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Phonon scattering by dislocations in metallic alloys

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The theory of phonon scattering by fluttering dislocations of Ninomiya is applied to the thermal conductivity of copper alloys. Modifications made are the inclusion of a Peierls potential and of a restoring force on the dislocation due to solute atmospheres around the dislocation. In addition to the reradiation of phonons, scattering by the strain field around the dislocation and by the phonon-electron scattering are included to obtain the overall phonon relaxation rate. This theory is applied in particular to the lattice thermal conductivity of copper-aluminum alloys. The effects of dispersal of the atmospheres by moderate annealing is discussed. Agreement with experiment in the vicinity of the "bow" around 2–3 K could be obtained.

I. INTRODUCTION

The lattice thermal conductivity of metallic systems has been studied extensively through the thermal conductivity of alloys.[1,2] At low temperatures the principal phonon scattering mechanisms are free electrons and, for plastically deformed specimens, dislocations. Both scattering mechanisms vary as the first power of frequency, and the corresponding thermal resistivity should vary as T^{-2}, where T is the absolute temperature. While early measurements conformed to that expectation, more recent and more detailed investigations[3-7] have shown deviations from a T^2 dependence of the lattice thermal conductivity at low temperatures. This deviation appears as a reduction in the lattice thermal conductivity, bowing the curve, and this bow is centered usually between 2 to 3 K. To explain it, one must invoke a different scattering mechanism than the anharmonic scattering by the static strain field around the dislocation, which is the basis of the earlier theory.[1]

Since dislocations are mobile, they respond dynamically to incident thermal phonons, resulting at low temperatures to dislocation flutter which can enhance scattering, especially near resonance frequencies, so that the thermal conductivity curve is depressed in the vicinity of the corresponding temperature. This scattering mechanism was proposed by Granato and Lücke[8] in analogy to the forced vibration of a stretched string with damping. Their model has proven particularly successful when applied to internal friction and ultrasonic attenuation. It has also been applied to thermal resistance due to phonon scattering by dislocations, particularly in the case of alkali haides, where the observed thermal resistances are much larger than would be expected from scattering by static dislocations. The experimental evidence has recently been reviewed in some detail by Anderson.[9]

The stretched string model is not complete, since it leaves indeterminate parameters such as line tension and mass. The treatment of Ninomiya[10] is self-consistent and more satisfactory, because it predicts these quantaties and also avoids other difficulties discussed by Ninomiya.

The present treatment is based on Ninomiya's theory, but considers additional factors needed to treat the lattice thermal resistivity of dislocations in alloys: (1) An appropriate weighting of the scattering cross section over angles, (2) the inclusion of scattering of phonons by electrons and by the static strain fields of the dislocations, (3) the difference between longitudinal and transverse phonons in their scattering not only by the mobile dislocations but also by the electrons, and (4) the restoring force acting on the vibrational dislocation not only owing to the Peierls potential but also arising from solute atmospheres. The theory is then applied to the case of Cu—10 at.% Al and compared to the results of Linz *et al.*[3]

II. MODEL

The problem of phonon scattering by a fluttering dislocation has an intimate connection with that of finding the eigenstates of lattice vibration in a dislocated crystal. Ninomiya investigated the eigenfrequencies of a dislocated crystal in an isotropic elastic continuum. He found that the introduction of a dislocation into a crystal shifts the perfect crystal's phonon band according to Rayleigh's theorem.[11] While most modes experience an inconsequential shift, the dislocation also causes localized waves lying below the bottom of the band. This must be understood as follows: Each localized wave has a wave number and must be compared to all modes of the perfect crystal whose wave-vector components are parallel to the dislocation axis and are equal to that wave number. The frequencies of those modes form a continuous band with a lower limit for each such wave number. If the frequency of the localized wave lies below that band the wave is truly orthogonal to all modes of the perfect crystal, and is a localized mode. If the frequency lies in the band the wave is not an independent mode, but gives rise to resonant scattering of the lattice waves.

The localized waves exist for both screw and edge dislocations. For edge dislocations the localized waves lie below the band of perfect crystal modes. They are thus orthogonal to those modes and are truly independent modes. For screw dislocations the localized waves lie closer to the band edge, and may even slightly overlap the band of perfect crystal modes of the same wave-vector component. As a result, screw dislocations will scatter phonons more strongly than edge dislocations, and some modes will even be scattered resonantly, because their wave-vector component matches the wave number of the localized wave of the same frequency. The localized wave is then no longer a normal mode of the system.

The resonant scattering occurs for a transverse phonon incident on a screw dislocation at some oblique angle. Longitudinal waves are scattered but cannot satisfy the conditions needed for resonance.

When the dislocation lies along the z axis and its slip plane is taken to be the xz plane, the differential cross section derived through the Ninomiya formalism is

$$\frac{d\sigma_{\text{tot}}}{d\Omega}=\frac{\mu^2\Phi^*(\vec{q}_0,s_0)\Phi(\vec{q}_0,s_0)}{8\pi|k^2T(k)F(\omega^2-i\epsilon)|}\times\sum_s\left(\frac{c_s}{c_{s_0}}\right)\left(\frac{c_t}{c_s}\right)^4\frac{1}{\rho q_s}\Phi^*(\vec{q}_s,s)\Phi(\vec{q}_s,s), \tag{1}$$

where $d\Omega=\rho\, d\sigma$ and (ρ,ϕ) are polar position coordinates lying in a plane perpendicular to the axis of the dislocation. The polarization index for incident and scattered waves is given, respectively, by s_0 and s, and the velocity c of a phonon before and after scattering depends upon polarization and is subscripted s_0 or s. A specific polarization (transverse or longitudinal) is denoted by t or l. The denominator $|k^2T(k)F(\omega^2-i\epsilon)|$ and the function Φ are defined and discussed in the Appendix. Here k is the wave number of a localized wave propagating along the dislocation, $\vec{q}$ is a phonon wave vector, and μ is the shear modulus of the material.

