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Lattice Thermal Resistivity due to Dense Arrays of Dislocations *

M. W. Ackerman and P. G. Klemens
Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268
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The scattering of phonons by dislocations is modified if the strain field of dislocations is cut off at a finite range. The lattice thermal resistivity of a dense dislocation array is calculated on the assumption that the cutoff radius is comparable to the average distance between dislocations. Phonons of very long wavelength are only weakly scattered, and phonon-electron scattering must be invoked to obtain a finite thermal resistivity. The lattice thermal conductivity of deformed alloys departs from the usual T^2 dependence. On a reduced plot the shape of the conductivity curve depends on the ratio of the lattice conductivity in the annealed state to that in the deformed state. Curves are given for two values of this parameter. In a typical case of a heavily deformed copper alloy, significant deviations from the T^2 dependence should occur at liquid-helium-three temperatures. The shape of the curves could be used to estimate dislocation densities independently of estimates requiring knowledge of the strength of the interaction between phonons and dislocations.

I. INTRODUCTION

The density of dislocations could be determined by means of lattice-thermal-conductivity measurements at very low temperatures if one knew the average strength of the interaction between phonons and dislocations. Unfortunately, this strength is difficult to estimate reliably from first principles, since it depends in detail on the anharmonicities. Measurements of dislocation densities by other methods are also difficult and uncertain in the high-density region. It would thus be advantageous to have a measure of dislocation densities using lattice thermal conductivities which is independent of any estimate of the interaction strength.

The suggestion made here is that the dislocations tend to arrange themselves so as to minimize the free energy and that, in a dense array, this results in cancellation of the long-range strain field. The ordinary theory of phonon scattering by dislocations[1] assumes an infinite-range strain field, but if the strain field is cut off at a finite distance R, the scattering phonons which have wavelengths on the order of or greater than R is reduced. One may relate the cutoff radius R to the dislocation density.[2] This cutoff of the strain field should therefore cause noticeable changes in lattice thermal conductivity at very low temperatures, namely, deviations from the T^2 temperature dependence ordinarily predicted.[1] Conversely, one should be able to deduce the average range of the strain field from such changes in the temperature dependence. This would provide an independent estimate of the density of dislocations, still using the lattice thermal conductivity, and consequently, this would also yield the average strength of the interaction between phonons and dislocations. It will be shown that, for the dislocation densities to be expected in deformed alloys, the important region for such studies are liquid-He^3 temperatures and it is suggested that the lattice thermal conductivity of cold-worked alloys should be measured at these temperatures.

Gruner and Bross[3] have proposed another model leading to the cancellation of the long-range strain field, namely, dislocation dipoles. Their results will be compared to ours in Sec. IV.

Other workers have dealt with dislocation arrangements which lead to reinforcement of scattering, either due to pile up or due to dislocation walls.[1,4] These arrangements have the opposite effect to the one discussed here.

Our model is reminiscent of one proposed by Carruthers,[5] who used an exponentially damped dislocation strain field, and then went to the limit

of vanishing damping. Unfortunately, he does not present the intermediate results, which should bear similarity to ours, but only the result for zero damping, which corresponds to the isolated dislocation.

II. LATTICE THERMAL CONDUCTIVITY

If the dislocation axis is taken as the axis of a system of cylindrical coordinates, the spatial dependence of the components of the strain field becomes $\sin\theta/r$ and $\cos\theta/r$. Since scattering by the core may be neglected at liquid-helium temperatures and the present model assumes that the strain field is zero for $r > R$, where R is the average range of the strain field, the Fourier transform of $\sin\theta/r$ is now

$$F(\sin\theta/r) = \int_0^{2\pi} d\theta \sin\theta \int_{r_0}^{R} dr\, e^{iqr\cos\alpha}, \tag{1}$$

where r_0 is the core radius, $r = r(\cos\theta, \sin\theta)$, the change in wave vector is $\vec{q} = \vec{q}_0 - \vec{q}' = q(\cos\phi, \sin\phi)$, and $\alpha = \theta - \phi$.

