Thermal Properties of Mobile Defects

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Using simplified models, calculations are made for the contribution of mobile dislocations and small-angle boundaries to the specific heat and thermal resistivity of crystals. The specific heat is found to be proportional to T and T^2, and the lattice resistivity approximately to T^{-n} (where n lies between 3 and $\frac{7}{2}$ for the usual range of measurements) and T^{-5} for mobile dislocations and mobile small-angle boundaries, respectively, over a range of low temperatures, but eventually both go to zero in the limit as the temperature approaches zero. The magnitudes of the effects are such that although the contribution of dislocations to the specific heat of some pure cold-worked nonconductors and superconductors may be measurable, that from small-angle boundaries is not. The effect of dislocations on the thermal resistivity is large and should compete with boundary scattering for temperatures of the order of 10^{-2} of the Debye temperature, with dislocation densities of the order of 10^7 cm^{-2} in specimens of a few millimeters in diameter. The predicted temperature dependence is in agreement with recent measurements on superconducting lead at low temperatures. At present a contribution from mobile boundaries to the thermal resistivity is not excluded as a possibility.

I. INTRODUCTION

THE influence of defects on thermal properties of crystalline materials has been receiving increasing attention. The specific heat can be affected by imperfections through their effect on the distribution of frequencies and modes of vibration of the lattice. The effect of point defects has been examined by Montroll and Potts.[1] Extended defects which are mobile even under the influence of small thermal stresses give rise to low vibration frequencies and may therefore be effective at low temperatures. One- and two-dimensional defects of this type will be considered here. The sensitivity of thermal conductivity to imperfections is well known. At low temperatures, the lattice conductivity of nonconductors and superconductors is primarily limited by the scattering of phonons at defects. A detailed discussion of the influence of many different types of static defects has been published by Klemens.[2] Available measurements show that there are components of resistivity which cannot as yet be accounted for on the basis of the so far known mechanisms. It is therefore appropriate to consider additional mechanisms. Klemens has computed the thermal resistivity arising from static dislocations and small-angle boundaries. We shall attempt here to determine the temperature dependence and order of magnitude of the thermal resistivity offered by mobile dislocations and small-angle boundaries.

Dislocations which do not lie along crystallographic directions where they are restricted by the Peierls' stress and which are not completely pinned down by point defects are free to move under the influence of thermal shear stresses. Their mode of motion still depends, however, on restrictions such as network points or the stress fields of other nearby dislocations. Anticipating that the largest effects occur when the dislocation densities are large, one would like to know the exact arrangement and distribution of obstacles for motion of the dislocation in the cold-worked state. There is little detailed information of this sort available, but one may expect that models in which dislocations are in networks, pileups, and small-angle boundaries would be appropriate. Dislocations which form elements of networks for which the average distance between dislocation segments is not small compared to the lengths of the segments may be treated as isolated dislocations pinned at the network points. (See Appendix I.) Dislocations in pileups have complicated modes of vibration when the interaction between the various dislocations are taken into account and will not be considered here. It is likely that such pileups do not have great mobility. Most small-angle boundaries are sessile. Simple tilt boundaries, however, which are mobile will be considered. In what follows, therefore, the models used will be isolated, pinned dislocations for one-dimensional defects and glissile tilt boundaries for two-dimensional defects. Sessile dislocations and small-angle boundaries will not concern us.

II. SPECIFIC HEAT

A. Pinned Dislocations

Consider a dislocation line segment of length L in an isotropic material as in Fig. 1, which is free to oscillate as a vibrating string in its slip plane. The equation of motion of this dislocation is given by

$$\frac{E}{C^2}\frac{d^2\xi}{dt^2}-E\frac{d^2\xi}{dx^2}=0, \tag{1}$$

where the boundary conditions are $\xi(0,t)=\xi(L,t)=0$, and where ξ is the displacement of the dislocation. E is

[1] E. W. Montroll and R. B. Potts, Phys. Rev. **100**, 525 (1955). See also Magnuson, Palmer, and Koehler, Phys. Rev. **109**, 1990 (1958), who find that a radiation of 2.5×10^{16} deuterons per square centimeter produces a decrease of 16°K in the Debye θ of copper.
[2] P. G. Klemens, Proc. Phys. Soc. (London) **A68**, 1113 (1955).