What is of interest in transport problems is the total weighted cross section. The differential cross section is first weighted by a factor which measures the relative change in the component of phonon velocity along the initial direction of motion and then integrated over the scattering angle, viz.,

$$\sigma=\int\left(1-\frac{n_s}{n_0}\right)\frac{d\sigma_{\text{tot}}}{d\Omega}\,d\Omega\,. \tag{2}$$

$n_s\alpha\vec{q}_s\cdot\vec{\nabla}T$ and $n_0\alpha\vec{q}_{s_0}\cdot\vec{\nabla}T$ are the deviations from equilibrium of the phonon distribution assumed in order to satisfy the Boltzmann equation assuming a relaxation time.

When the differential cross section (1) is substituted into (2) with the standard assumption and averaged over the polar scattering angle the second term in (2) is zero. The resulting cross section due to the first term before averaging over the scattering angles is

$$\sigma_{\text{tot}}=\frac{\mu^2b^2|\Phi(\vec{q}_0,s_0)|^2}{8|k^2T(k)F(\omega^2-i\epsilon)|^2}\left(\frac{c_t}{c_s}\right)^4q_s^{-3}\{\beta_x^2(q_t^4-k^4)+\beta_z^2(q_t^4-3k^2q_t^2+4k^4)+H(q_l^2-k^2)[\beta_x^2(q_l^2-k^2)+4\beta_z^2(q_l^2-k^2)]\}\,, \tag{3}$$

where

$$H(y)=\begin{cases}1 & \text{if } y>1\\ 0 & \text{if } y<1\end{cases}$$

and $c_tq_t=c_lq_l=c_sq_s$. The β's are the direction cosines of the Burgers vector $\vec{b}$ with the dislocation axis, x indicating an edge component and z a screw component.

As pointed out in the Appendix, the denominator of (3) has the form

$$k^2T(k)F(\omega^2-i\epsilon)=m\omega^2+k^2T+\text{Im term}. \tag{4}$$

Here m and T are dynamical, frequency-dependent, dislocation mass, and line tension, respectively. When the real part is equal to zero, resonant scattering occurs. However, the condition $q_0\geqslant k$ must be also met.

It is now evident from Figs. 1 and 2 that a resonance condition is satisfied for a transverse-phonon incident at some angle on a screw dislocation, but is not satisfied for an edge dislocation. If the mass curve for the edge dislocation were lower the resonance condition could be satisfied. The addition of a potential field in which the dislocation vibrates can create just this effect, as will be seen below.

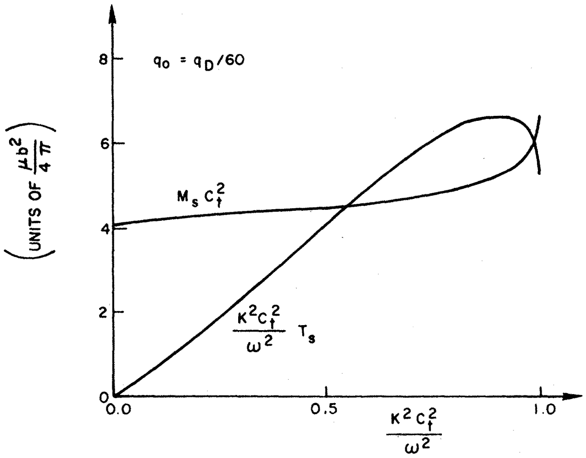

FIG. 1. Plot of $m_S c_t^2$ and $(k^2c_t^2/\omega^2)T_S$ versus $k^2c_t^2/\omega^2$ for a transverse-phonon incident on a screw dislocation. Resonance occurs where the two curves cross, at $\theta_0 \simeq 43°$, since this is equivalent to the condition $-m_S\omega^2 + k^2T_S = 0$. The curves also intersect at near parallel incidence. This intersection makes a lesser contribution to the weighted cross section and, furthermore, implies the phase velocity along the dislocation is approximately equal to the transverse-phonon velocity. q_D is the Debye wave vector.

III. THE INFLUENCE OF A PEIERLS POTENTIAL AND A SOLUTE ATMOSPHERE

A dislocation vibrating in a real crystal experiences a potential due to the discreteness of the crystal, called the Peierls potential. In addition, if the material is an alloy, solute atoms tend to rearrange themselves about the dislocation, forming solute or Cottrell atmospheres; this results in yet another potential field for the dislocation. The addition of these two potentials will change the equations of motion of the dislocation and thus change its dynamical scattering properties.