Integrating over r, we have

$$F(\sin\theta/r) = \int_0^{2\pi} d\theta \sin\theta (e^{iqr\cos\alpha}/iq\cos\alpha)_{r_0}^{R}, \tag{2}$$

and changing variables from θ to α

$$F(\sin\theta/r) = (-i/q)\int d\alpha(\tan\alpha\cos\phi + \sin\phi)(e^{iqr\cos\alpha})_{r_0}^{R}. \tag{3}$$

Since $\tan\alpha$ is odd in α while the exponential terms are even, the expression reduces to

$$F(\sin\theta/r) = (\sin\phi/iq)\int_0^{2\pi} d\theta (e^{iqr\cos(\theta-\phi)})_{r_0}^{R}. \tag{4}$$

Noting that the Bessel function may be represented by

$$J_0(qr) = (2\pi)^{-1}\int_0^{2\pi} d\theta\, e^{iqr\cos(\theta-\phi)}, \tag{5}$$

the Fourier transform becomes finally

$$F(\sin\theta/r) = (2\pi i \sin\phi/q)[J_0(qr_0) - J_0(qR)]. \tag{6}$$

Since r_0 is on the order of a lattice spacing and q is also small at low temperatures, $J_0(qr_0) \cong 1$ and

$$F(\sin\theta/r) \cong (2\pi i \sin\phi/q)[1 - J_0(qR)]. \tag{7}$$

A similar calculation yields

$$F(\cos\theta/r) \cong (2\pi i \cos\phi/q)[1 - J_0(qR)]. \tag{8}$$

The perturbation energy per phonon caused by the strain field is of the form $\hbar q_0 \delta v$, where δv varies as $v\sin\theta/r$ or $v\cos\theta/r$ for each component of strain, so that from second-order perturbation theory $\sigma_d(\theta_s)$, the differential cross section for phonon scattering by dislocations, is of the form

$$\sigma_d(\theta_s) \propto \frac{q_0^2[|F(\sin\theta/r)|^2 + |F(\cos\theta/r)|^2]\rho}{d\theta_s}, \tag{9}$$

where θ_s is the scattering angle and ρ is the density of final states which, in this two-dimensional formulation, is proportional to $q_0 d\theta_s$. Thus, we have

$$\sigma_d(\theta_s) \propto q_0^3[1 - J_0(qR)]^2/q^2, \tag{10}$$

where $q = 2q_0 \sin(\frac{1}{2}\theta_s)$.

The reciprocal of the effective mean free path for scattering by dislocations is

$$\Lambda_d^{-1} \propto N_d \pi \int_0^{\pi} d\theta_s \sin\theta_s (1 - \cos\theta_s)\sigma_d(\theta_s), \tag{11}$$

where N_d is the dislocation density. Since $\theta_s = \pi - 2\phi$, this becomes, upon changing the variable of integration to $\mu = \cos\phi$,

$$\Lambda_d^{-1} \propto \pi N_d \int_0^1 d\mu\, \mu^3 \sigma_d(\mu), \tag{12}$$

$$\Lambda_d^{-1} \propto N_d \int_0^1 d\mu\, \mu^3 q_0^3 [1 - J_0(qR)]^2/(2q_0\mu)^2,$$

$$\Lambda_d^{-1} \propto N_d q_0 [1 + J_0^2(2q_0R) + J_1^2(2q_0R) - 4J_1(2q_0R)/2q_0R]. \tag{13}$$

For convenience, we denote the quantity in the square brackets by $f(2q_0R)$ or simply f.

Define a parameter p by $R = p\Theta_D a$, where Θ_D is the Debye temperature and a^3 is the volume per atom. Following Ref. 2, we relate the dislocation density to the cutoff radius of the strain field by $N_d = 1/\pi R^2$, so that

$$\Lambda_d^{-1} \propto q_0 f(2q_0R)/p^2 \tag{14}$$

or

$$\Lambda_d = Dp^2/q_0 f(2q_0R). \tag{15}$$

The constant of proportionality D has been estimated elsewhere[1,6]; its value is not needed for the present purposes.

The cutoff of the long-range strain field has the consequence that long-wavelength phonons are scattered only very weakly by dislocations and, if dislocation scattering were the only resistive mechanism, the expression for the thermal conductivity would diverge at low frequencies. It is thus necessary to consider dislocation scattering in combination with another scattering mechanism which removes the divergence. In metals and alloys such a mechanism is always provided by the scattering of phonons by electrons.[6]

Writing the effective mean free path for phonon scattering by electrons, Λ_e, in the form E/q_0, the effective mean free path for phonon scattering by both dislocations and electrons is

$$\Lambda_g = \Lambda_e\Lambda_d/(\Lambda_e + \Lambda_d) = Dp^2/q_0(f+g), \tag{16}$$

where $g = Dp^2/E$.

