Temperature dependence of the cross section for electron scattering by dislocations in metals

V. F. Gantmakher and G. I. Kulesko

Solid State Institute, USSR Academy of Sciences

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The temperature dependence of the additional electrical resistance that arises when dislocations are introduced into a metal is examined for single-crystal and polycrystalline specimens of copper, molybdenum, and zinc. In all cases a stepped curve is obtained, the position of the step on the temperature scale being independent of the degree and mode of deformation. The possibility is discussed that a temperature dependence of this type may result from a temperature dependence of the cross section for scattering of electrons by the dislocation themselves, either on account of inelastic scattering via quasilocal vibrational modes, or on account of changes in the elastic scattering cross section because of filling of electron levels localized at the dislocations.

More than a decade has now passed since it was first reported[1] that the additional electrical resistivity ρ_d that arises when dislocations are introduced into a metallic conductor increases sharply as the temperature is raised through a comparatively narrow interval. Here we present the results of an experimental study of this phenomenon, mainly as it appears in copper and molybdenum, and discuss some of its possible causes.

MEASUREMENTS

A potentiometric method (sensitivity 10^{-8} V, measuring current 1–2 A) was used for the resistance measurments. The specimens were rectangular strips 70–90 mm long and (4–5) × (0.1–0.5) mm in cross section. The potential electrodes were never more than 40 mm apart. Since ρ_d is much smaller than the total resistivity of the specimen even at temperatures of the order of 30–40 K and higher, unstrained standard specimens, cut from the same material as the specimens being investigated, were put in the thermostat along with the investigated specimens. Then the formula

$$\rho_d(T)=\left[\frac{R(T)}{R^*(273\mathrm{K})}-\frac{R_{st}(T)}{R_{st}(273\mathrm{K})}\right]\rho(273\mathrm{K}), \tag{1}$$

where R and R_{st} are the resistances of the measured and standard specimens, respectively, and ρ is the resistivity of the metal, was used to determine ρ_d. After the measurements the deformed (i.e., strained beyond the elastic limit) specimen was so annealed that recrystallization took place and the dislocation density consequently fell by several orders of magnitude. The resistance at 0°C of this annealed specimen is the quantity R*(273 K) in Eq. (1).

Dislocations were introduced into the specimen by straining it in various ways: by rolling, stretching, and bending. After straining the specimens were subjected to mild heat treatment to remove the vacancies produced by the deformation (the copper specimens were held for an hour at 100°C, the molybdenum specimens were held for an hour at 400–450°C, and the zinc specimens were held for a day at room temperature). The dislocation distribution and its dependence on the mode and degree of deformation were examined in preliminary electron-microscope studies[2, 3].

Copper. About 20 single-crystal and polycrystalline specimens were measured. The specimens differed in manner and degree of deformation (bending of a 0.4 mm thick strip on a 2.5 mm radius, rolling and stretching to a strain of 5 to 40%), orientation (rolling on the (110) plane in the [1$\bar{1}$2] direction, stretching along the [100] and [1$\bar{1}$2] axes), and purity (resistivity ratio γ = R(273 K)/R(4.2 K) ranging from 220 to 3500). For all the specimens the ρ_d(T) curve had a single step (see Fig. 1) with most of the rise taking place within the same 30–90 K temperature interval.

For some of the specimens a small but noticeable decrease in ρ_d with increasing temperature can be seen at temperatures above ~150 K. As Eq. (1) shows, however, ρ_d is the small difference between two quantities that increase rapidly with increasing temperature, so that the systematic error may well increase with increasing temperature. An estimate based on comparison of the resistances of various standard specimens indicates, however, that this error does not exceed 5% of $\rho_{d\,\max}$.

It is convenient to use the dimensionless quantity

$$r(T)=[\rho_d(T)-\rho_d(0)]/\rho_d(0). \tag{2}$$

in place of ρ_d(T). The basic datum on the r(T) curve—the height $r_{\max}$ of the step—is plotted on Fig. 2 for a number of specimens. The following comments may be made:

1. The step on the r(T) curve is higher the straighter the dislocations in the specimen. In a series of specimens that have been deformed in the same manner, therefore, $r_{\max}$ increases with decreasing degree of deformation; further, this increase in $r_{\max}$ depends on the type of deformation. Deforming single crystals by rolling or stretching along [1$\bar{1}$2] results in a structure having long interlacing regions in which the dislocations lie preferentially along [110] and [1$\bar{1}$2]. This feature becomes less marked with increasing degree of deformation.

