alpha}} G^{\circ}(n_{\alpha}; \omega) e^{-iq_{\alpha} n_{\alpha} b} = \frac{1}{\omega^2 - \omega_{q_{\alpha}}^2}, \quad (14)$$

$$G_{\alpha}^{\circ}(n_{\alpha}; \omega) = \sum_{n_{\alpha}} G^{\circ}(n_{\alpha}; \omega) \exp(-iq_{\alpha} n_{\alpha} b) = \frac{1}{N_{\alpha}} \sum_{n_{\alpha}} \frac{\exp(iq_{\alpha} n_{\alpha} b)}{\omega^2 - \omega_{q_{\alpha}}^2};$$

N_{α} is the number of atoms in the plane perpendicular to the α axis, and $\omega_{q_{\alpha}}$ is the natural frequency of the oscillations of a perfect lattice and corresponds to the wave vector q_{α} ; within the framework of our approximations we can assume that $\omega_{q_{\alpha}} = sq_{\alpha}$, where s is a certain effective speed of sound; q_{α} is the projection of q on the direction of the dislocation line.

The other terms of (11) depend on Green's functions with lattice indices that fall on dislocation lines. The averaged value of this function, which we shall label with the superscript d , is

$$\langle G^d(n, n'; \omega) \rangle_c = \frac{1}{N_{\alpha}} \sum_{q_{\alpha}} \frac{\exp[iq_{\alpha}(n_{\alpha} - n'_{\alpha})b] G_{q_{\alpha}}^{\circ}(n_{\alpha} - n'_{\alpha}; \omega)}{1 - U_{q_{\alpha}} G_{q_{\alpha}}^{\circ}(0; \omega)}, \quad (15)$$

where N_{α} is the number of atoms on the dislocation line ($N_{\alpha} N_{\alpha'} = N$).

Using (12) and (15), we obtain for $\langle S_{inel} \rangle_c$

$$\langle S_{inel} \rangle_c = -\frac{2q^2}{M}(n_\omega + 1) \operatorname{Im} \left\{ a_0^2 G_{\alpha}^{\circ}(\omega + i\delta) \right. \\ \times \left[1 + \frac{\sum_{\alpha} c_{\alpha} \chi_{\alpha}(\omega + i\delta) G_{\alpha}^{\circ}(\omega + i\delta)}{1 - \sum_{\alpha} c_{\alpha} \chi_{\alpha}(\omega + i\delta) G_{\alpha}^{\circ}(\omega + i\delta)} \right] + 2a_0 \Delta a \sum_{\alpha} c_{\alpha} \frac{G_{\alpha}^{\circ}(\omega + i\delta)}{1 - U_{q_{\alpha}} G_{q_{\alpha}}^{\circ}(0; \omega + i\delta)} \\ \left. + (\Delta a)^2 \sum_{\alpha} c_{\alpha} \frac{G_{q_{\alpha}}^{\circ}(0; \omega + i\delta)}{1 - U_{q_{\alpha}} G_{q_{\alpha}}^{\circ}(0; \omega + i\delta)} \right\}. \quad (16)$$

We have already separated in the first term the part that leads to the ordinary Bloch law for the resistivity of an ideal metal due to scattering by phonons (the unity term in the square brackets). The contributions of all other terms of (16) to ρ are proportional to the dislocation density, i.e., they correspond to the inelastic part of ρ^d .

The elastic part of ρ^d , which is obtained by substituting in (8) the structure factor (10), contains the temperature-independent residual resistivity $\rho^d(0)$, which is connected with the first term of (10), and also parts that depend on T via the Debye-Waller factors W_1 and W_0 . The latter are given by

$$W_0 = -\frac{q^2}{\pi M} \int_{-\infty}^{\infty} d\omega (n_{\omega} + 1) \operatorname{Im} G^{\circ}(0; \omega + i\delta), \quad (17)$$

$$W_1 = -\frac{q^2}{\pi M} \int_{-\infty}^{\infty} d\omega (n_{\omega} + 1) \operatorname{Im} \langle G^d(n, n; \omega + i\delta) \rangle_c.$$

In the calculation of the integrals with respect to $dkdk'$ or $dkdq = dk k^2 d\theta \times \sin\theta d\varphi dq^2 d\theta' \sin\theta' d\varphi'$ in (8) it is useful to change over to the integration variables

$$k_{\perp} = k^2/2m, \quad \omega = (-q^2 + 2kq)/2m, \quad q, q_{\alpha}, \varphi, \varphi'.$$

We assume henceforth that the electric field \mathbf{E} (which enters in $\varphi_{\mathbf{k}}$ (9)) is oriented along a definite crystallographic axis, i.e., it is parallel or perpendicular to various sets of dislocation lines. This assumption simplifies the analysis of the anisotropy effects, which undoubtedly must arise in the presence of some preferred orientation in the dislocation system.

