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Scattering of Phonons by Elastic Strain Fields and the Thermal Resistance of Dislocations

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A theory of the scattering of phonons by static elastic strain fields is presented. It is found that the Fourier component of the strain field plays a role similar to that of the potential in the external field approximation. All quantities (except the strain field) in the formulas obtained refer to specifically atomic characteristics, allowing in principle the examination of the influence or crystal structure, interatomic potentials, etc., and also scattering between different polarization modes. A Boltzmann equation is found.

The results of the theory are used to estimate the low temperature thermal resistance (in nonconductors) due to dislocations. This is done by finding a relaxation time τ; with some simplifying assumptions one finds for an edge dislocation $\tau^{-1}=A\sigma[\ln(nb^{-1}\sigma^{-\frac{1}{2}})]^2q$. In this equation σ is the density of dislocations, n is the average number in a slip plane, b is the Burgers vector, q is the wave vector of the phonon, A is a constant. This result differs from that obtained previously by Klemens by essentially the presence of the logarithm. This latter factor seems to be essential in explaining the experimental observations of Sproull *et al.* that the thermal resistance due to dislocations in LiF is three orders of magnitude greater than predicted by Klemens. For a screw dislocation τ^{-1} lacks the logarithm term so that the scattering is much smaller than for an edge dislocation.

INTRODUCTION

THE extreme sensitivity of low-temperature thermal conductivity to the presence of crystalline imperfections has led to a revival of interest in thermal conductivity as a means of investigating these imperfections. Klemens[1–4] has carried out an extensive analysis of the many factors involved. In particular he has calculated the magnitude and temperature dependence of the lattice resistivity due to a number of different imperfections. In general Klemens' results account for the experiments in a satisfactory way. For a survey of the experimental situation and further references the reader may consult the review articles of Klemens[3,4] and Berman[5] and also the work of Slack.[6]

However, recent work by Sproull, Moss, and Weinstock[7] has indicated that the thermal resistivity in lithium fluoride is roughly 10^3 as great as predicted by Klemens' theory.[8,9] This observation motivated the present investigation, which is devoted to a general formulation of the problem of phonon scattering by arbitrary static elastic strain fields; application is made to the strain fields of dislocations and an approximate value of the thermal conductivity coefficient $\kappa(T)$ is found.

The present calculation differs from that of Klemens[2] in the following respects. The present theory is similar to the usual results for scattering in an external field in that the Fourier component of the strain field displacement enters into the scattering matrix elements. In Klemens' theory the corresponding quantity is the Fourier component of the dilatation (or rotation). In arriving at this result Klemens made an approximation which is in fact invalid for the logarithmic variation of the strain field of an edge dislocation.[10]

Another difference is that all physical quantities (except of course the strain field, which is computed from elastic theory) of the present calculation refer to atomic quantities, e.g., interatomic force constants. Further one can examine the effect of crystal symmetries on the scattering. On the other hand, Klemens uses a Grüneisen-type anharmonic potential from the beginning. Since the anharmonic forces in most materials are rather poorly known, and because of the difficulty of taking into account the anharmonic coupling of distant atoms, the more rigorous atomic approach has at present only the slight advantage of deferring the necessary approximations to the end of the calculation. However, in the present formulation one may examine the scattering between different modes of polarization. Furthermore, in the theory presented here, all phase information is retained, so that the interference effects of competing scattering processes may be evaluated, although that is not done in this paper. In Appendix 1 the effect of an arbitrary array of identical scatterers is found to be given by essentially a form factor in the appropriate matrix elements. Such interference effects are known to exist at low temperatures.

Finally, if the atomic anharmonicities are related to Grüneisen's γ as described by Klemens,[4] the essential difference between the two theories applied to scattering by edge dislocations (aside from a numerical factor) is

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[1] P. G. Klemens, Proc. Roy. Soc. (London) **A208**, 108 (1951).

[2] P. G. Klemens, Proc. Phys. Soc. (London)**A68**, 1113 (1955).

[3] P. G. Klemens, *Handbuch der Physik* (Spinger-Verlag, Berlin, 1956), second edition, Vol. 14, Part 1, p. 198.

[4] P. G. Klemens, *Solid-State Physics*, edited by F. Seitz and D. Turnbull (McGraw-Hill Book Company, New York, 1958), Vol. 8, p. 1.

[5] R. Berman, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1953), Vol. 2, p. 103.

[6] G. A. Slack, Phys. Rev. **105**, 829, 832 (1957).