The lattice thermal conductivity when limited by electrons alone is of the form

$$K_{ge} = \tfrac{1}{3} v \int_0^{q_D} dq_0 c(q_0) \Lambda_e(q_0), \tag{17}$$

where v is the average phonon speed, q_D is the Debye wave number, and $c(q_0)dq_0$ is the specific heat of the phonons in the wave-number interval dq_0 about q_0. Since phonons have energy $\hbar v q_0$ and the number of states in dq_0 is proportional to q_0^2,

$$c(q_0) \propto q_0^4 e^{\hbar v q_0/kT} (e^{\hbar v q_0/kT} - 1)^{-2}/T^2, \tag{18}$$

where $\hbar$ and k are the modified Planck and the Boltzmann constants.

Changing the variable of integration to the reduced frequency $x = \hbar v q_0/kT$, K_{ge} may be written

$$K_{ge} = CT^2 E \int_0^{\Theta_D/T} dx\, x^3 e^x/(e^x - 1)^2 = CT^2 E J_3(\Theta_D/T), \tag{19}$$

where C is the product of all those proportionality constants omitted in the above discussion and J_3 is the standard transport integral.

Similarly, the lattice thermal conductivity, when dislocation scattering is included, becomes

$$K_g = \tfrac{4}{3} \pi v \int_0^{q_D} dq_0\, c(q_0) \Lambda_g(q_0, 2q_0 R). \tag{20}$$

Since q_0 is given by $x q_D T/\theta$, R by $p\Theta_D a$, and q_D by $3.9/a$, then

$$f(2q_0 R) = f(2xpTq_D/a) = f(7.8pTx), \tag{21}$$

so that, upon changing the variable of integration, Λ_g is a function of pT as well as x, and K_g becomes

$$K_g = CT^2 Dp^2 \int_0^{\Theta_D/T} dx\, x^3 e^x / \{(e^x - 1)^2 [f(7.8pTx) + g]\}. \tag{22}$$

The modified transport integral in (22) will be denoted by J_3'.

For large values of argument $f(7.8pTx)$ approaches unity while for small values it approaches zero. Thus, the above expression for K_g predicts that K_g should begin to depart from T^2 behavior at some low temperature and that this temperature increases as N_d increases.

III. NUMERICAL EXAMPLES

To estimate typical temperatures at which K_g in copper alloys should have values noticeably greater than those for a T^2 temperature dependence, use was made of some recent measurements of thermal conductivity[7] in specimens of Cu-10% Al and of a theoretical relation[8] between N_d and W_d, the dislocation thermal resistance, in a copper alloy. The value of N_d in deformed specimens obtained from this relation was, typically, 2.7×10^{11} cm^{-2}. In Refs. 8 and 9 it is noted that values of N_d obtained from this relation, in specimens of Cu-30% Zn, are six times those obtained from electron micrographs[9]; hence, N_d should be taken, more realistically, as 4.5×10^{10} cm^{-2}.

The relation

$$K_{ge}/K_g = CT^2 E J_3/CT^2 Dp^2 J_3' = J_3/gJ_3' \tag{23}$$

does not provide a means for calculating the ratio $g = Dp^2/E$ because the value of J_3' depends on g. However, it does provide a useful check on the validity of approximations used in estimating g.

To estimate g it is noted that the additive resistance approximation holds at temperatures above 3 °K so that

$$K_{ge}/K_g = 1 + K_{ge}/K_{gd}, \tag{24}$$

where K_{gd} is the lattice thermal conductivity as limited by dislocations alone. In the present case, the ratio of K_{ge} to K_g is about 2.1. The additive resistance approximation holds only when the scattering rates have the same frequency dependence. It was assumed that, at temperatures above 3 °K

$$K_{gd} = CT^2 Dp^2 J_3(\theta/T). \tag{25}$$

On this assumption, $K_{ge}/K_{gd} = 1/g$ so that from (24), g is approximately 0.9. Since the resulting value of J_3/gJ_3' is within 1% of 2.1 at values of pT corresponding to temperatures above 3 °K, this approximation is valid.

For the same value of K_{ge}, ratios of K_{ge} to K_g of 3 and 4 correspond to N_d values of 8.2×10^{10} and 1.2×10^{11} cm^{-2}, respectively, and K_g departs significantly from T^2 behavior at higher temperatures for these cases.