The integration with respect to $d\varphi d\varphi'$ and $d\mathbf{e}_{\mathbf{k}}$ can be carried out immediately, and the Fermi statistics impose the usual limitation $q_0 = 2k_F$ on the interval of the integration with respect to dq . The expression for $\rho^d(T)$ obtained by subtracting from (8) the phonon resistivity of the ideal metal can be represented in the form

$$\rho^d(T) = \rho_{el}^d + \rho_{inel}^d \quad (18)$$

where

$$\rho_{el}^d = \rho_1 \sum_{\alpha} c_{\alpha} \int_{\alpha} dQ Q^2 [(\Delta \bar{a})^2 - W_1 (\Delta \bar{a})^2 - \bar{a}_0 \Delta \bar{a} (W_1 - W_0)]; \quad (19a)$$

$$\rho_{inel}^d = -\rho_2 \sum_{\alpha} c_{\alpha} \int_{\alpha} dQ Q^2 \int_0^{\Theta} dQ_{\alpha} F_{\alpha} \int_{-\infty}^{\infty} d\Omega \Omega n_{\Omega} (n_{\Omega} + 1) I(\Omega, Q, Q_{\alpha}), \quad (19b)$$

$$I(\Omega, Q, Q_{\alpha}) = \operatorname{Im} \left\{ [(\Delta \bar{a})^2 \frac{(bk_F)^2}{\pi} \bar{G}_{\alpha}(\Omega + i\delta) + \frac{2\bar{a}_0 \Delta \bar{a}}{(\Omega + i\delta)^2 - Q^2} + \frac{\bar{a}_0^2 \pi}{(k_F b)^2} \frac{V_{\alpha}}{[(\Omega + i\delta)^2 - Q^2]^2}] \frac{1}{1 - V_{\alpha} \bar{G}_{\alpha}(\Omega + i\delta)} \right\}.$$

We have used here the following notation for the parameters:

$$\Theta = \hbar \omega_0, \quad \omega_0 = sq_0; \\ \rho_1 = \frac{p_F}{e^2} a_0^2(0) \frac{72\pi^4}{(k_F b)^4}, \quad \rho_2 = \rho_1 \frac{8k_F b}{\pi^2} \frac{p_F}{M s}, \quad (20)$$

and also for the variables:

$$Q = q/q_0, \quad Q_{\alpha} = q_{\alpha}/q_0, \quad \Omega = \omega/\omega_0$$

and the functions (see (14)):

$$\begin{aligned} \tilde{a}_0 &= \frac{a_0(q)}{a_0(0)}, \quad \Delta \tilde{a} = \frac{\Delta a(q)}{\Delta a(0)}, \quad V_\alpha = \frac{b^2}{4\pi s^2} U_{q_\alpha}, \\ \tilde{G}_\alpha(\Omega + i\delta) &= \frac{\pi \omega_0^2}{(bk_F)^2} G_{q_\alpha}^0(0; \omega + i\delta) = \int_0^{1-q_\alpha} \frac{dx}{(\Omega + i\delta)^2 - Q_\alpha^2 - x} = I_\alpha - i\pi g_\alpha \text{sign } \Omega, \\ I_\alpha &= \ln \left| \frac{\Omega^2 - Q_\alpha^2}{1 - \Omega^2} \right|, \\ g_\alpha &= \theta(1 - \Omega^2) \theta(\Omega^2 - Q_\alpha^2) + [\theta(\Omega^2 - 1) + \theta(Q_\alpha^2 - \Omega^2)] \delta, \quad \delta \rightarrow +0; \end{aligned} \quad (21)$$

θ is the unit step function (the integral in (21) is cut off at the upper limit in the spirit of the Debye model). The prime at the summation sign and at ρ_{el}^d means that it is necessary to take only the α corresponding to directions perpendicular to the electric field E ; the function F_α is given by

$$F_\alpha = \begin{cases} Q_\alpha^2, & E \parallel \alpha \\ (Q_\alpha^2 - 2), & E \perp \alpha \end{cases}$$

(we recall that the cubic-axes index α labels also the directions of the dislocation lines).