[7] Sproull, Moss, and Weinstock, J. Appl. Phys. (to be published).

[8] There also seems to be some question about point defects. See A. Toxen, Phys. Rev. **110**, 585 (1958). This case is not discussed here.

[9] Klemens[4] has recently indicated that the anharmonicities may be greater than previously thought. This accounts for a factor of 15.

[10] See Eq. (30) of reference 2.

the presence of the factor $[\ln(R/r_0)]^2$ in the expression for $\tau(q)^{-1}$ in the present theory.[11] R is the range of the strain field of the disloaction, r_0 is the radius of the dislocation core, and $\tau(q)$ is the relaxation time for a phonon of wave number q. For screw dislocations and other imperfections the two approaches should agree to an order of magnitude. It should be noted that the present approach predicts a vastly greater scattering by edge dislocations in comparison with screw dislocations [roughly the factor $[\ln(R/r_0)]^2$], while Klemens' results show that the scattering is roughly equal (to $\sim 10\%$) for the two cases.

It should be pointed out that the results obtained here will need modification if the temperature is so high that collective modes (due to the imperfections) can be easily excited, leading to appreciable inelastic scattering. The thermal oscillations of dislocations are well known and, for example, seem to be the essential feature in understanding the temperature dependence of the yield strength of iron.[12] However the calculations of Granato[13] for mobile dislocations yield a temperature dependence $\kappa \propto T^5$, while T^2 is roughly what is observed in dielectric solids.

The present paper is concerned with crystalline solids in which the conduction of heat by electrons is negligible, so that it is not necessary to consider electron-phonon interactions. All statements concerning thermal conductivity refer to low temperatures, i.e., temperatures appreciably below the Debye temperature.

I. GENERAL FORMULATION

The potential energy of a crystal can be written as a Taylor series in the relative displacements of the atoms. In the case of scattering by static strain fields the phonon energy is conserved, so that the lowest order term in the expansion that contributes is cubic in the displacements. Higher order terms are neglected as small.

The anharmonic potential is chosen to be

$$V_c=(3!)^{-1}\textstyle\sum_{\mathbf{mn}} B_{\mathbf{mn}}{}^{ijk}(u_{\mathbf{m}}{}^i-u_{\mathbf{n}}{}^i)\times(u_{\mathbf{m}}{}^j-u_{\mathbf{n}}{}^j)(u_{\mathbf{m}}{}^k-u_{\mathbf{n}}{}^k). \quad (1)$$

The summation convention is used for the indices $i,j,k=x,y,z$. The sum $\mathbf{m},\mathbf{n}$ proceeds over all pairs of atoms in the crystal. The coefficients $B_{\mathbf{mn}}{}^{ijk}$ depend on the difference of the position vectors $\mathbf{m}-\mathbf{n}$. This form explicitly emphasizes the dependence of the potential on the relative displacements of the atoms, which fact must be considered when a nonuniform strain field is present. This potential was also used by Pomeranchuk.[14]

The total displacement of an atom from its equilibrium site in the unstrained lattice is the sum of the static strain field displacement $\mathbf{v}_{\mathbf{m}}$ (as computed from elastic theory) and the running-wave phonon displacement $\mathbf{u}_{\mathbf{m}}{}^0$. For the latter it is supposed that there is only one atom per unit cell since only the general features of the problem are of interest.[15] Then we have

$$\mathbf{u}_{\mathbf{m}}{}^0=\textstyle\sum_{\mathbf{q}\lambda}\left(\dfrac{\hbar}{2\rho\Omega\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}}\times[a_{\mathbf{q}\lambda}\exp(i\mathbf{q}\cdot\mathbf{m})+a_{\mathbf{q}\lambda}{}^*\exp(-i\mathbf{q}\cdot\mathbf{m})]\boldsymbol{\varepsilon}_{\mathbf{q}\lambda}. \quad (2)$$

Here ρ is the density, Ω is the volume of the crystal, $\mathbf{q}$ the wave vector of the phonon, λ its polarization index, $\omega_{\mathbf{q}\lambda}$ the frequency, $\boldsymbol{\varepsilon}_{\mathbf{q}\lambda}$ the (unit) polarization vector. $a_{\mathbf{q}\lambda}{}^*(a_{\mathbf{q}\lambda})$ creates (destroys) a phonon of wave vector $\mathbf{q}$ and polarization λ. In the following the polarization index λ will often be omitted, with the understanding that the sum over q (without the vector symbol) includes the sum over λ, etc. The operators $a_{\mathbf{q}\lambda}{}^*$, $a_{\mathbf{q}\lambda}$ are characterized by

$$a_q{}^*\Psi(n_q)=(n_q+1)^{\frac{1}{2}}\Psi(n_q+1), \quad (3a)$$

$$a_q\Psi(n_q)=(n_q)^{\frac{1}{2}}\Psi(n_q-1), \quad (3b)$$

where $\Psi(n_q)$ is the phonon wave function.