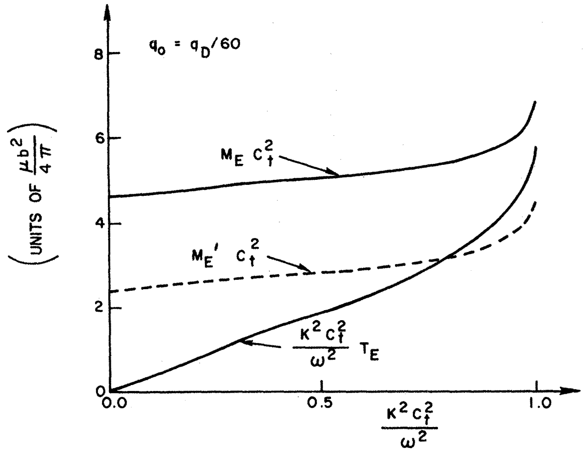

FIG. 2. Plotting $m_E c_t^2$ and $(k^2c_t^2/\omega^2)\ T_E$ against $k^2c_t^2/\omega^2$ for a transverse-phonon incident on an edge dislocation does not show a resonance condition. The two curves do not cross and the condition $-m_E\omega^2 + k^2T_E = 0$ cannot be met. It is evident, however, that a lowering of the mass curve would result in resonance as illustrated by $m_E' c_t^2$. The introduction of a Cottrell atmosphere or the Peierls potential produces this effect. q_D is the Debye wave vector.

In modifying Eq. (3) to accomodate these additional effects we confine ourselves to infinitesimal vibrations of the dislocation so that only the harmonic terms in these potentials will be considered. Then, just as in the case of a simple harmonic oscillator, the potential per unit length of dislocation will be equal to one half the spring force constant times the square of the dislocation amplitude. Here the spring force constant is a measure of the "strength" of the interaction. For the Peierls potential we shall designate this strength by P and for the Cottrell atmosphere by K. The addition of these potentials into the equation of motion has the effect of replacing $k^2T(k)$ in the denominator of (3) by

$$k^2T(k) \to k^2T_S(k) + P_S \quad \text{(screw)}, \tag{5a}$$

$$k^2T(k) \to k^2T_E(k) + P_E + K \quad \text{(edge)}. \tag{5b}$$

The quantities P_S, P_E, and K will be discussed later. The atmosphere term has been omitted for screw dislocations. In alloys where the strain field of the solute can be regarded as having spherical symmetry, there is no interaction between it and the strain field of a screw dislocation. There is, however, a strong interaction between the dilatational strain of an edge dislocation and the solute.

We now return to Eq. (3) to calculate the scattering cross section. For computational purposes we make the following approximations for edge and screw dislocations, respectively (see Appendix):

$$[k^2T_E(k) + P_E + K]F(\omega^2 - i\epsilon)$$

$$\simeq m_E(\omega_{PE}^2 + \omega_K^2 - \omega^2) + k^2T_E + i\frac{m_E\omega^2}{\eta}, \tag{6a}$$

$$[k^2T_S(k) + P_S]F(\omega^2 - i\epsilon)$$

$$\simeq m_S(\omega_{PS}^2 - \omega^2) + k^2T_S + i\frac{m_S\omega^2}{\eta}, \tag{6b}$$

where η is 5 and 2.5 for transverse and longitudinal waves, respectively, and we have defined the $\omega_{P,K}^2$ by $m\omega_{P,K}^2 = P$ and K, respectively. The values of the m's and T's are suitable averages chosen in accordance with the particular system and will be discussed shortly.

Now consider (6a) for the edge dislocation. The mass term may be factored as

$$-m_E(1 - \Omega^2/\omega^2)\omega^2 = -m_E'\ \omega^2, \tag{7}$$

defining m'_E, where $\Omega^2 = \omega_{PE}^2 + \omega_K^2$. The effective mass m'_E is frequency dependent and for $\omega > \Omega$, $m'_E < m_E$ thus lowering the mass curve as shown in Fig. 2 and introducing a frequency-dependent resonance condition. This is similarly the case for a screw dislocation.

If dislocations are randomly oriented the cross section must be averaged over all possible incident phonon directions, and since the k dependence is almost entirely in the denominator of the cross section this can be approximated as

$$\sigma_E(\omega, s_0) \simeq \frac{76}{81} \frac{\mu^2 b^2}{q^3} \frac{|\langle \Phi_E(\vec{q}_0, s_0)\rangle_k|^2}{8T_E^2} I_E(\omega) , \tag{8a}$$

$$\sigma_S(\omega, s_0) \simeq \frac{44}{81} \frac{\mu^2 b^2}{q^3} \frac{|\langle \Phi_S(\vec{q}_0, s_0)\rangle_k|^2}{8T_S^2} I_S(\omega) . \tag{8b}$$

The numerical factors of 76/81 and 44/81 arise from an averaging over the scattering angles θ_s and ϕ_s. Also $I(\omega)$ is an integral of form

$$I(\omega) = \int \frac{dx}{(x^2 - \delta)^2 + \gamma^2} , \tag{9}$$

where $x = k/q_0$, $\delta = (mc_s^2/T)(1 - \Omega^2/\omega^2)$, and $\gamma = mc_s^2/\eta T$.