the dislocation line energy, $C^2=G/\rho$,[3] E/C^2 is the effective mass per unit length of the dislocation, ρ is the density, and G is the shear modulus. The resonant frequency of the dislocation is given by

$$\omega_0=\pi C/L. \tag{2}$$

The number of modes of oscillation of the dislocation is given by L/a, where a is the lattice spacing along the dislocation line. Although the vibrations of this oscillating system are transverse, the problem is mathematically equivalent to that of the determination of the internal energy of a one-dimensional crystal. The internal energy U of such a system is well known[4] to be

$$U=\sum_\kappa \frac{\hbar\omega_\kappa}{\exp(\hbar\omega_\kappa/\kappa T)-1}, \tag{3}$$

where the sum is over all the normal modes of the vibrating dislocation; κ is Boltzmann's constant.

If we approximate the sum by an integral in the usual way, Eq. (3) becomes

$$U=\int_{k_0}^{k_m}\frac{\hbar\omega}{\exp(\hbar\omega/\kappa T)-1}\omega(k)\frac{dk}{d\omega}d\omega, \tag{4}$$

where $\omega(k)dk$ is the number of modes between k and $k+dk$. For a one-dimensional line, the density of modes is given by

$$\omega(k)=L/\pi. \tag{5}$$

We are interested in the temperature dependence of (4) for low temperatures. For these long wavelengths we may take $dk/d\omega=1/C$, and (4) becomes

$$U=\frac{L}{\pi C}\int_0^\infty\frac{\hbar\omega d\omega}{\exp(\hbar\omega/\kappa T)-1}. \tag{6}$$

Now, upon letting $x=\hbar\omega/\kappa T$, Eq. (6) may be expressed as

$$U=\frac{L}{\pi C}\frac{(\kappa T)^2}{\hbar}\int_0^\infty\frac{xdx}{e^x-1}, \tag{7}$$

or, since the integral has the value $\pi^2/6$,

$$U=\frac{\pi}{6}\frac{L}{C}\frac{\kappa^2T^2}{\hbar}. \tag{8}$$

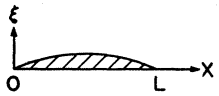

FIG. 1. Dislocation line of length L bowed out by an applied stress, but fixed at its end points.

[3] This equation holds for a screw dislocation. For an edge dislocation, C^2 will have a slightly different value. [See A. Seeger, *Handbuch der Physik* (Springer-Verlag, Berlin, 1955), Vol. VII, p. 1.]

[4] See, for example, C. Kittel, *Introduction to Solid State Physics* (John Wiley and Sons, Inc., New York, 1953), p. 72, or M. Blackman, Proc. Roy. Soc. (London) **A148**, 365 (1935).

The contribution of the loop L to the specific heat is therefore

$$c_v=\frac{\pi}{3}\frac{L}{C}\frac{\kappa^2T}{\hbar}. \tag{9}$$

This can be put in terms of the Debye Θ once the relation between C and v_0, the velocity of sound in the perfect lattice, is determined. Θ is defined by

$$\kappa\Theta=h\nu_m, \tag{10}$$

and therefore

$$\Theta=v_0\pi\hbar/\kappa a=p C\pi\hbar/\kappa a, \tag{11}$$

where $p=v_0/C$, and ν_m is the limiting frequency in the perfect lattice. Upon using (11), Eq. (9) becomes

$$c_v=\frac{p\pi^2}{3}\frac{L}{a}\frac{T}{\Theta}\kappa. \tag{12}$$

Finally, to obtain the specific heat per mole (C_v), we multiply (12) by the number of loop segments L per unit volume (Λ/L), by the volume per atom (a^3/Z), and by the number of atoms per mole (N), where Λ is the dislocation density and Z is the number of atoms per unit cell. Then (12) becomes

$$C_v=\frac{p\pi^2}{3}\frac{\Lambda a^2}{Z}\frac{T}{\Theta}N\kappa. \tag{13}$$

The magnitude of this contribution to the specific heat will be discussed in a later section. For the present, we simply note that Eq. (13) predicts a specific heat which is proportional to the dislocation density and the temperature at low temperatures. Equation (13), however, is not valid in the limit as $T\rightarrow 0$, since for very low temperatures ($\kappa T\ll\hbar\omega_0$) even the lowest mode (ω_0) is not fully excited. For this case, only the first term of the sum (3) need be used and one obtains

$$C_v=\frac{\Lambda}{L}\frac{a^3}{Z}N\kappa\left(\frac{\hbar\omega_0}{\kappa T}\right)^2\exp(-\hbar\omega_0/\kappa T), \tag{14}$$

so that the specific heat goes to zero exponentially at very low temperatures.