2. The dislocation structure as such has little effect on the height of the step: it is not important whether the dislocations are collected into interlacing regions with high density (rolling single crystals to large deformations) or are concentrated in cell walls (rolling and stretching polycrystalline specimens, stretching single crystals along [100]).

3. The size of the cells is not important either. For example, in a series of polycrystalline specimens deformed by rolling, the size of the cells varied with increasing deformation from 5–3 to ~1 μm.

4. A tenfold change in the impurity content had no effect on the height of the step. Irradiating deformed

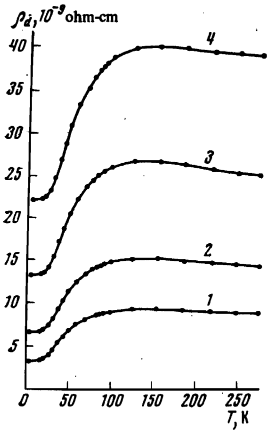

FIG. 1

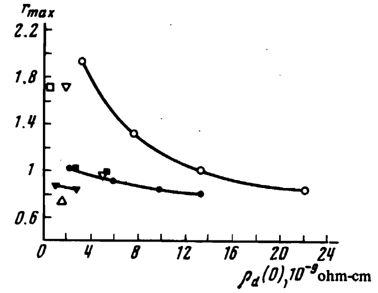

FIG. 2

FIG. 1. $\rho_d(T)$ curves for copper single crystals ($\gamma = 2700$) deformed by rolling on the (110) plane in the $[1\bar{1}2]$ direction to the following deformations δ: 1–15%, 2–21%, 3–44%, 4–70%.

FIG. 2. r_{max} vs $\rho_d(0)$ for polycrystalline (black symbols) and single-crystal (open symbols) copper specimens: ●—rolled, $\gamma = 220$; ▼—stretched, $\gamma = 220$; ■—stretched, $\gamma = 1900$; ○—rolled on (110) along $[1\bar{1}2]$, $\gamma = 2700$; ▽—stretched along $[1\bar{1}2]$, $\gamma = 3700$; △—stretched along [100], $\gamma = 3000$; □—bent on a 2.5 mm radius (bending axis [111]), $\gamma = 3200$.

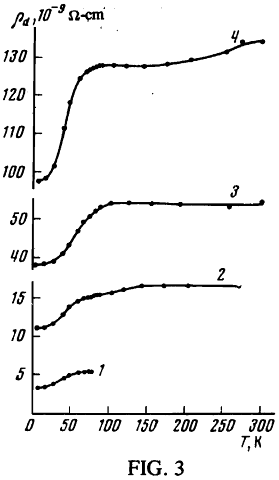

FIG. 3

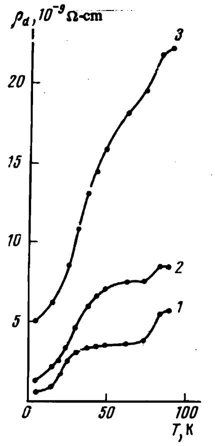

FIG. 4

FIG. 3. $\rho_d(T)$ curves for polycrystalline (curve 1) and single-crystal (curves 2–4) molybdenum specimens: 1–stretched, $\delta = 6\%$, $\gamma = 650$; 2–rolled on (100) along [011], $\delta = 80\%$, $\gamma = 800$; 3–rolled in a random direction, $\delta = 99\%$, $\gamma = 22$; 4–rolled on (110) along [110], $\delta = 90\%$, $\gamma = 1000$.

FIG. 4. $\rho_d(T)$ curves for zinc, $\gamma = 4500$: 1–stretched, $\delta = 4.3\%$; 2–stretched, $\delta = 10\%$; 3–rolled, $\delta = 90\%$.

specimens with 300 mR of cobalt gamma radiation, which leads to pinning of the dislocations, did not change r_{max} either.