Expanding the elastic strain field in Fourier series we have

$$\mathbf{v}_{\mathbf{m}}=\textstyle\sum_{\mathbf{q}}\mathbf{v}_{\mathbf{q}}\exp(i\mathbf{q}\cdot\mathbf{m}), \quad (4)$$

$$\mathbf{v}_{\mathbf{q}}=\Omega^{-1}\int\mathbf{v}_{\mathbf{m}}\exp(-i\mathbf{q}\cdot\mathbf{m})d^3m. \quad (5)$$

Note that the expansion of Eq. (1) involves a sum over four types of terms. The first is a sum over cubic terms in $\mathbf{v}$, i.e., a constant shift in the energy which we ignore. Secondly there are terms linear in a_q and $a_q{}^*$. Such terms cannot conserve energy and give zero contribution. The terms quadratic in the creation and annihilation operators contain the scattering processes of primary interest. Finally, the terms cubic in a_q, $a_q{}^*$ are present in the unstrained crystal and are responsible for ordinary 3-phonon processes (important in establishing thermal equilibrium) and Umklapp processes.[16] Therefore the effective perturbstion due to the presence of the strain field is (omitting 2 terms not conserving energy):

$$V=\frac{\hbar}{4\rho\Omega}\sum_{qq'q''}(\omega_q\omega_{q'})^{-\frac{1}{2}}v_{\mathbf{q}''}{}^i\epsilon_q{}^j\epsilon_{q'}{}^k\times\{a_qa_{q'}{}^*\textstyle\sum_{\mathbf{mn}}B_{\mathbf{mn}}{}^{ijk}F_{\mathbf{q}''}F_{\mathbf{q}}F_{\mathbf{q}'}{}^*+a_q{}^*a_{q'}\textstyle\sum_{\mathbf{mn}}B_{\mathbf{mn}}{}^{ijk}F_{\mathbf{q}''}F_{\mathbf{q}}{}^*F_{\mathbf{q}'}\}, \quad (6)$$

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[11] See Eq. (50) and (51).

[12] A. Cottrell and B. A. Bilby, Proc. Phys. Soc. (London) **A62**, 49 (1949).

[13] A. Granato, Phys. Rev. **111**, 740 (1958).

[14] I. Pomeranchuk, J. Phys. U.S.S.R. 4, 259 (1941); **6**, 237 (1942).

[15] In more complicated crystals (2) will be adequate at low temperatures since only the lowest branch of the phonon spectrum is excited.

[16] R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, Oxford, 1954), Chap. 2.

where

$$F_{\mathbf{q}} \equiv \exp(i\mathbf{q}\cdot\mathbf{m}) - \exp(i\mathbf{q}\cdot\mathbf{n}). \qquad (7)$$

Consider the functions $b_{ijk}(\mathbf{q},\mathbf{q}',\mathbf{q}'')$ defined by

$$b_{ijk}{}^{(1)} \equiv \sum\nolimits_{\mathbf{mn}} B_{\mathbf{mn}}{}^{ijk} F_{\mathbf{q}''} F_{\mathbf{q}} F_{\mathbf{q}'}{}^{*}, \qquad (8a)$$

$$b_{ijk}{}^{(2)} \equiv \sum\nolimits_{\mathbf{mn}} B_{\mathbf{mn}}{}^{ijk} F_{\mathbf{q}''} F_{\mathbf{q}}{}^{*} F_{\mathbf{q}'}. \qquad (8b)$$