For temperatures such that $\hbar\omega_0=\kappa T$, the approximation of replacing the summation by an integration should not be accurate. To determine the error introduced, we evaluate this case separately. The value obtained by direct summation of Eq. (3) is

$$C^{(\Sigma)}=2.88N\kappa\Lambda a^3/LZ,$$

so that the ratio of the specific heat as computed by summation of Eq. (3) to that determined approximately by integration, $C^{(S)}$ is

$$C^{(\Sigma)}/C^{(S)}=0.88. \tag{15}$$

We therefore see that no great error is introduced by using Eq. (13) for temperatures $\kappa T\gtrsim\hbar\omega_0$.

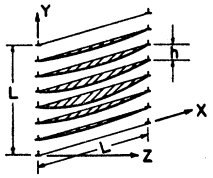

FIG. 2. Small-angle boundary consisting of parallel edge dislocations spaced a distance h apart. Under a stress, the individual dislocations bow out, but are restricted at the edges of the boundary.

The temperature defined by $\kappa T=\hbar\omega_0$ depends on the length of the dislocation segment, according to Eq. (2). Taking an average value of C to be $\sim 10^5$ cm/sec for most metals, one finds

$$\kappa T=\hbar\pi C/L\sim\hbar\pi 10^5/L,$$

or

$$LT\sim 2.4\times 10^{-6}.$$

Thus for loop lengths L of 2.4×10^{-6}, 2.4×10^{-5}, and 2.4×10^{-4} cm, Eq. (13) should be valid for temperatures greater than 1.0°K, 0.1°K, and 0.01°K, respectively (but only for temperatures which are also much smaller than the Debye Θ).

B. Simple Tilt Subgrain Boundaries

As a model here, we consider a simple tilt boundary composed of edge dislocations arrayed as in Fig. 2, separated by a distance h and supposed to be clamped down at the ends. The tilt angle of the boundary is given by

$$\Theta=b/h.$$

Under the action of a shear stress σ, the boundary will bow out, but be constrained at the ends. The dislocations will not be able to bow out independently but will be coupled through their mutual stress fields. In general, the tension in the two coordinate directions will be different although of the same order of magnitude. For the purposes of the following estimate, this difference will be ignored and the tension will be taken to be the grain boundary energy per unit area (A). The equation of motion of the dislocation is then

$$\frac{E}{C^2h}\frac{\partial^2\xi}{\partial t^2}-A\left(\frac{\partial^2\xi}{\partial x^2}+\frac{\partial^2\xi}{\partial y^2}\right)=0. \tag{16}$$

Thus the natural frequency of the system is given by

$$\omega_0=\frac{\pi C}{L}\left(\frac{Ah}{E}\right)^{\frac{1}{2}}, \tag{17}$$

which is of the same order of magnitude as that for the dislocation segment.

Proceeding now in the same way as before, but using a two-dimensional distribution of modes $\omega(k)=k/2\pi$, and the resonant frequency (17), one obtains

$$U=\frac{(kT)^3}{2\hbar^2\pi v_0^2}\int_0^{x_m}\frac{x^2dx}{e^x-1},$$

or $U=\pi\kappa T^3I_2/2a^2\Theta^2$ per unit area of boundary per unit volume, where

$$I_2=\int_0^\infty\frac{x^2dx}{e^x-1},$$

or

$$C_v=I_2\left(\frac{3\pi}{2}\right)N\kappa\left(\frac{T}{\Theta}\right)^2\frac{aS}{Z}, \tag{18}$$

where S is the total area of simple tilt boundary found in unit volume of the specimen. The two-dimensional aspect of the vibration is reflected in the T^2 temperature dependence.

III. THERMAL CONDUCTIVITY

We start with the expression for the thermal conductivity in the form

$$K=\tfrac{1}{3}\textstyle\sum_k v_kc_kl_k. \tag{19}$$

Since we shall be interested in the results for low temperatures, we can take v_k to be a constant, v_0. The contribution to the specific heat from the mode with wave vector k is found by differentiation of the kth term of Eq. (3) with respect to T to be

$$c(\omega)=\frac{\kappa x^2e^x}{(e^x-1)^2}, \tag{20}$$

where $x=\hbar\omega/\kappa T$. The distribution of modes to be used is that for the lattice phonons, or

$$\omega(k)=3k^2/2\pi^2=3\omega^2/2\pi^2v_0^2. \tag{21}$$

We then need only find the mean free path l_k for the two cases of incident thermal phonons on isolated dislocations and on small-angle boundaries.