Table I shows the temperatures $T(10\%)$ and $T(50\%)$ at which the value of K_g exceeds the value for T^2 dependence by 10 and 50%, respectively, for three ratios of K_{ge} to K_g. The estimated values of N_d are also shown and it may be seen that the relationship between N_d and the temperature at which there is a given fractional deviation from T^2 dependence is roughly a linear one.

Figures 1 and 2 show the departure of K_g/T from linear dependence on T at liquid-helium-three temperatures.

TABLE I. Temperatures at which K_g is 10 and 50% greater than the value for T^2 dependence in three cases.

K_{ge}/K_g at 3 °K	N_d (10^{10} cm^{-2})	$T(10\%)$ (°K)	$T(50\%)$ (°K)
2.1	4.5	0.63	0.29
3	8.2	1.10	0.53
4	12.0	1.52	0.77

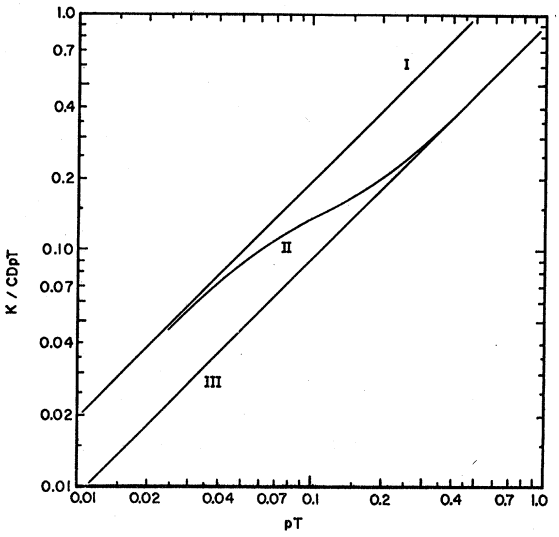

FIG. 1. Reduced lattice thermal conductivity $K/CDpT$ vs reduced temperature pT: curve I as limited by phonon-electron scattering only; curve II with dislocations according to the present model; and curve III with randomly arranged dislocations. This figure assumes the ratio of K_{ge} to K_g to be 2.1 at liquid-He^4 temperatures.

IV. CONCLUSION

The predicted departure of K_g from its T^2 temperature dependence, if it occurs, should be measurable at liquid-He^3 temperatures in alloy specimens which have undergone severe plastic deformation, provided the solute concentration of the alloy is sufficient to reduce the electronic component of thermal conductivity to the level of the lattice component.

Such measurements would make it possible to determine p and thus N_d. It would then be possible to obtain the average strength of the phonon-dislocation interaction by comparing N_d and the lattice thermal resistivity due to dislocations at liquid-He^4 temperatures, thus making it possible to obtain the value of N_d in other specimens of the alloy from measurements of lattice thermal conductivity in the range 1–4 °K. There are, however, some difficulties in addition to those of making accurate measurements of K_g at liquid-He^3 temperatures.

First, the relation $N_d = 1/\pi R^2$ is open to question. There is some evidence that the average range of the strain field is approximately equal to the average dislocation spacing.[2] However, one might expect πR^2 to be somewhat greater than the area per dislocation, particularly in specimens which have not been aged at elevated temperatures, because of incomplete cancellation of the long-range strain fields. Since the method proposed here is essentially based on a measurement of R, it would therefore underestimate N_d. Since the concensus is that the other method[8,9] of obtaining N_d from thermal-conductivity measurements overestimates its value, it would be interesting to compare the results from the two methods for the same specimens.

A second difficulty is the formation of atmospheres around edge dislocations; in a sufficiently concentrated alloy this can change the strength of phonon scattering by dislocations.[10] The effect depends on the temperature at which the atmosphere attained equilibrium and can be separated from the scattering by bare dislocations by a series of measurements after annealing at low temperatures, as was done, for example, by Mitchell in Ref. 7.