Let $\mathbf{a}$ be some arbitrary lattice vector. From the equalities

$$B_{\mathbf{m+a}\ \mathbf{n+a}}{}^{ijk} = B_{\mathbf{mn}}{}^{ijk} \qquad (9)$$

$$\bar{F}_{\mathbf{q}''} \bar{F}_{\mathbf{q}} \bar{F}_{\mathbf{q}'}{}^{*} = \exp[i(\mathbf{q}''+\mathbf{q}-\mathbf{q}')\cdot\mathbf{a}] F_{\mathbf{q}''} F_{\mathbf{q}} F_{\mathbf{q}'}{}^{*}, \qquad (10)$$

where

$$\bar{F}_{\mathbf{q}}(\mathbf{m},\mathbf{n}) \equiv F_{\mathbf{q}}(\mathbf{m}+\mathbf{a},\, \mathbf{n}+\mathbf{a}), \qquad (10')$$

one finds the relations

$$b_{ijk}{}^{(1)} = \exp[i(\mathbf{q}''+\mathbf{q}-\mathbf{q}')\cdot\mathbf{a}] b_{ijk}{}^{(1)}, \qquad (11a)$$

$$b_{ijk}{}^{(2)} = \exp[i(\mathbf{q}''+\mathbf{q}'-\mathbf{q})\cdot\mathbf{a}] b_{ijk}{}^{(2)}. \qquad (11b)$$

Thus it follows that

$$b_{ijk}{}^{(1)}(\mathbf{q},\mathbf{q}',\mathbf{q}'') = \Delta(\mathbf{q}''+\mathbf{q}-\mathbf{q}') b_{ijk}{}^{(1)}(\mathbf{q},\mathbf{q}',\mathbf{q}'').$$

$\Delta(\mathbf{q})$ is defined by[8]

$$\begin{aligned} \Delta(\mathbf{q}) &= 0, \quad \mathbf{q} \neq \mathbf{G} \\ &= 1, \quad \mathbf{q} = \mathbf{G}, \end{aligned} \qquad (12)$$

where $\mathbf{G}$ is a reciprocal lattice vector. The processes with $\mathbf{G} \neq 0$ correspond to the usual Umklapp processes.[16] Since wave vector is already not conserved for $\mathbf{G}=0$ (in contrast to the normal 3-phonon processes) and since $\mathbf{q}$'s large enough for Umklapp-type processes decrease exponentially at low temperatures[16] (and also for most strain fields $\mathbf{V}_{\mathbf{q}}$ decreases with increasing $\mathbf{q}$) we consider only the case $\mathbf{G}=0$ for the present, remembering that one can always include the terms $\mathbf{G}\neq 0$ if necessary, by inserting the appropriate factors in $\mathrm{b}_{ijk}(\mathbf{q},\mathbf{q}',\mathbf{q}'')$ and summing over $\mathbf{G}$. Summing over $\mathbf{q}''$ Eq. (6) becomes

$$\begin{aligned} V = \frac{\hbar}{4\rho\Omega} \sum\nolimits_{qq'} (\omega_q \omega_{q'})^{-\frac{1}{2}} \epsilon_q{}^{j} \epsilon_{q'}{}^{k} \\ \times \{ a_q a_{q'}{}^{*} v_{\mathbf{q}'-\mathbf{q}}{}^{i} b_{ijk}{}^{(1)}(\mathbf{q},\mathbf{q}',\mathbf{q}'-\mathbf{q}) \\ + a_q{}^{*} a_{q'} v_{\mathbf{q}-\mathbf{q}'}{}^{i} b_{ijk}{}^{(2)}(\mathbf{q},\, \mathbf{q}',\, \mathbf{q}-\mathbf{q}') \}. \end{aligned} \qquad (13)$$

We observe that

$$b_{ijk}{}^{(2)}(\mathbf{q},\mathbf{q}',\, \mathbf{q}-\mathbf{q}') = b_{ijk}{}^{(1)*}(\mathbf{q},\, \mathbf{q}',\, \mathbf{q}'-\mathbf{q}), \qquad (14)$$

$$\mathbf{v}_{\mathbf{q}} = \mathbf{v}_{-\mathbf{q}}{}^{*}. \qquad (15)$$

It is then found that the perturbation takes the form

$$\begin{aligned} V = \frac{\hbar}{4\rho\Omega} \sum\nolimits_{qq'} (\omega_q \omega_{q'})^{-\frac{1}{2}} \epsilon_q{}^{j} \epsilon_{q'}{}^{k} v_{\mathbf{q}'-\mathbf{q}}{}^{i} \\ \times b_{ijk}{}^{(1)}(\mathbf{q},\, \mathbf{q}',\, \mathbf{q}'-\mathbf{q}) a_q a_{q'}{}^{*} + \mathrm{H.c.} \end{aligned} \qquad (16)$$

This equation has a very simple meaning; for example the first term in Eq. (16) may be read as follows: a phonon of wave number $\mathbf{q}$ interacts (a_q) with the Fourier component $v_{\mathbf{q}'-\mathbf{q}}$ of the strain field displacement and is scattered ($a_{q'}{}^{*}$) to a state with wave vector $\mathbf{q}'$, giving up an amount of wave vector $\mathbf{q}'-\mathbf{q}$ to the strain field.