Formulas (18) and (19) are the general (within the framework of our model) expressions for the dislocation resistivity $\rho^d(T)$. It is due, as follows from (19a) and (19b), to three processes: direct scattering by dislocations (terms with $(\Delta \tilde{a})^2$), scattering by the distorted phonon spectrum (terms proportional to a_0^2), and interference of these two effects (the part with $\tilde{a}_0 \Delta \tilde{a}$). The residual resistivity is obviously determined by the first term of (19a):

$$\rho^d(0) = \rho_1 \sum_\alpha' c_\alpha \int_0^1 dQ Q^2 (\Delta \tilde{a})^2. \quad (22)$$

All other terms introduce a temperature dependence. The concrete results for $\rho^d(T)$ depend on the form of the functions $\Delta \tilde{a}(Q)$ and $V_\alpha(Q_\alpha)$, which characterize respectively the change of the scattering amplitude and the distortion of the interatomic-interaction forces by the dislocation line (all other functions and parameters of our model are given in (18)–(21), and the form of $\tilde{a}_0(Q)$ can be borrowed from pseudopotential theory).

3. RESULTS AND DISCUSSION

In the limiting case of high temperatures $T \gg \Theta$ we can progress quite far in an analysis of $\rho^d(T)$ without involving greatly the concrete forms of $\Delta \tilde{a}$ and V_α . We replace the product of the Planck functions in (19) by $T^2/(\Theta\Omega)^2$ and consider by way of example the integral of the first term of (19b) with respect to $d\Omega$:

$$\begin{aligned} Y_1 &= \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega} \text{Im} \frac{\tilde{G}_\alpha(\Omega + i\delta)}{1 - V_\alpha \tilde{G}_\alpha(\Omega + i\delta)} = \frac{1}{2i} \int_0^1 \frac{d\Omega^2}{\Omega^2} \left[\frac{\tilde{G}_\alpha(\Omega + i\delta)}{1 - V_\alpha \tilde{G}_\alpha(\Omega + i\delta)} - \text{c.c.} \right] \\ &= \frac{1}{2i} \int_{C_1} \frac{dx}{x} \frac{\tilde{G}_\alpha(x)}{1 - V_\alpha \tilde{G}_\alpha(x)}. \end{aligned}$$

The contour C_1 is made up of the lines $(0 + i\delta, \infty + i\delta)$ and $(\infty - i\delta, 0 - i\delta)$, with $\delta \rightarrow +0$. Closing it with arcs of the circles C_0 of radius $r \rightarrow 0$ and C_R of radius $R \rightarrow \infty$ (see Fig. 1), we obtain

$$\begin{aligned} Y_1 &= \frac{1}{2i} \left[\oint_{c_0+c_1+c_\infty} \frac{\tilde{G}_\alpha(x)}{x} - \oint_{c_\infty} \frac{\tilde{G}_\alpha(x)}{x} \right] \frac{dx}{1 - V_\alpha \tilde{G}_\alpha(x)} \\ &= \pi \frac{\tilde{G}_\alpha(0)}{1 - V_\alpha \tilde{G}_\alpha(0)} + \pi \sum' \text{Res} \frac{\tilde{G}_\alpha(x)}{x(1 - V_\alpha \tilde{G}_\alpha(x))}. \end{aligned}$$

Here \sum' contains only the residues of the poles outside the real positive axis.

It is easy to verify, by using (21), that such a pole is possible only on the negative axis under the conditions $V_\alpha < 0$ and $\exp(1/V_\alpha) > Q_\alpha^2$. As a result we have

$$\begin{aligned} Y_1 &= \pi \frac{\ln Q_\alpha^2}{1 - V_\alpha \ln Q_\alpha^2} + \pi \theta(-V_\alpha) \theta \left(\exp\left(\frac{1}{V_\alpha}\right) - Q_\alpha^2 \right) \\ &\quad \times \frac{\exp(1/V_\alpha) (1 - Q_\alpha^2)}{V_\alpha^2 (\exp(1/V_\alpha) - 1) (\exp(1/V_\alpha) - Q_\alpha^2)}. \end{aligned} \quad (23)$$