IV. PEIERLS POTENTIAL

Owing to lattice discreteness and the periodicity of a real crystal, a dislocation will experience a periodic variation in its misfit energy as function of position x in the slip plane. For simplicity let $W(x)$, the potential energy per unit length of dislocation due to the misfit, vary sinusoidally with the period of the lattice parameter b. It may then be expressed as

$$W(x) = W_0 + W_P(x) . \tag{10}$$

W_0 is some reference energy, $W_P(x)$ is

$$W_P(x) = \frac{W_P}{2}\left(1 - \cos\frac{2\pi}{b} x\right) , \tag{11}$$

and W_P is the Peierls potential.

When the dislocation vibrates with infinitesimal amplitude (11) may be expanded keeping only the harmonic term so that

$$W_P(x) \simeq \frac{\pi^2}{b^2} W_P x^2 . \tag{12}$$

The strength of the potential P in Eq. (4) can be identified with

$$P = \frac{2\pi^2}{b^2} W_P . \tag{13}$$

Associated with $W(x)$ is a periodic stress $\sigma(x)$ given by

$$\sigma(x) = \frac{1}{b} \frac{dW(x)}{dx} . \tag{14}$$

The maximum stress is called Peierls stress σ_P and is

$$\sigma_P = \frac{1}{b} W_P . \tag{15}$$

It is a phenomenological parameter and the potential strength can be related to it by using (13) and (15)

$$P = 2\pi \sigma_P . \tag{16}$$

Thus with the use of (16) and using the expression for mass given in the Appendix, the resonant frequency due to the Peierls potential becomes

$$\omega_{P_j}^2 = \frac{P_j}{m_j} = \frac{8\pi^2 c_t^2}{b^2 M_j} \frac{\sigma_P}{\mu} , \tag{17}$$

where $j = E$ or S (edge or screw dislocations), and M is a dimensionaless quantity containing the frequency dependence of m_j which is defined in the Appendix.

V. COTTRELL ATMOSPHERE

When a dislocation is at rest, solute atoms migrate to and distribute themselves around it to form a Cottrell atmosphere. Because of cylindrical symmetry this distribution may be conveniently described in terms of the polar coordinates (ρ, ϕ). As the dislocation is displaced, in the x direction, it experiences a potential per unit length $V(x)$ due to the presence of the solute atmosphere. Since the dislocation oscillates with a frequency much higher than the jump frequency of the solutes the atmosphere is considered to be stationary. Thus with respect to the new position of the dislocation the distribution of the solutes may be described in terms of the coordinates (ρ', ϕ'). The transformation between the two sets of coordinates is $\vec{\rho}' = \vec{\rho} - \vec{x}$.

The potential energy per unit length is given by

$$V(x) = \int_{r_0}^{R} \int_0^{2\pi} [c(\rho, \phi) - c_0] U_{\text{int}}(\rho', \phi') \rho \, d\rho \, d\phi . \tag{18}$$

Here $c(\rho, \phi)$ is the distribution of solutes about the dislocation and c_0 the average concentration of solutes in the crystal. The interaction energy between a solute and the dislocation is $U_{\text{int}}(\rho', \phi')$.

In order to evaluate (18) the functional form of U_{int} and $c(\rho, \phi)$, which in turn depends on U_{int}, must be known. There are two contributions to the interaction energy: the size effect and the bulk modulus effect.

First consider the size effect. By inserting an impurity of different size than the atoms of the matrix, a local strain field is created which interacts with the strain field of the dislocation. The interaction energy is

$$U(\rho, \phi) = \Gamma \delta v \frac{\sin\phi}{\rho} . \tag{19}$$

δv is the external change in volume due to the insertion of the solute, and in a continuum approximation is given by[12]

$$\delta v = (v_s - v_m) \frac{1 + 4\mu/3B_m}{1 + 4\mu/3B_s} , \tag{20}$$

where the subscripts m and s refer to matrix and solute and the quantities v and B are the atomic volume and bulk modules, respectively. The factor Γ in (19) is

$$\Gamma = \frac{\mu}{3\pi}\left(\frac{1+\nu}{1-\nu}\right), \tag{21}$$

where ν is the Poisson ratio.

The modulus effect arises because solutes have different bonding properties with matrix atoms than matrix atoms have with themselves. In a continuum model the solute and matrix atoms are ascribed different elastic moduli as though they were elastic balls of different materials. Consequently, the solute atoms relax the strain field of the dislocation differently than the matrix atoms. If the volume of the strained solute is taken to be approximately equal to that of the matrix atom it replaces, the interaction energy between it and an edge dislocation is[12]

$$U'(\rho, \phi) = -\tfrac{1}{2} V_m B_{ms} \Gamma^2 \sin^2\phi/\rho^2 , \tag{22}$$

where $B_{ms} = (B_m - B_s)/B_m B_s$ is the fractional change in the elastic constant.

The concentration of solute atoms around an edge dislocation is thus

$$c(\rho, \phi) = c_0 \exp[-(U + U')/k_B T] , \tag{23}$$

where k_B is the Boltzmann constant and T the absolute temperature. The potential energy per unit length may now be calculated with the aid of (19), (22), and (23).

The potentials are singular at $\rho = 0$, since continuum theory fails at the dislocation core. When evaluating $V(x)$ the core region must be excluded. This can be done simply by choosing an inner cutoff radius, r_0 for ρ. If r_0 is large enough, $c(\rho, \phi)$ may be expanded in a power series and only first-order terms need be considered. In order to justify retaining only first-order terms r_0 must be chosen such that it has a value larger than ρU and $(\rho^2 U')^{1/2}$ simultaneously. For Cu—10 at.% Al this reduces numerically to

$r_0 > \Gamma \delta v / k_B T = 1.95b$ size effect,

$r_0 > (\Gamma v_m B_{ms} / 2k_B T)^{1/2} = 0.596b$ modulus effect.