This physical result shows that, once having chosen running wave phonons, the most natural way to represent the transfer of wave vector to the lattice is indeed to expand $\mathbf{v}_{\mathbf{m}}$ in a Fourier series, since this gives directly the "conservation" laws represented by Eq. (12).

The matrix elements corresponding to the change in the number of phonons due to scattering by the strain field are, using Eq. (3),

$$\mathfrak{M}_{q'\to q} = \frac{\hbar}{4\rho\Omega} C_{qq'} \left(\frac{(n_q+1) n_{q'}}{\omega_q \omega_{q'}} \right)^{\frac{1}{2}}, \qquad (17a)$$

$$\mathfrak{M}_{q\to q'} = \frac{\hbar}{4\rho\Omega} C_{qq'}{}^{*} \left(\frac{n_q (n_{q'}+1)}{\omega_q \omega_{q'}} \right)^{\frac{1}{2}}, \qquad (17b)$$

$$C_{qq'} = \sum\nolimits_{ijk} v_{\mathbf{q}'-\mathbf{q}}{}^{i} \epsilon_q{}^{j} \epsilon_{q'}{}^{k} b_{ijk}{}^{(1)}(\mathbf{q},\, \mathbf{q}',\, \mathbf{q}'-\mathbf{q}). \qquad (18)$$

One can now write down the rate of change of the number of phonons in state $\mathbf{q}$ due to the scattering by the strain field. For the moment other scattering processes are ignored. It should be noted that the equations are valid even when there are different types of imperfections present in the crystal, since the displacements are additive. Using the standard formula of time-dependent perturbation theory[16] it is found that

$$\begin{aligned} \left(\frac{\partial n_{\mathbf{q}\lambda}}{\partial t} \right)_{\mathrm{collision}} = \frac{1}{64\pi^2 \rho^2 \Omega} \int d^3 q' \frac{\delta(\omega_q - \omega_{q'})}{\omega_q \omega_{q'}} \\ \times |C_{qq'}|^2 (n_{q'} - n_q). \end{aligned} \qquad (19)$$

Equation (19) is easily converted to a Boltzmann equation.[1–4,16] The problem is then reduced to that of the solution of an integral equation of n_q. One can also easily write Eq. (19) in the form of a surface integral in q' space owing to the delta function.

II. SCATTERING BY DISLOCATIONS

Using the results of the preceding sections we investigate the scattering of phonons by dislocations, and derive an approximate expression for the thermal conductivity. For screw and edge dislocations the strain field displacements in elastically isotropic crystals are given by[17]

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[17] W. T. Read, Jr., *Dislocation in Crystals* (McGraw-Hill Book Company, New York, 1953), Chap. 8.

edge dislocation:

$$v_x = \frac{b}{2\pi}\left(\theta + \frac{\sin 2\theta}{4(1-\nu)}\right), \tag{20}$$

$$v_y = -\frac{b}{2\pi}\left(\frac{(1-2\nu)}{2(1-\nu)}\ln(r/r_0) + \frac{\cos 2\theta}{4(1-\nu)}\right), \tag{21}$$

$$v_z = 0, \tag{22}$$

screw dislocation:

$$v_z = b\theta/2\pi, \tag{23}$$

$$v_x = v_y = 0. \tag{24}$$

In these expressions r,θ are plane polar coordinates, b is the Burgers vector, ν is Poisson's ration and r_0 is the radius of the core of the dislocation ($\approx b$).