A. Dislocation Line Segment

The scattering cross section σ for a thermal wave incident normally on a screw dislocation has already been computed by Nabarro[5] for a different purpose. Nabarro gives

$$\sigma=2\pi^2C/\{\omega[\ln(4/kb)-1.077]^2\}, \tag{22}$$

as the scattering width per unit length of dislocation. Multiplying (22) by the dislocation density Λ, we obtain the attenuation α of the incident sound wave. The mean free path l is the reciprocal of α and is therefore given by

$$l(\omega)=\omega[\ln(4/kb)-1.077]^2/2\pi^2C\Lambda. \tag{23}$$

Now using (23), (21), and (20) in (19) and replacing the summation by integration, we find

$$K=\frac{v_0}{3}\int_0^{\omega_m}\frac{\kappa x^2e^x}{(e^x-1)^2}\frac{[\ln(4/kb)-1.077]^2\kappa Tx}{2\pi^2C\Lambda\hbar}\times\frac{3(\kappa T)^2x^2}{2\pi^2v_0^2\hbar^2}\frac{\kappa T}{v_0\hbar}dx. \tag{24}$$

[5] F. R. N. Nabarro, Proc. Roy. Soc. (London) **A209**, 279 (1951).

For the purpose of the integration, we regard the logarithmic factor as an average value and find

$$K=\frac{k[\ln(4/kb)-1.077]^2}{4\pi^4}\frac{v_0^2}{C\Lambda}\left(\frac{\kappa T}{\hbar v_0}\right)^4 J_5(x),$$

where

$$J_n(x)=\int_0^x \frac{z^n dz}{(e^z-1)(1-e^{-z})}.$$

To express the results in terms of the Debye Θ, we use the relation[4]

$$\Theta=\hbar v_0(6\pi^2 N)^{\frac{1}{3}}/\kappa, \tag{25}$$

in terms of which K may be written as

$$K=\frac{3}{2\pi^2}N\kappa[\ln(4/kb)-1.077]^2 J_5\frac{v_0\kappa}{C\hbar}\frac{T^4}{\Lambda\Theta^3}, \tag{26}$$

where

$$\lim_{T/\theta\to 0} J_n = n!\sum_{r=1}^{\infty}\frac{1}{r^n}.$$

Tables of the values of $J_n(x)$ have been tabulated by Sondheimer.[6] J_5, as $T\to 0$, is given by 124.3. We note that the conductivity is a very strong function of the temperature and inversely proportional to the dislocation density. The magnitude given by Eq. (26) will be discussed in a later section.

B. Simple Tilt Boundary

To find the mean free path, we first determine the energy irradiated by the boundary when it oscillates with amplitude d. Consider the tilt boundary of Fig. 3. The stress field surrounding a simple edge boundary is very complicated in the immediate vicinity of the boundary, but goes to zero quickly at points distant from the boundary larger than the spacing h of the dislocations in the boundary because the stress fields of the individual dislocations tend to cancel at large distances.[7] The strain field is therefore very simple for distances $z>h$. If the boundary moves a distance ξ, then the displacement at points $z>h$ will be given by

$$v/2=\xi\tan(\theta/2). \tag{27}$$

The displacements u and w (in the x and z directions) are zero, and for small-angle boundaries we have

$$v=\theta\xi. \tag{28}$$

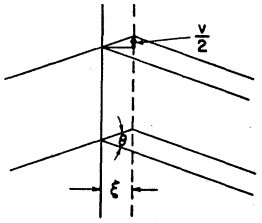

FIG. 3. Schematic figure showing the displacement v when a small-angle boundary (solid line) of angle θ is displaced a distance ξ.