The other parts of (19) are calculated similarly. We present the formulas for the high-temperature limit of ρ^d , with terms similar to the second term of (23) omitted²⁾:

$$\begin{aligned} \rho_{el}^d(T) - \rho^d(0) &= \rho_2 (bk_F)^2 \frac{T}{\Theta} \sum_\alpha' c_\alpha \int_0^1 dQ Q^2 \left[\int_0^1 dQ_\alpha \frac{\ln Q_\alpha^2}{1 - V_\alpha \ln Q_\alpha^2} (\Delta \tilde{a})^2 \right. \\ &\quad \left. + \left(1 + \int_0^1 dQ_\alpha \frac{\ln Q_\alpha^2}{1 - V_\alpha \ln Q_\alpha^2} \right) \tilde{a}_0 \Delta \tilde{a} \right], \end{aligned} \quad (24)$$

$$\begin{aligned} \rho_{inel}^d(T) &= \rho_2 \frac{T}{\Theta} \sum_\alpha' c_\alpha \int_0^1 dQ Q^2 \int_0^1 dQ_\alpha \frac{F_\alpha}{1 - V_\alpha \ln Q_\alpha^2} \\ &\quad \times \left[-(bk_F)^2 (\Delta \tilde{a})^2 \ln Q_\alpha^2 + \frac{2\pi \tilde{a}_0 \Delta \tilde{a}}{Q^2} - \frac{\pi^2 \tilde{a}_0^2 V_\alpha}{(bk_F)^2 Q^4} \right]. \end{aligned} \quad (25)$$

Let us ascertain first whether our results (24) and (25) can ensure at $T \sim \Theta$ a value of $\rho^d(T)$ of the same order as $\rho^d(0)$ (22), as is the case in the experiments. We used for the purpose the maximum-screening approximation, in which $a(Q) = a(0)$, and put in (22), (24), and (25)

$$\tilde{a}_0 = 1, \quad \Delta \tilde{a} = \text{const.}$$

The potential V_α is taken in the long-wave approximation³⁾:

$$V_\alpha = -\lambda Q_\alpha^2. \quad (26)$$

At $|\lambda| < e$ the integrand in (24) and (25) has no singularities, and the calculations yield (at $|\lambda| \leq e$)

$$\rho^d(0) = \rho_1^* \sum_\alpha' c_\alpha, \quad \rho_1^* = \rho_1 (\Delta \tilde{a})^2 / 3$$

and next

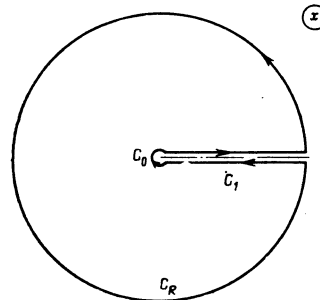


FIG. 1.

$$r(T) = \frac{\rho^d(T) - \rho^d(0)}{\rho^d(0)} \approx \frac{p_F}{Ms} \frac{T}{\Theta} \left\{ \frac{4}{\pi} \frac{bk_F}{\Delta\tilde{a}} \left(1 + \frac{c_{\parallel}}{c_{\perp}} \right) + \frac{2}{5} \frac{\lambda}{bk_F(\Delta\tilde{a})^2} \left(1 + \frac{3c_{\parallel}}{c_{\perp}} \right) - \frac{4}{5\pi^2} (bk_F)^3 \left(1 - \frac{5c_{\parallel}}{3c_{\perp}} \right) \right\}. \quad (27)$$

Here $c_{\parallel(\perp)}$ is the density of the dislocations parallel (perpendicular) to the electric field.

For $|\lambda| \gg e$ we have (we retain only the principal terms in λ^{-1})

$$r(T) \approx 6 \frac{T}{\Theta} \frac{p_F}{Ms} \left\{ \frac{2}{\pi} \frac{bk_F}{\Delta\tilde{a}} \left(\frac{\pi(bk_F)^2}{15} - \frac{\ln 2}{\lambda} \frac{c_{\parallel}}{c_{\perp}} \right) - \frac{1}{bk_F(\Delta\tilde{a})^2} \left(\frac{1}{2} \ln \frac{4}{3} + \frac{c_{\parallel}}{c_{\perp}} \ln \frac{3}{2} \right) - \frac{3}{5} \frac{(bk_F)^3}{\pi^2 \lambda} \left(1 - \frac{5}{3} \frac{c_{\parallel}}{c_{\perp}} \right) \right\}. \quad (28)$$