The required Fourier components are given by

$$(\ln(r/r_0))_q = (2\pi/x^2)\{xJ_1(x)\ln(R/r_0) + J_0(x) - 1\}\Delta(q_z), \tag{25}$$

$$(\cos 2\theta)_q = (\cos\phi/x^2)\{xJ_1(x) + 2[J_0(1)-1]\}\Delta(q_z), \tag{26}$$

$$(\sin 2\theta)_q = (\sin\phi/x^2)\{xJ_1(x) + 2[J_0(x)-1]\}\Delta(q_z), \tag{27}$$

$$\theta_q \cong (2\pi^2/x^2)\{xJ_1(x)\}\Delta(q_z). \tag{28}$$

$\pi+\phi$ is the angle made by $\mathbf{q}$ with the x axis. The x and y axis are perpendicular to the dislocation line, The x axis lies in the direction of the Burgers vector; the origin is chosen in the center of the dislocation. J_0 and J_1 are the zeroth and first order Bessel functions; $x = qR$, $R = \Omega^{\frac{1}{3}}$. In Eq. (25) note the presence of the factor $\ln(R/r_0)$. When applying the theory to a real crystal, one must take for R a distance representing the range of the strain field; for example R will be the order of the diameter of a single slip band. Thus in most cases of practical interest Eq. (25) is very much larger than Eqs. (26), (27), or (28). Equation (25) arises from the y component of the displacement in the strain field of an edge dislocation. Observing that the coefficients in Eq. (20) to (23) are all roughly equal, one concludes that: (1) edge dislocations are much better scatterers than screw dislocations; (2) the scattering by an edge dislocation proceeds almost entirely by the y-component of the displacement. Both results are plausible from consideration of the nature of the distortion of a crystal due to the presence of edge or screw dislocations. (Actually conclusion (1) is reinforced by consideration of the factor $C_{qq'}$ for the two cases.) It seems unlikely that a more detailed model of the atomic arrangement in the core of the dislocation would change these conclusions, since most of the scattering occurs at long distances from the core, where the elastic theory results are quite good. We ignore completely the scattering of the core.[2]

In order to make further progress one must make an estimate of the term $C_{qq'}$. This is difficult primarily because the anharmonic forces in crystals are rather poorly known. (For example, a measure of the anharmonicity such as Grüneisen's γ is not necessarily an accurate reflection of the coefficients $B_{\mathrm{mn}}{}^{ijk}$, except in an average sort of way.)

In view of this situation we adopt the simplest possible model consistent with reality: a central force, nearest neighbor interactions only. For such forces

$$B_{ijk} = \frac{\partial^3\phi(r)}{\partial r_i \partial r_j \partial r_k}, \tag{29}$$

where $\phi(r)$ is the interatomic potential and the right-hand side of Eq. (29) is evaluated at the equilibrium position. Then it is found that[18]

$$B_{ijk} = (g' - 3f/a)a_i a_j a_k/a^3 + (f/a^2)(\delta_{ij}a_k + \delta_{ik}a_j + \delta_{jk}a_i), \tag{30}$$

where $g' = \phi'''(a)$, $f = \phi''(a)$; a is the interatomic spacing, a_i, etc. being the appropriate Cartesian components. $g'a/f$ is small[18] so that only the first term is retained: $g = g' - 3f/a \approx g'$,

$$B_{ijk} \cong g a_i a_j a_k/a^3. \tag{31}$$

Comparing Eqs. (31), (A-5), and (18) one finds

$$C_{\mathbf{q}\lambda,\,\mathbf{q}'\lambda'} = (Nig/2a^3)\sum(\mathbf{v}_{\mathbf{q}'-\mathbf{q}}\cdot\mathbf{a})(\boldsymbol{\varepsilon}_{\mathbf{q}\lambda}\cdot\mathbf{a})(\boldsymbol{\varepsilon}_{\mathbf{q}'\lambda'}\cdot\mathbf{a}) \times(\mathbf{q}\cdot\mathbf{a})(\mathbf{q}'\cdot\mathbf{a})(\mathbf{q}'-\mathbf{q})\cdot\mathbf{a}. \tag{32}$$

where the sum is taken over nearest neighbors; N is the number of atoms in the crystal. $\mathbf{a}$ represents the position vectors of the neighbor atoms with respect to the chosen atom.

In order to evaluate Eq. (32) for an edge dislocation a further simplification is made; it is supposed that the lattice is simple cubic. It is then seen that the predominance of Eq. (25) greatly simplifies the evaluation of Eq. (32). Further, take the Z axis of the edge dislocation to lie along a cube edge. For the time being also suppose that the phonons are incident perpendicularly in the dislocation. Note from the calculation of the Fourier components [Eqs. (20)–(23)] that the component of wave vector along the dislocation (q_z) is conserved. From this one can conclude that there is no scattering of phonons incident in the z direction along the dislocation line between *the same polarization modes*. However scattering between *different* modes may be allowed. For instance, energy and q_z are conserved as in the transition (long. → transverse). [In the Debye approximation the perpendicular component of the scattered (transverse) phonon is $q_\perp' = ((C_l/C_t)^2 - 1)^{\frac{1}{2}} q_z$]. Similarly a transverse phonon incident along the z direction cannot be scattered by the dislocation, except in Umklapp type processes [see Eqs. (25)–(28)].