We can now find plane-wave solutions for the irradiated wave with the required properties for small and large z. For example, the solution

$$v=\theta d\exp[i(kz-\omega t)], \tag{29}$$

satisfies the wave equation and reduces to the proper stress field $v=\theta d e^{-i\omega t}$ for $h\ll z\ll\lambda/2\pi$. The rate at which energy is irradiated by this oscillating surface per unit area is given by $\sigma_{zy}(\partial v/\partial t)$. Since $\sigma_{zy}=G\epsilon_{zy}=G(\partial v/\partial z)$, we have

$$W=Gd^2\theta^2\omega\pi/C, \tag{30}$$

as the energy irradiated away per unit area of boundary per cycle. We determine d in terms of the applied thermal stress σ_0 from the differential equation for the motion of the boundary:

$$\frac{E}{C^2 h}\frac{\partial^2\xi}{\partial t^2}=\frac{b\sigma_0}{h}\exp[i\omega t], \tag{31}$$

where it has been assumed that the motion is mass-limited. From (31), we find that

$$d=\sigma_0 bC^2/E\omega^2. \tag{32}$$

The attenuation α is conveniently found in terms of the decrement Δ by means of the relation

$$\Delta=\alpha\lambda. \tag{33}$$

The decrement is a measure of the damping of a sound wave commonly used in internal friction studies and is given by the ratio of the energy lost per cycle by irradiation to twice the maximum stored energy in the lattice by the sound wave. Taking $E=Gb^2\ln(h/b)/[4\pi(1-\nu)]$ as the line energy of the dislocation and an average value of $\nu=\frac{1}{3}$ for Poisson's ratio, we find

$$\Delta=128\pi C^3 S/[\ln(h/b)]^2 h^2 b^2\omega^3, \tag{34}$$

where S is the boundary area per unit volume of specimen. The mean free path is then

$$l(\omega)=h^2\omega^2[\ln(h/b)]^2/64C^2 S. \tag{35}$$

Now, using (35), (21), and (20) in (19), we obtain in the same manner as for the previous calculation

$$K=\frac{3}{64}Nk[\ln(h/b)]^2\frac{h^2 J_6}{S}\frac{v_0}{C^2}\frac{\kappa^2}{\hbar^2}\frac{T^5}{\Theta^3}, \tag{36}$$

where $J_6=731.2$.

IV. DISCUSSION

We consider first the contribution to the specific heat given by dislocations in detail for a specific case. There seems to be reliable evidence that dislocation densities of the order of 10^{10} cm^{-2} are achieved in the case of

[6] E. H. Sondheimer, Proc. Roy. Soc. (London) **A203**, 75 (1950).
[7] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Oxford University Press, Oxford, 1953), p. 93.

cold-worked aluminum.[8] We therefore take $\Lambda=10^{10}$ cm^{-2}, $L=1.7\times10^{-5}$ cm (roughly estimated from the relation, $\Lambda L^2=3$, for a cubic array), $\Theta=398$°K, $G=2.5\times10^{11}$ dynes/cm^2, $\rho=2.69$ g/cm^3, $b=2.86\times10^{-8}$ cm, $a=4.04\times10^{-8}$ cm, and $Z=4$, from which we find that $p=2.21$, using $v_0=ak\Theta/\pi\hbar$. Then from Eq. (13) we find that the dislocation contribution to the specific heat is

$$C_D=29.7\times10^{-6}N_K(T/\Theta),$$

whereas the lattice contribution is

$$C_L=233.8N_K(T/\Theta)^3.$$

The two should have the same size, therefore, at $T=0.142$°K.

The product LT is close to the critical value of $LT=2.4\times10^{-6}$ so that Eq. (13) will give a value slightly too high. For aluminum in its normal state, both of these contributions will be overshadowed by the electronic specific heat. However, in the superconducting state, the electronic specific heat becomes small at these temperatures. Using the data of Goodman[9] for aluminum, the electronic specific heat, C_{el}, is given by

$$C_{el}=b\gamma T_c\exp[-bT_c/T],$$

where $\gamma=3.34\times10^{-4}$ cal/mole deg^2, $b=6.9$, $b=1.28$, and $T_c=1.18$°K; so one finds that

$$C_{el}(0.142\text{°K})=7.45\times10^{-8}\text{ cal/mole deg},$$
$$C_L=2.17\times10^{-8}\text{ cal/mole deg},$$
$$C_D=C_L.$$

Therefore nearly 20% of the measured specific heat at this temperature could be due to the dislocations. For slightly lower temperatures (or higher dislocation densities) the dislocation contribution could be a larger fraction of the total, but at very low temperature C_D also goes to zero exponentially according to Eq. (14).