The theory of dislocation dipoles[3] is similar to that presented here in that it also leads to cancellation of the long-range strain field. However, while it also leads to the prediction that, at very low temperatures, the value of K_g is larger than the value it would have if it remained proportional to T^2, the theory leads to a temperature dependence of K_g which is quite different from that predicted here. Further, the cancellation of the long-range strain field is assumed to be the result of the pairing of dislocations of opposite signs, which is more restrictive than the assumption underlying the present model. While such pairing is probably a very important mechanism in the reduction of the average range of the strain field, it may be unnecessary to make such a detailed assumption for the purpose of constructing a theory of the

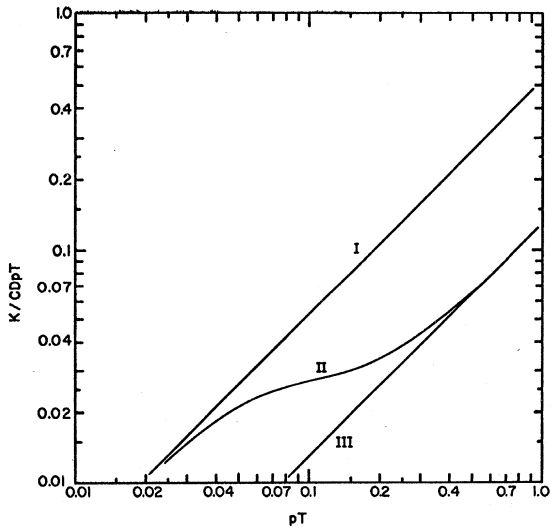

FIG. 2. Curves similar to those in Fig. 1, except that the ratio of K_{ge} to K_g is assumed to be 4.0 at liquid-He^4 temperatures.

temperature dependence of lattice thermal conductivity at liquid-He^3 temperatures.

Comparison of the temperature dependence of the two models is complicated by the fact that Gruner and Bross used three-phonon N processes instead of phonon-electron interactions to prevent low-frequency divergence. However, the two models also differ in other respects and lead to different temperature dependences. First, since the spacing of the dislocations forming the dipole must be less than the average distance between dislocations, deviations from the T^2 behavior should begin at a higher temperature. Second, for very long wavelengths in our model, the strained regions on either side of a single dislocation (compressed and dilated regions in the case of an edge dislocation) form a dipole which scatters as q_0^5, whereas the corresponding regions of a dislocation dipole form a quadrupole which scatters as q_0^7. Hence, the lattice thermal conductivity in the case of dipoles would change more rapidly away from a T^2 behavior than in our model, even if the same cutoff mechanism is invoked.

No measurements appear to have been made to date on the lattice thermal conductivity of deformed alloys below 1 °K. Such measurements would test the present theory and may provide information on dislocation densities.

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Knight Shift in Cadmium: Field and Temperature Dependence*

R. G. Goodrich, S. A. Khan, and J. M. Reynolds
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803
(Received 18 November 1970)

Measurements have been performed of the Knight shift in cadmium as a function of field between 1 and 20 kG at 1.2 °K and as a function of temperature between 1.2 and 300 °K at 9.4 kG. The field-dependent studies show an oscillatory behavior of the Knight shift at the de Haas-van Alphen frequency appropriate to the first band in the higher-field ranges. In the low-field region the average value of the Knight shift is found to exhibit a strong anisotropic field dependence. The temperature-dependent measurements show that the anisotropy in the Knight shift reverses sign between 1.2 and 300 °K. Measurements of the amplitude of the de Haas–van Alphen signals were performed in the same field range and orientation as the oscillatory Knight-shift measurements. All of the measurements reported are accounted for by the detailed field and temperature dependence of the topology of the cadmium Fermi surface.

I. INTRODUCTION

There have been several measurements of the Knight shift σ in Cd over the past few years, but only recently have the measurements yielded consistent results and has a reasonable interpretation been given for them.[1] Cadmium is an interesting metal on which to compare measurements of σ with theory because the band structure[2] and particularly the Fermi surface[3] (FS) are extremely well known. In a series of recent papers, the results of field-dependent measurements of σ on single crystals of Sn,[4] Cd,[5] and Al[6] have been reported. It has been found that σ oscillates at the de Haas–van Alphen (dHvA) frequencies of electrons on the FS, and that through measurements of the amplitude of this oscillatory behavior one can determine wave-function amplitudes for selected groups of electrons on the FS. The wave-function amplitudes of conduction electrons can be determined through this technique at different points in the Brillouin zone once the FS and the amplitude of the dHvA signals are known. The purpose of this paper is to report on field- and temperature-dependent measurements of σ in Cd from which information about the conduction-electron wave functions can be obtained.