The expression for $r(T)$ contains the small parameter $p_F/Ms \sim s/v_F \ll 1$, which characterizes (together with $\Delta\tilde{a}$ and T/Θ) the magnitude of the temperature part of the cross section relative to the static part. It is therefore clear that a large temperature effect cannot be produced by pure dislocation scattering, without allowance for the changes of the phonon spectrum (the last terms of (27) and (28)).³⁾ Noticeable changes can be ensured in our problem by interference and phonon processes (the first two terms in (27) and (28)) provided that $\Delta\tilde{a}$ is small enough. We shall retain henceforth only these terms. The sign of the effect or the direction of the slope of the $r(T)$ plot is determined in this case by the ratio of the parameters $\Delta\tilde{a}$ and λ and by their signs. At $|\lambda| \ll 1$ the interference term predominates and $r(T)$ is independent of λ , while the sign of the effect is the sign of the parameter $\Delta\tilde{a}$. At $|\lambda| \gg e$ both the phonon term and the interference term are practically independent of λ ,⁴⁾ the sign of the latter is connected as before with the sign of $\Delta\tilde{a}$, and the contribution of the phonon term is negative.

We present numerical estimates for the parameters of copper (in the calculations of a_0 we used the limiting value of the Fourier component of the pseudopotential $w_0(0) = -2/3\epsilon_F$,^[11] and for $\rho^d(0)/D_{\perp}$ we assumed the value $2 \times 10^{-19} \Omega\text{-cm}^2$,^[1] which yielded $|\Delta\tilde{a}| \approx 0.1$):

$$r(T) \approx \frac{T}{\Theta} \text{sign } \Delta\tilde{a} \cdot 0.5 \left(1 + \frac{c_{\parallel}}{c_{\perp}} \right), \quad |\lambda| \ll 1, \quad (29)$$

$$r(T) \approx \frac{T}{\Theta} \left[\text{sign } \Delta\tilde{a} \left(3.8 - \frac{2}{\lambda} \frac{c_{\parallel}}{c_{\perp}} \right) - \left(0.9 + 1.7 \frac{c_{\parallel}}{c_{\perp}} \right) \right], \quad |\lambda| \gg e.$$

The estimates (29) show that it is possible in principle to attribute the large (~ 1) values of $r(T)$ to the scattering processes considered by us.

The temperature functions that describe the electron-phonon scattering and take a linear asymptotic form usually become linear long before the values $T/\Theta \sim 1$ are reached. One can expect formulas (27) and (28) to remain in force also at $T/\Theta \lesssim 1$. The analysis of the low-temperature limit ($T/\Theta \ll 1$) of the expressions (18) and (19) for $\rho^d(T)$ is much more cumbersome. A distinction must be made between the contributions due to scattering by bound and by resonant phonon states. The former are formally connected with the poles of the function $(1 - V_{\alpha} \tilde{G}_{\alpha})^{-1}$ in (19b), which appear in the region $\Omega^2 < Q_{\alpha}^2$,⁵⁾ i.e., the roots of the equation $1 - V_{\alpha} I_{\alpha} = 0$, and are equal to

$$\Omega^2 = \Omega_{\text{loc}}^2 = \frac{Q_{\alpha}^2 - \exp(1/V_{\alpha})}{1 - \exp(1/V_{\alpha})}. \quad (30)$$

The roots (39) fall in the region $\Omega^2 < Q_{\alpha}^2$ only if $V_{\alpha} < 0$ [i.e., $\lambda < 0$ in (26)]. The resonant scattering takes place in the region $Q_{\alpha}^2 < \Omega^2 < 1$, in which $(1 - V_{\alpha} \tilde{G}_{\alpha})^{-1}$ gives the resonant denominator $(1 - V_{\alpha} I_{\alpha})^2 + \pi^2 V_{\alpha}^2$.

In the region where bound states exist, the integration with respect to $d\Omega$ in (19b) is carried out with the aid of a δ -function that replaces Ω with $\Omega_{\text{loc}}(Q_{\alpha})$. In the maximum-screening approximation we can carry out directly also the integration with respect to dQ . The greatest difficulties are raised by the integration with respect to dQ_{α} , but asymptotic estimates can be obtained by the saddle-point method. For resonant scattering, the calculations are more difficult (two integrations with respect to dQ_{α} and $d\Omega$ remain), but for a number of limiting cases it is nevertheless possible to obtain analytic solutions. We shall not present the cumbersome and hard-to-visualize results for the low-temperature limit, and merely note their characteristic features.