It is therefore concluded that dislocations can have a measurable effect on the specific heat of some pure deformed superconductors. In general, however, the effect appears to be a small one and is probably not detectable in most materials with present techniques.

For a dielectric material the electronic component would be absent, but it may be more difficult to achieve the same dislocation densities that are obtained in metals. The effect would appear at lower temperatures for lower dislocation densities. The writer is not aware of any measurements which could be examined for this effect.

For the magnitude of the contribution of the mobile small-angle boundaries to the specific heat, we note that Eq. (18) yields, for a rough order of magnitude,

$$C_B\sim10^{-7}SN_K(T/\Theta)^2,$$

while

$$C_L\sim2\times10^2N_K(T/\Theta)^3.$$

Therefore, the two contributions would have the same order of magnitude when

$$T/\Theta\sim5\times10^{-10}S.$$

Taking a typical Debye Θ value of $\Theta=300$°K, we have $T=0.15\times10^{-6}S$. Thus, in order for the specific heat contribution from the boundaries to be appreciable even at 0.1°K, we would require a surface area of boundary of $\sim10^6$ cm^2 per cubic centimeter of specimen. This is exceedingly large and could be achieved only if mosaic blocks with average dimension of 10^{-6} cm permeated the crystal and if the boundaries of these blocks consisted entirely of simple mobile small-angle boundaries. Even if this were so, the dimension of 10^{-6} cm implies that the natural frequency of the system would be much higher than the average phonon frequency at this temperature, so that Eq. (18) would not apply and the exponential form of this equation would have to be used. We conclude, therefore, that although dislocation line segments can contribute to the specific heat at low temperatures, mobile low-angle boundaries cannot.

In discussing the thermal conductivity due to dislocations, it is of interest to consider the order of magnitude of the mean free path given by Eq. (23). Using $\hbar\omega=3_K T$ and $v_0=a_K\Theta/\pi\hbar$, we find that the factor, $\ln(4/kb)-1.077$, may be written approximately as $\ln(\Theta/5T)$. Then Eq. (23) may be expressed as

$$l=3p[\ln(\Theta/5T)]^2T/(\Theta2\pi a\Lambda),$$

where $p=v_0/C$. Using typical values of $p=2.5$ and $a=4.0\times10^{-8}$ cm for metals, we find that for $T=10^{-2}\Theta$,

$$l\sim2.7\times10^6/\Lambda,$$

so that for a dislocation density of 2.7×10^7 cm^{-2} the mean free path should be about one millimeter in a typical metal. At low temperatures the thermal conductivity of nonconductors and superconductors is usually limited by boundary scattering. This process has been considered by Casimir,[10] who showed that the conductivity should be proportional to dT^3, where d is the diameter of the specimen. From our expression it is clear that even moderate dislocation densities ($\sim10^7$ cm^{-2}) should compete with boundary scattering at low temperatures for specimens of the usual diameters (say, several millimeters).

We now express Eq. (26) for the conductivity in a somewhat more useful form. Multiplying (26) by $(Z/Na^3)\times10^{-7}$ to obtain units of watt/sec-cm-deg, and introducing Θ through $v_0=ak\Theta/\pi\hbar$, we obtain

$$K=5.7\Theta^2F(T/\Theta)/a^2C\Lambda,$$

[8] P. B. Hirsch, *Progress in Metal Physics* (Pergamon Press, Ltd., New York, 1956), p. 236.

[9] B. B. Goodman, *Conférence de Physique de Basses Temperatures Paris, 1955* (Centre National de la Recherche Scientifique and UNESCO, Paris, 1956), Supplement to the Bulletin de l'Institut International du Froid, 1955, p. 506.

[10] H. B. G. Casimir, Physica **5**, 495 (1938).