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[18] G. Leibfried, *Handbuch der Physik* (Springer-Verlag, Berlin, 1955), second edition, Vol. 7, Part I, p. 299.

Maximum scattering is expected for phonons incident perpendicular to the dislocation, since all possible scattering processes can occur and also because of the angular dependence of the geometrical factor $C_{qq'}$.

The rest of the calculation is made assuming the phonons to be incident perpendicular to the dislocation, both to simplify the calculation and to make comparison with Klemens results[2–4] more direct. (Klemens makes the same assumption.)

Equation (32) is now evaluated for an edge dislocation, under the stated assumptions. As discussed previously only the large term (Eq. (25)) is considered, keeping only the part containing $\ln(R/r_0)$. Thus

$$\begin{aligned}\mathbf{v}_{\mathbf{q}'-\mathbf{q}}&=\alpha b\ln(R/r_0)[J_1(x)/x]\mathbf{j},\\ \alpha&=(1-2\nu)/2(1-\nu),\end{aligned}\tag{33}$$

with $x=R|\mathbf{q}'-\mathbf{q}|$; $\mathbf{j}$ is a unit vector in the y direction. $\theta+\pi$ is defined as that angle which $\mathbf{q}$ makes with the positive y axis, similarly for θ'. The polarization vectors are chosen to be $\boldsymbol{\varepsilon}_{\mathbf{q}l}=\mathbf{q}/|\mathbf{q}|$ for longitudinal phonons and $\boldsymbol{\varepsilon}_{\mathbf{q}t}=\boldsymbol{\xi}\ \ \mathbf{q}/|\mathbf{q}|$, where $\boldsymbol{\xi}$ is some unit vector perpendicular to $\mathbf{q}$. $\boldsymbol{\varepsilon}_{\mathbf{q}t}$, in general, lies out of the plane of x and y. The projection in the y direction contains a factor $\sin\theta\sin\varphi$, where φ is some azimuthal angle about $\mathbf{q}$. When $C_{qq'}$ is squared there appears a factor of $\sin^2\varphi$ for each transverse phonon under consideration. Averaging over φ, one can uplace each $\sin^2\varphi$ by a factor of $\frac{1}{2}$. Table I for $|C_{\mathbf{q}\lambda,\mathbf{q}'\lambda'}|^2$ is found in this way.

$$A(\mathbf{q},\mathbf{q}')=(Nga^3q^3v_{\mathbf{q}'-\mathbf{q}}{}^{(y)})^2.\tag{34}$$

η, ζ are equal to q'/q for their respective cases. q' and q are related by $\omega_{\mathbf{q}\lambda}=\omega_{\mathbf{q}'\lambda'}$ in all calculations. Thus for instance in the Debye approximation $\eta=\zeta^{-1}=c_l/c_t$.

We now assume the validity of the Debye approximation, and also put $c_l=c_t=c=$ velocity of sound, so that $\eta=\zeta=1$. In view of the approximations made in evaluating $C_{qq'}$ there is nothing to be gained by keeping the more general expressions. In order to calculate the thermal current rigorously one should first solve the Boltzmann integral equation [resulting from Eq. (19)] for n_q. We shall only do this assuming a relaxation time approximation. The thermal conductivity then follows from knowledge of[1–4] $\tau(\mathbf{q})$. This will also allow a more direct comparison with the results of Klemens.[2–4] It must be pointed out that the following calculation assumes the scattering by dislocations to be the dominant scattering mechanism, so that further considerations are necessary when there are competing mechanisms. The observations of Sproull *et al.*[7] of the great decrease of thermal conductivity due to the introduction of dislocations into LiF indicate that this approximation may be quite realistic. It is assumed that other processes (especially ordinary 3-phonon processes which in themselves cause no resistivity)[16] act only to maintain the steady state conditions.[4]

TABLE I. Dependence of the structure factor $|C_{\mathbf{q}\lambda,\mathbf{q}'\lambda'}|^2$ on the polarization indices λ,λ'.