It is evident that the size effect sets the lower limit on r_0. When the entire integrand is considered those terms which include the modulus effect are relatively small and may well be neglected. We chose $r_0 = 2b$. Based on a relation between dislocation density and its strain field cutoff given by Kocks and Scattergood,[13] the outer cutoff is taken as $R \simeq 50 r_0$.

We now expand (23) and substitute this along (19) and (22) into (18). Transforming coordinate variables we obtain

$$V(x) \simeq \frac{c_0 \Gamma^2 \delta v^2}{k_B T} \int_{r_0}^{R} \int_0^{2\pi} \frac{\rho\, d\rho \sin^2\phi \, d\phi}{\rho^2 + x^2 - 2\rho x \cos\phi} , \tag{24}$$

which takes the form

$$V(x) \simeq -\frac{c_0 \Gamma^2 \delta v^2}{k_B T} \pi \left[\ln\left(\frac{R}{r_0}\right) - \tfrac{1}{4} x^2 \frac{R^2 - r_0^2}{R^2 r_0^2} \right] \tag{25}$$

for $x \ll r_0$. The first term is just the average binding energy of the dislocation to the solute atmosphere. The second term is the restoring potential due to the harmonic approximation. Hence the coefficient K in (5b) becomes

$$K = \frac{c_0 \Gamma^2 \delta v^2 \pi}{2 k_B T} \frac{(R^2 - r_0^2)}{R^2 r_0^2} \tag{26}$$

from which one finds the resonance frequency

$$\omega_K^2 = \frac{K}{m_E} = \frac{2\pi c_0 \Gamma^2 \delta v^2 c_t^2}{\mu b^2 M_E k_B T} \frac{(R^2 - r_0^2)}{R^2 r_0^2} . \tag{27}$$

VI. NUMERICAL EVALUATION OF RESONANCE FREQUENCIES

In order to numerically evaluate resonance frequencies a value of dynamical dislocation mass as defined in the Appendix, $m(\omega) = (\mu b^2 / 4\pi c_t^2) M(\omega)$, must be obtained. Thermal conductivity experiments on Cu—10 at.% Al indicate that resonance scattering occurs between 2 and 3 K. This corresponds to a dominant phonon frequency of about $\frac{1}{60}$th of the Debye frequency.

From Figs. 1 and 2 it can be seen that resonance occurs at a different angle of incidence for each frequency. For parallel incidence the mass becomes infinite. To circumvent this difficulty the angular range is arbitrarily cut off at $k^2 c_t^2 / \omega^2 = 0.9$ and then averaged over the range. The same procedure is adopted for the dynamical line tension.

The value of the resonance frequency due to the Peierls potential depends on the ratio of σ_P / μ as seen from Eq. (17). As reported by Seeger *et al.*[14] this ratio has the value of 4.0×10^{-4} for polycrystalline copper. This value is approximately 200 times larger than observed by Young[15] in a single crystal of pure copper. A possible explanation for the discrepancy is that Young may have observed the stress needed in order to translate a kink over the Peierls barrier. At any rate, Seeger *et al*. measured some type of locking mechanism in polycrystalline copper, and if it is not the Peierls potential it may be interpreted as an effective Peierls potential for the present purpose.

Using Eq. (17) and the above information the resonance frequencies due to Peierls potential are

	edge	screw	
$\omega_p^2 =$	4.58	5.14	transverse
	5.62	6.39	longitudinal

and those due to the solute atmospheres (27) are

$\omega_k^2 = 5.52$ transverse

6.67 longitudinal

all in units of 10^{23} (rad/sec)^2.

VII. THERMAL CONDUCTIVITY

For the isotropic Debye continuum the lattice thermal conductivity is given by

$$K_g = \frac{k_B \omega_D^3}{6\pi^2}\left(\frac{T}{\Theta}\right)^3 \sum_{s_0} \int_0^{\Theta/T} \frac{x^4 e^x}{(e^x - 1)^2}\, \frac{\tau_{s0}(\omega)}{c_{s_0}}\, dx\,, \tag{28}$$

where $x = h\omega/k_B T$, Θ is the Debye temperature, and τ_{s_0} is the relaxation time.

The predominant scattering mechanisms at low temperatures are phonon-electron scattering and both the resonant and the anharmonic scattering of phonons by dislocations. At these temperatures umklapp-processes are very weak and may be neglected. Normal processes may also be disregarded since none of the scattering mechanisms being considered are strongly dependent on frequency. Thus the total relaxation rate $1/\tau$ is equal to the sum of the relaxation rates for the individual scattering processes.