where

$$F(T/\Theta)=(T/\Theta)^4[\log(\Theta/5T)]^2.$$

The effect of the slowly varying logarithmic term is to decrease the temperature dependence somewhat. Inspection of a log-log plot of F shows that it can be represented to within 10% by

$$F\approx F_1=9.0\times10^{-8}[T/(\Theta\times10^{-2})]^{3.3},$$

for the range $0.005<T/\Theta<0.02$, or by

$$F\approx F_2=9.4\times10^{-8}[T/(\Theta\times10^{-2})]^{7/2}$$

for the range $0.002<T/\Theta<0.008$. Upon using F_2, our expression for the conductivity becomes (in watt units)

$$K=5.4[T/\Theta]^{7/2}\Theta^2/a^2C\Lambda.$$

Using the values, $\Theta=398$°K and 88°K, $a=4.04\times10^{-8}$ and 4.94×10^{-8} cm, $C=3.05\times10^5$ and 0.715×10^5cm/sec, for aluminum and lead, respectively, one obtains $K=1.7\times10^8/\Lambda$ and $0.24\times10^8/\Lambda$, respectively, when $T=10^{-2}\Theta$. Thus the order of magnitude of the dislocation resistivity is unity (in watt units) for dislocation densities of $\sim10^8$ cm^{-2} at one percent of the Debye Θ. This result is in contrast to that found by Klemens[2] for the thermal conductivity resulting when phonons are scattered by static dislocations. In that case a T^2 law is found and dislocation densities of the order of 10^{11} cm^{-2} are required for observable effects.

Although it is often reported that there seems to be more thermal resistivity in some specimens than can be accounted for by boundary scattering, there seems to be little systematic work along this line at the present date. One experiment, however, reported by Mendelssohn and Montgomery[11] provides us with some evidence for dislocation resistivity of the foregoing type. Lead specimens were deformed and the conductivity was measured before and after, in both the normal and superconducting states between 1 and 4°K. The normal conductivity, which is believed to be mostly by electrons, was unaffected, but the conductivity in the superconducting state was reduced from 0.2 to 0.033 watt units as a result of the deformation. Furthermore, the temperature dependence of the conductivity was increased as a result of the deformation. Since the conductivity in the superconducting state is believed to be primarily by phonons, it is reasonable to suppose that the increased resistivity is a result of the increased density of dislocations. According to the expressions written above, a dislocation density of about 7×10^8 cm^{-2} would be required to account for the added resistivity at 1°K. The measured temperature dependence, however, is only $T^{2.7}$. It is likely that the measured resistivity in this range contains components from other sources since the measurements are near a maximum, and measurements over a wider and lower temperature range should be more informative. In measurements on superconducting lead below 1°K by Felix, Passell, and Silsbee,[12] a conductivity of $AT^{3.7\pm0.2}$ was found, where the values of A for three specimens lie between 0.1 and 0.2 for the range from $T=0.15$°K to 0.8°K. This is in good agreement with the temperature dependence predicted here for this temperature range. It should be pointed out that there are no other known mechanisms which predict such a large temperature dependence and the magnitude of the dislocation density required ($\sim2\times10^8$ cm^{-2}) appears to be reasonable.

We shall limit our discussion of the contribution of mobile small-angle boundaries to a discussion of the magnitude of the mean free path, as there seems to be no experimental evidence of such a large temperature dependence at present. From Eq. (35), making the same substitutions as before, and using $\bar{p}=2.5$ and $h=3\times10^{-6}$cm for the dislocation spacing (corresponding to a boundary of 0.6 degree), we find

$$l\sim8.7\times10^4(T/\Theta)^2[\ln(h/b)]^2/S,$$

where S is the small-angle boundary area per unit volume of crystal. Then, at $T/\Theta=10^{-2}$, one has $l=200/S$. Thus to achieve a mean free path of the order of two millimeters, one would need $S\sim10^3$ cm^2/cm^3. If the entire crystal were broken into mosaic blocks of linear dimension L, and if the fraction of boundaries that are mobile is called f, then S would be given by $6f/L$. For $f=\frac{1}{2}\%$ and $L\sim10^{-5}$cm, the above conditions can be met so that we cannot exclude this possibility.

There are a number of assumptions and simplifications in the estimates made here which require comment. For example, it has been assumed that the modes of vibration of the lattice could be split into those associated with dislocations and those connected with running waves in the lattice. Since there are only $3N$ normal modes, those connected with the dislocations must be subtracted from the total number. The total number connected with dislocations is given by $N\Lambda a^2/Z$, which is, under ordinary circumstances, negligible compared with $3N$. Some evidence that this dissociation of the modes may be valid is given by the fact that deformation does not seem to affect the Debye Θ as measured in the usual manner.[13]

The loop lengths L have been assumed to be constant, and an improved model would consider a distribution of loop lengths and also the effect of mild amounts of pinning. The materials have been assumed to be isotropic, whereas it is known that such quantities as the dislocation energies depend on the degree of anisotropy of the crystal. For the case of the contribution of mobile tilt boundaries to the specific heat, it seems to be not worthwhile to improve the model by considering the tension forces in detail since they cannot make a measurable contribution.