Molybdenum. The basic features of the $\rho_d(T)$ curves noted above for copper are also found for the molybdenum specimens (Fig. 3). The various deformation modes were chosen as to obtain the most diverse dislocation distributions in the crystals. Rolling single crystals along [110] in the (110) plane (specimen 4) results in a sharp cellular structure, while rolling in the (100) plane results in a uniform distribution of dislocations throughout the body of the crystal (specimen 2). The height of the step r (80°) is the same for these two specimens, but the trends of the two r(T) curves differ at higher temperatures, r increasing further in different temperature intervals.

Zinc. Our measurements on zinc are much less detailed and may be regarded in a certain sense as preliminary. At the same time they are very important since zinc does not have cubic symmetry. This circumstance leads to additional difficulties, however, for the resistivity of a zinc single crystal is anisotropic and the degree of anisotropy is temperature dependent. We therefore made measurements only on polycrystalline specimens, and the results can be regarded as reliable only at temperatures below ~100 K. As is evident from Fig. 4, the curve has a step at $T < 50$ K and apparently a second step in the interval 80–100 K.

DISCUSSION

Thus, in all the cases that we investigated the r(T) curve has a step, and for zinc, it probably has two. We feel that there must be some specific reason for a dependence of this sort. The r(T) curve is usually discussed in terms of deviations from Matthiessen's rule, i.e., it is attributed to nonadditivity of the scattering from scatterers of different types. Such nonadditivity could arise, for example, from differences in the angular dependences of the differential scattering cross sections or from differences in the dependences of the total scattering cross sections on the position of the electron on the Fermi surface. It seems unlikely, however, that the steplike form of the r(T) curve could be explained in this manner. In addition, the interference between scattering from phonons and scattering from dislocations should be affected by the introduction of scattering centers of a third type–impurities. As was noted above, however, experiment shows that there is no such effect, even when passing from specimens for which the residual resistivity $\rho(0)$ is much smaller than ρ_d to specimens for which $\rho(0) \gg \rho_d$.

An attempt was made some time ago[4] to explain the shape of the curves in terms of a nonuniform distribution of dislocations throughout the body of the crystal, it being assumed that such a distribution would lead to a periodic variation of the local resistivity $\rho(r)$. For specimens with a cellular structure, however, the electron mean free path l at low temperatures is greater than the linear dimensions of a cell and is much greater than the wall thickness, and this invalidates the theoretical model advanced in[4]. In copper, l remains greater than the wall thickness even at liquid nitrogen temperatures. Moreover, as we saw above, the r(T) curve has a step even for specimens with a uniform dislocation distribution (copper deformed by bending[5], molybdenum rolled in the (100) plane).

We would like to call attention to the possibility of explanations of a different type, based on the idea that the dependence of r on T may be determined by the temperature dependence of the scattering of electrons by the dislocations themselves.

Various mechanisms may be proposed for the temperature variation of the scattering. First, if the dislocations have quasilocal vibrational modes of characteristic frequency ω, a new inelastic scattering channel–scattering with absorption or emission of a quasilocal phonon–may open up at elevated temperatures. From the position of the step on the r(T) curve it follows that ω must be of the order of 70°, i.e., just a few times lower than the Debye frequency. Such vibrational frequencies have not been observed for dislocations, but, generally speaking, we can suggest reasonable physical models for such modes. For example, there may be a branch $\omega(k)$

of the optical type corresponding to vibrations of dislocations near one minimum of the Peierls surface with a characteristic frequency of the order of a few degrees[1]. In addition, one can imagine vibrational modes in the cores of dislocations near points at which the dislocations are pinned whose frequencies are determined by parameters associated, not with the defect, but with the dislocation itself. This possibility, however, was apparently not realized in our experiments: otherwise, altering the impurity concentration and γ-ray irradiation of the specimens would have affected r_{max} since they affect the concentration of pinning points.