The phonon-electron relaxation time varies in direct proportion to the wavelength[1] and may be written as

$$\tau_{pe} = E_{s_0}/q_0 \tag{29}$$

for each polarization. The parameter of E_{s_0} is inversely proportional to the square of the phonon-electron coupling parameter, which is difficult to calculate from first principles. However, it can be deduced from thermal conductivity data. At low temperature the value of (28) which corresponds to a well annealed sample where only phonon-electron interactions are important becomes[16]

$$K_g = 7.18 k_B \omega_D^2 T^2 E / 6\pi^2 \Theta^2\,, \tag{30}$$

where $E = \sum_{s_0} E_{s_0}$. Comparing this to the low-temperature lattice thermal conductivities of well annealed dilute copper alloys E is found to be 1.12×10^{-2} sec/cm. Since longitudinal waves suffer most of the scattering it will be assumed 95% of the thermal conductivity is due to the transverse modes, hence, $E_l \simeq E/21$ and $E_t \simeq (10/21)E$.

For anharmonic dislocation scattering, two relaxation times must be considered, one for scattering by an edge dislocation and the other by a screw dislocation. They are

$$\begin{aligned} \tau_E &= 4z/(13 N_E b^2 \omega_D^2)\,, \\ \tau_S &= z/(2 N_S b^2 \omega_D^2)\,, \end{aligned} \tag{31}$$

where $z = \omega/\omega_D$ and N_E and N_S are the densities of edge and screw dislocations. The total density is then $N_d = N_E + N_S$. Dislocations of edge character are predominant.[17] Thus we assume there are twice as many edge as screw dislocations, as would be the case of a Burgers vector which is randomly oriented with respect to the dislocation line,[18] $N_E = (\frac{2}{3}) N_d$ and $N_S = (\frac{1}{3}) N_d$.

Since the solute atoms around dislocations are themselves capable of scattering phonons[19] it will be further assumed that the static strain field scattering is enhanced by a factor of 2, in rough accord with observation.[6]

Finally the relaxation time for the resonance mechanism is

$$\tau_R = [N_d\, c_s\, \sigma_R(\omega, s_0)]^{-1}. \tag{32}$$

As in the case of anharmonic scattering the assumption of twice as many edge than screws dislocations require

$$\sigma_R(\omega, s_0) = \tfrac{2}{3}\sigma_E(\omega, s_0) + \tfrac{1}{3}\sigma_S(\omega, s_0)\,, \tag{33}$$

where σ_E and σ_S are given by Eq. (8).

Using the above relaxation times in (28), theoretical values of lattice thermal conductivity were calculated. These values, shown in Fig. 3 as solid lines, have been plotted for three dislocation densities. The dashed curves are the experimental curves of Linz *et al*.[3] Their lowest temperature values were omitted since that data is now considered in doubt (private communication). A reasonably good fit between experimental data and theory is obtained when a dislocation density of $N_d = 4.0 \times 10^{11}$ cm^{-2} is used in the calculations.

If the effects of the solute atmosphere are removed by annealing the sample so as to disperse the atmospheres but leave the bare dislocations,[6,20] the resonant frequency of the dislocation is lowered. This decrease in resonant frequency which shifts the bow is shown by the dashed curve in Fig. 4. With the elimination of the atmospheres comes a slight increase in the magnitude of K_g since the strain field scattering is no longer enhanced by the solutes. The net effect is that the