Of course, the small parameter p_F/Ms is retained here, too, in the expression for $r(T)$, but the temperature dependence is more complicated. At $|\lambda| \ll 1$ the principal role is played by terms with a power-law temperature dependence, which are proportional to $(T/\Theta)^4$, $(T/\Theta)^5$, and $(T/\Theta)^6$, but there are also exponential terms $\propto \exp[-3(\Theta^2/\lambda T^2)^{1/3}]$ (they appear at $T < \lambda\Theta$). At larger values of the parameter λ the temperature terms have a greater variety of forms. Depending on the relations between T , Θ , and λ , power-law terms appear (from the first to the sixth power of T/Θ) as well as exponentials such as $\exp(-2\Theta/T(\lambda \ln \lambda)^{1/2})$ [at $T < \Theta/(\lambda \ln \lambda)^{1/2}$]. The principal role is played, just as at high temperatures, by the interference and phonon terms, but the relation between them differs from that in (27) and (28).

The character of the transition of the function $r(T)$ to the linear limit depends on the value of λ . The transition becomes steeper with increasing λ . Typical plots of $r(T)$ for $\Delta\tilde{a} > 0$, $c_{\parallel} = c_{\perp}$, and for λ equal 10 and 100, are shown in Fig. 2.

We note one more important feature of the temperature part of the dislocation resistivity: the quantity $\rho^d(T)$ depends on dislocations of all orientations, in contrast to the residual resistivity $\rho^d(0)$, which is not influ-

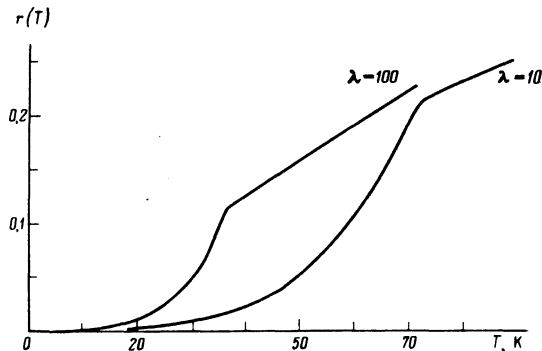


FIG. 2.

enced by dislocations parallel to the applied field. A study of the anisotropy of $\rho^d(T)$ may permit a more reliable determination of the role of the scattering mechanism considered by us. For example, a situation is possible with $\rho_{\parallel}^d(T) < 0$ but $\rho_{\perp}^d(T) > 0$ (the symbols \parallel and \perp mark the contributions from dislocations parallel and perpendicular to the electric field). This should occur if $\lambda \gg 1$ and $\Delta\tilde{a} > 0$. For high temperatures this follows from (29); for low temperatures this behavior should take place at $\lambda > 4(\Delta\tilde{a})(\hbar k_F)^2$, when the main contribution to ρ_{\parallel}^d is made by resonant states. At $\Delta\tilde{a} < 0$, ρ_{\parallel}^d and ρ_{\perp}^d are negative, but the anisotropy at large λ remains; thus, at high temperatures the dislocations parallel to the field scatter three times more strongly than the perpendicular ones. At low values of λ the anisotropy decreases.

The foregoing results demonstrate the important role played in the qualitative picture of the effect considered here by the parameter λ , which characterizes the local distortion of the force constants. The value of this phenomenological parameter of the Lifshitz-Kosevich model is unknown. As shown in this paper, the phonon modes distorted by the dislocations should exert a most noticeable influence on the temperature dependence of the dislocation resistivity regardless of the parameter λ (see (29)). It is possible that the experimental results^[2-5] are explained by the described mechanism. This can be established more reliably by carrying out a more detailed investigation of the character of $\rho^d(T)$ in the low-temperature region. Then a comparison of the experimental data with the numerical calculations will make it possible to estimate the value of λ .

¹It is assumed that the parameter $a_1(q)$ takes into account the possibility of formation of bound electronic states on the dislocations. The corresponding change in the electron scatter-

ing can depend in principle also on the temperature. This effect, however, calls for a special analysis and will not be considered here.

²In the long-wave approximation for the potential V_{α} (we confine ourselves in the estimates to this approximation) the contribution of such terms can be shown to be negligible. On the other hand, the Lifshitz-Kosevich model, which we use to calculate the Green's function and the spectrum, does not cover the case of sufficiently short waves.

³We are not considering cases with $c_{\parallel} \gg c_{\perp}$.

⁴It is of interest to note that the main contribution to the interference part of (28) is due to the Debye-Waller factor—the last term of (24).

⁵The function $(1 - V_{\alpha} \tilde{G}_{\alpha})^{-1}$ has poles also in the region $\Omega^2 > 1$. They lead to a contribution $\propto \exp(-\Theta/T)$ to the resistivity, but the Lifshitz-Kosevich model is not valid in the region of their existence.

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Translated by J. G. Adashko