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[12] Felix, Passell, and Silsbee, Phys. Rev. **100**, 1808(A) (1955).

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The contribution of dislocation segments to the thermal conductivity, however, seems to be large enough to provide a serious difficulty to workers who would like to avoid it. It is remarkable to find the result of this simplified calculation to be in such good agreement with the data so far available. The result holds strictly only for a phonon incident normally on a screw dislocation. If edge dislocations are more effective than screw dislocations in scattering the phonons, then Λ in Eq. (31) will have to be replaced by a factor $(\Lambda_s+g\Lambda_e)$, where Λ_e is the edge dislocation density and g is the ratio of the effectiveness of the edge to the screw components. The scattering by dislocations is directional, and this as well as the distinction between longitudinal and shear thermal waves should be taken into consideration in a more accurate treatment. Also, for an oblique angle of incidence, the dislocations will be bent and tension forces should be taken into account. The expressions derived here for the mean free paths should only hold at frequencies much higher than the resonant frequencies. For frequencies much smaller than the resonant frequencies, the mean free path should increase again, so that as $T\rightarrow 0$, the dislocation resistivity should eventually go to zero, and the thermal conductivity should finally be limited only by the boundary scattering. It may be possible to measure the resonant frequencies of dislocations by this approach.

V. CONCLUSIONS

Simple models have been used to estimate the contributions of mobile dislocation segments and mobile low-angle boundaries to the specific heat and thermal lattice resistivity. Dislocations and boundaries have T and T^2 specific-heat temperature dependence and approximately T^n and T^5 thermal-conductivity temperature dependences, where n lies between 3.3 and $\frac{7}{2}$ for the usual range of measurements. Dislocations may be able to make contributions to the specific heat of superconductors and nonconductors at very low temperatures. Low-angles boundaries cannot. Dislocations can make relatively large contributions to the thermal resistivity of nonconductors and superconductors at low temperatures. It seems to be possible to interpret the available data with reasonable dislocation densities. It is at present uncertain whether or not mobile low-angle boundaries can be available in sufficient quantities in crystals to influence the measured thermal conductivity.

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APPENDIX I

We wish to demonstrate that two parallel edge dislocations of length L, which are separated by a distance L, have displacements which are approximately independent of small displacements of either. Consider the displacement y of a pinned dislocation when acted upon by a shear stress σ. One has

$$b\sigma=Td^2y/dx^2,$$

where T is the tension of the dislocation line. Solving this with the boundary conditions $y(0)=y(L)=0$ gives

$$y=(b\sigma/2T)x(L-x).$$

The interaction stress, σ_i, between two parallel edge dislocations is given by[7]

$$b\sigma_i=\frac{Gb^2}{2\pi(1-\nu)}\frac{1}{R},$$

where R is the distance between them, and ν is Poisson's ratio. R is given by $L+y_2-y_1$, where y_1 and y_2 are the displacements of the first and second dislocations, respectively. We shall assume that y_1/L and y_2/L are small, and can take R to be $L+\bar{y}_2-\bar{y}_1$, where $\bar{y}_2$ is the average displacement of the second dislocation. Also, taking the approximate values, $T=\frac{1}{2}Gb^2$ and $\nu=\frac{1}{3}$, we obtain

$$b\sigma_i\approx T/[2(L+\bar{y}_2-\bar{y}_1)],$$

and

$$\bar{y}=\frac{1}{L}\int_0^L y(x)dx=\frac{b\sigma L^2}{12T}.$$

Consider the dislocation numbered (2). Because of the interaction force, it will bow out until the interaction force is just balanced by the tension force. The total interaction force is given by $b\sigma_iL$ and the tensile restoring force by $T(d^2y/dx^2)L$. For equilibrium the net force on dislocation (2) must be zero, and we have

$$TL/[2(L+\bar{y}_2-\bar{y}_1)]-12T\bar{y}_2/L=0,$$

or

$$y_2=(L/24)[1-(\bar{y}_2-\bar{y}_1)/L+\text{terms of order}(\bar{y}/L)^2].$$

Therefore, to a first approximation, the average displacement $\bar{y}_2$ is unaffected by variations in $\bar{y}_1$.