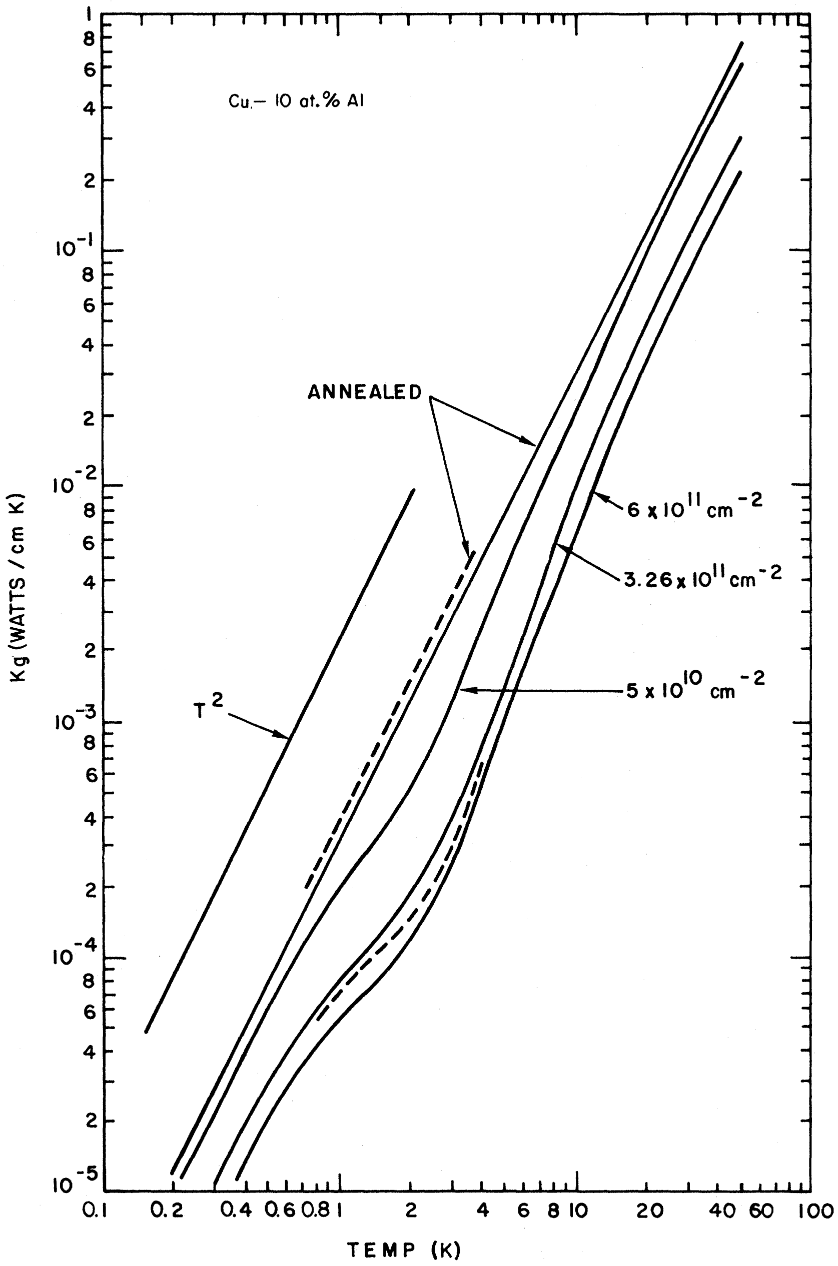

FIG. 3. Lattice thermal conductivity versus temperature. The solid lines are theoretical curves. As indicated, they are shown as a function of dislocation density, N_d. The dotted lines are experimental curves, Linz *et al.* For $N_d = 4\times10^{11}$ cm^{-2} the theoretical curve is a close fit to the deformed specimen experimental curve.

thermal conductivity curves with and without atmospheres overlap each other in the vicinity of the bow.

This crossing phenomenon is consistent with the experimental results of Friedmann[20] for Cu—7 at.% Ge. His data indicates a crossover at about 3.4 K which appears to be close to the value shown in Fig. 4. Unfortunately Friedmann's data do not extend to low enough temperatures to see the second crossover point which the present theory predicts. The trend of his data indicates that this may occur; but it was, in any case, not expected at that time.

The present paper has applied Ninomiya's theory of the scattering of phonons by mobile dislocations to the case of metallic alloys, with particular reference to copper alloys, for which extensive experimental data exists. If the other scattering mechanisms are taken into account, such as the anharmonic effect of the strain field and the large

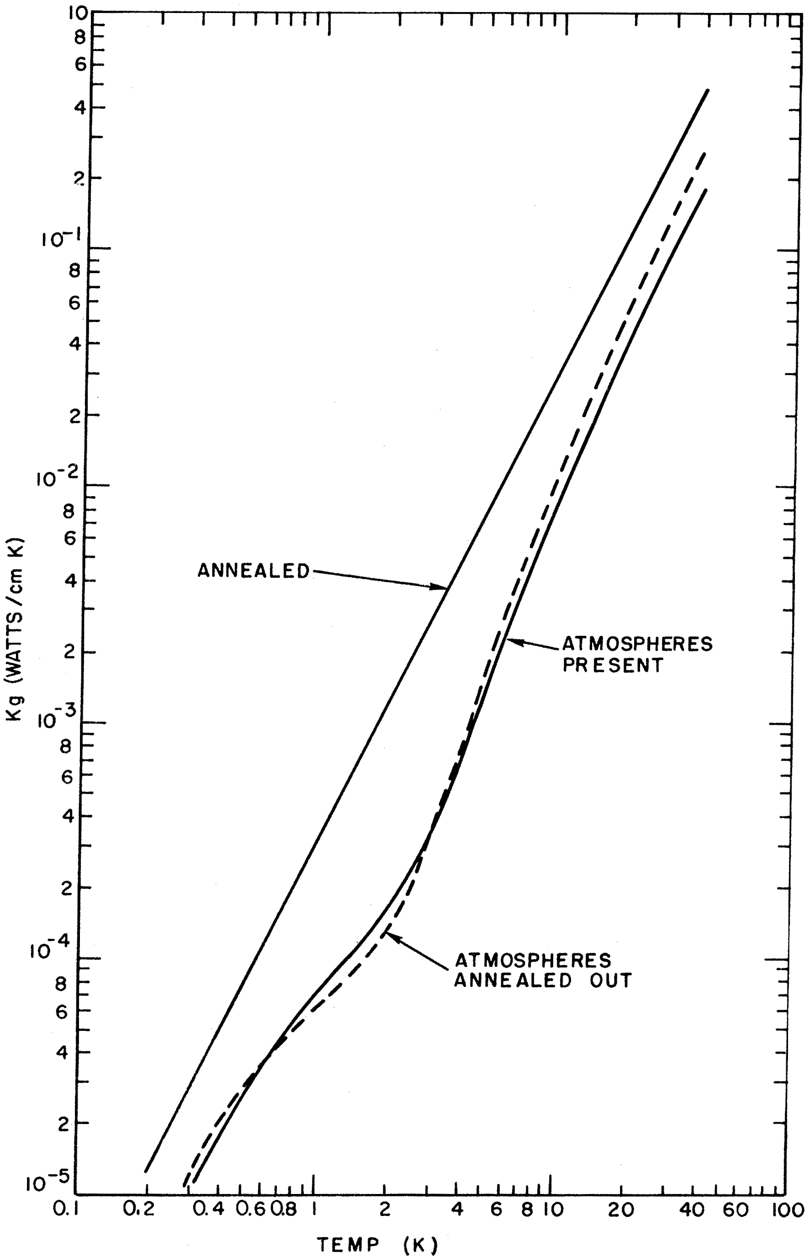

FIG. 4. This figure illustrates the effect on the lattice thermal conductivity of a deformed specimen produced by removing from the theory the potential due to the Cottrell atmospheres. Experimentally this corresponds to a deformation and then an annealing of the sample. The solid curve was calculated with atmospheres and the dashed curve without atmospheres. Both curves were calculated for a dislocation density of $N_d = 4 \times 10^{11}$ cm^{-2}. The straight line "annealed" curve was calculated with just phonon-electron interactions.

background of phonon-electron interactions, it appears that the theory can adequately describe the scattering of phonons by dislocations.