Regardless of the specific model, the change in the nonequilibrium addition Δf to the electron distribution function f due to collisions with phonons is proportional to the quantity (see, e.g.,[6])

$$2\varphi_\omega+1+f_{E+\hbar\omega}-f_{E-\hbar\omega}, \qquad (3)$$

in which φ_ω is the phonon distribution function. Assuming that the distribution functions in (3) differ little from the equilibrium ones;

$$\varphi=(e^\xi-1)^{-1}, \quad f=(e^\alpha+1)^{-1},$$
$$\xi=\hbar\omega/kT, \quad \alpha=(E-E_f)/kT$$

(E_f is the Fermi energy and k is Boltzmann's constant), we can average (3) over the energies of the electrons occurring in Δf. Then we find that the collision frequency (and therefore also the additional electrical resistance, provided the scattering is isotropic) is proportional to the quantity

$$r(T)\sim\xi e^\xi(e^\xi-1)^{-2}. \qquad (4)$$

The low-temperature parts of the experimental curves are in satisfactory agreement with (4), but a linear dependence of expression (4) on temperature resulting from the linear increase in the number of excited phonons sets in as early as $\xi \approx 1$. It should be borne in mind, however, that in the first approximation the number of degrees of freedom of the crystal does not change when dislocations are introduced, so that as T increases, the growth in the inelastic scattering from dislocations should be compensated by a decrease in the growth of the resistance of the ideal part of the crystal. In order to test the proposed model for inelastic scattering from dislocations, therefore, one must calculate both the vibrational modes themselves and the phonon part of the electrical resistance of the entire deformed crystal.

We feel that a different assumption is to be preferred: namely, that the temperature dependence of the electron elastic scattering cross section is due to the presence at the dislocations of additional electron levels at some height ϵ above the Fermi level; these levels are unoccupied at low temperatures but begin to become occupied as the temperature rises. In metals, charge is screened at interatomic distances, i.e., precisely at distances of the order of the dimensions of dislocation cores. Thus, the change in the elastic scattering cross section can be appreciable when the charge on the core changes:

$$r(T)=a[1+\beta e^{\epsilon/kT}]^{-1}, \qquad (5)$$

where β is the spin degeneracy of the level and a is a proportionality constant. Of course Eq. (5) is also applicable when the level lies below the Fermi level and the dislocations become positively charged when the temperature is raised.

Although Eq. (5) contains three parameters (a, β, and ϵ), the possibilities for fitting it to the experimental curve are quite limited. In fact, if the r(T) curve can be represented by Eq. (5), the plot of $\ln(a/r-1)$ against 1/T must be a straight line. This condition allows us to determine a region of possible values of a ($a \geq r_{max}$), and the position of the line for each value of a gives the corresponding values of ϵ and β. The procedure is illustrated in Fig. 5, using one of the copper specimens (for curve 1 of Fig. 1) as an example. It will be seen that ϵ depends little on a over the range of a values in which it is reasonable to use Eq. (5) at all: $\epsilon \approx 93°$. On the other hand, β depends strongly on a, and there are no serious grounds for preferring one value of β in the interval $0.3 < \beta < 1.5$ to another.

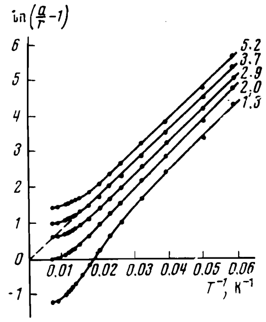

FIG. 5. Process of fitting Eq. (5) to the experimental points of curve 1, Fig. 1 (copper single crystal). The corresponding values of a/r_{max} are given at the curves.

The existence of electron levels localized near dislocations has been repeatedly discussed[7]. In our model, however, it remains unclear why these levels lie at about the same place with respect to the Fermi level in different metals. We merely note that in principle the collective properties of the Fermi gas may play a decisive part in bringing about such a correlation.

CONCLUSION

It must be said that at present there is no satisfactory theory of the contribution to electrical resistance from scattering of electrons by dislocations. We still do not understand why dislocations introduced by bending have very large scattering cross sections[8]. In fact, there is no explanation for the $\rho_d(T)$ curve either. The models proposed here can probably serve only as a point of departure for the theory. As regards experiment, it hardly seems possible that further information can be extracted from electrical resistance measurements; hence new, more direct experiments must be sought.

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[1] V. Ya. Kravchenko called our attention to this possibility. He made preliminary estimates, which however, gave ω values several times smaller than the experimental values.

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