To be fully successful, the theory would also have to describe the thermal resistance due to dislocations in insulators, particularly alkali halides. The large body of experimental data has recently been reviewed by Anderson.[9] There is no doubt that strain-field scattering alone is inadequate to explain the observed thermal resistivities. It is not clear whether Ninomiya's theory, suitably modified for pinning of dislocations at nodes and other special sites, can adequately describe the data, for the consequences of that theory have not yet been fully explored. One difficulty is that in a resonance theory the conductivity depends not on the strength of the scattering, but on the mean free path of those phonons which are not strongly scattered by the dislocations. In the case of alloys, this problem is not as critical, owing to the background interaction between phonons and electrons, and also owing to the higher densities of dislocations which makes strain-field scattering significant.

VIII. SUMMARY

Using the theory of Ninomiya for phonon-dislocation interactions it was found that the introduction of the Peierls potential and a Cottrell atmosphere will shift the localized modes of dislocations. This shift gives rise to resonance scattering by edge dislocations whereas before the introduction of these potentials only screw dislocations could scatter resonantly. The resonance scattering by a screw dislocation requires a transverse wave incident obliquely on it. The introduction of the additional potentials makes the resonance condition depend on frequency rather than direction of incidence.

Resonance frequencies were calculated for both the Peierls potential and a Cottrell atmosphere. At low temperatures the dislocation flutters with infinitesimal amplitudes and only the harmonic terms in these potential were considered in the calculation of the resonance frequencies.

The introduction of dislocation reduces the magnitude of the lattice thermal conductivity. In general its T^2 temperature dependence at low temperatures may be explained by the scattering of thermal phonons by the static strain field surrounding the dislocation. There is, however, in the 2–3 K range, a drastic change in the slope of the K_g versus T plot as reported by Linz *et al.*,[3] Leaver and Charsley,[4] and Vorhaus and Anderson[5] for Cu—10 at.% Al. The theory of resonance scattering gives rise to an interaction between dominant phonons and fluttering dislocations in this temperature interval which is substantially stronger than the anharmonic mechanism. The result is a bow in the K_g curve. Here the dynamic model of phonon scattering seems not only to be a reasonable one but is in good agreement with experiment.

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APPENDIX

There arise two quantities in the formalism of Ninomiya which are used in the differential cross section of Eq. (1). In order to make things more transparent we present some of the details of these quantities in this Appendix.

The first of these quantities is

$$\Phi(\vec{q}_0, s_0) = -i[(\hat{\epsilon}\cdot\vec{b})(\vec{q}_0\cdot\hat{n}) + (\vec{b}\cdot\vec{q}_0)(\hat{\epsilon}\cdot\hat{n})]\,. \tag{A1}$$

In brief Φ contains the information of how a particular wave $\vec{q}_0$ of polarization $\hat{\epsilon}$ interacts with a dislocation of character $\vec{b}$ which oscillates in a slip plane defined by a unit normal vector $\hat{n}$.

The second quantity is quite lengthy and the full expression may be found in the Appendix of Ninomya's paper.[10] It suffices here to give an abbreviated form

$$k^2 T(k) F(\omega^2 - i\epsilon) = -\omega^2 \frac{\rho b^2}{4\pi} M(\omega) + k^2 \frac{\mu b^2}{4\pi} t(\omega) + i\pi\omega^2 \frac{\rho b^2}{4\pi} g(\omega)\,. \tag{A2}$$

Here $T(k)$ is an instantaneous dislocation line tension calculated for just one particular mode of vibration. $M(\omega)$, $t(\omega)$, and $g(\omega)$ are functions of the frequency of vibration ω and are dimensionless.

When M and t are combined with the other factors to make up to coefficients of ω^2 and k^2 in (A2) the results are identified as dynamical mass and dynamical line tension since these coefficients are frequency dependent and carry the proper units. These dynamical quantities are

$$m(\omega) = -\frac{\mu b^2}{4\pi}\frac{1}{c_t^2} M(\omega)\,,$$

$$T(\omega) = \frac{\mu b^2}{4\pi} t(\omega)\,.$$

Thus we may write

$$k^2 T(k) F(\omega^2 - i\epsilon) = -m\omega^2 + k^2 T + \mathrm{Im\ term}\,,$$

which is analogous to a force vibrating string with damping. When the real part of this expression is zero resonance occurs.

Finally, it should be noted that the coefficient of ω^2 in the imaginary term carries units of mass per unit length. For each frequency it has the value of some fraction of the dynamical mass. It then turns out to be extremely convenient for computational reasons to write it as $im/\eta\omega^2$, where $1/\eta$ is the appropriate fraction.

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