λ	λ'	$\lvert C_{\mathbf{q}\lambda,\mathbf{q}'\lambda'}\rvert^2$
l	l	$A(\mathbf{q},\mathbf{q}')\cos^4\theta\cos^4\theta'(\cos\theta-\cos\theta')^2$
l	t	$\frac{1}{2}A(\mathbf{q},\mathbf{q}')\eta^2\cos^4\theta\sin^2\theta'\cos^2\theta'(\cos\theta-\eta\cos\theta')^2$
t	l	$\frac{1}{2}A(\mathbf{q},\mathbf{q}')\zeta^2\sin^2\theta\cos^2\theta\cos^4\theta'(\cos\theta-\zeta\cos\theta')^2$
t	t	$\frac{1}{4}A(\mathbf{q},\mathbf{q}')\sin^2\theta\cos^2\theta\sin^2\theta'\cos^2\theta'(\cos\theta-\cos\theta')^2$

Following Klemens,[4] the deviation from equilibrium of the phonon distribution in the presence of a heat current is of the form

$$n_q=-\frac{\boldsymbol{\lambda}\cdot\mathbf{q}}{kT}\frac{\exp(\hbar\omega/kT)}{[\exp(\hbar\omega/kT)-1]^2},\tag{35}$$

where $\boldsymbol{\lambda}$ is a vector in the direction of the heat current and k is Boltzmann's constant. We suppose $\boldsymbol{\lambda}$ to be essentially independent of polarization; if it were not there would be some process to erase the difference in anisotropy.

From Eq. (19) one can write the rate of change of the number of phonons of wave number $\mathbf{q}$ for each polarization λ in detail. Then

$$\dot{n}_{\mathbf{q}}=\dot{n}_{\mathbf{q}l}+2\dot{n}_{\mathbf{q}t};\tag{36}$$

$$\tau(\mathbf{q})^{-1}=-\dot{n}_{\mathbf{q}}/n_{\mathbf{q}}.\tag{37}$$

For economy of writing it is now stated that the processes of Table I $(\lambda,\lambda')=(l,t)$, (t,t) are negligible. This is found by numerical integration of integrals similar to (40). Then, noting that the 2 associated with the transverse modes cancels the $\frac{1}{2}$ arising from the average, transforming Eq. (19) yields

$$\tau(\mathbf{q})^{-1}=Dq^3\cos\theta I(2qR,\theta);\tag{38}$$

$$D=[gb\alpha\ln(R/r_0)]^2/(96\pi\rho^2c^3),\tag{39}$$

$$I(x,\theta)=\int_0^{2\pi}d\theta' J_1{}^2\left[x\sin\left(\frac{\theta'-\theta}{2}\right)\right]\times\cos^4\theta'\sin^2\left(\frac{\theta'+\theta}{2}\right)(\cos\theta-\cos\theta').\tag{40}$$

In deriving Eq. (38) Eqs. (33)–(37) have been used, and also the relations

$$|\mathbf{q}'-\mathbf{q}|=2q\sin\tfrac{1}{2}(\theta'-\theta),\tag{41}$$

$$\cos\theta-\cos\theta'=2\sin\tfrac{1}{2}(\theta'+\theta)\sin\tfrac{1}{2}(\theta'-\theta),\tag{42}$$

$$\Omega=Na^3.\tag{43}$$

Equations (38)–(40) represent the special case in which the phonon current parameter $\boldsymbol{\lambda}$ is in the y direction. Later a factor of the order of unity will be introduced to account for a random orientation of the dislocation with respect to $\boldsymbol{\lambda}$. Note that with regard to the phonon current, the dependence of the integrand of $I(X,\theta)$ on $\boldsymbol{\lambda}$ is contained in the factor $(\cos\theta-\cos\theta')$, which removes the contribution for $\theta\approx\theta'$. This factor is largest for backwards scattering of the phonons. The factor $\cos^4\theta'$ enhances the peaking about the backwards direction.

The integral (40) was evaluated numerically, for $\theta = 0°$, $30°$ and $60°$. It was found that $I(x,\theta)$ does not vary rapidly with θ. A good average value of $I(x,\theta)$ is $I(x) = I(x,0)$. In the region of interest $x > 2$ (i.e., $q > R^{-1}$; the minimum q that corresponds to a phonon is $\approx R^{-1}$) a good approximation is $I(x) = 2/x^2$. This variation really arises from the Bessel function, which for large x gives $x^{-1}\cos^2[x \sin\frac{1}{2}(\theta'-\theta) - 3\pi/4]$. The oscillations (as well as the angular dependence of the rest of the integrand) cut this down to approximately x^{-2}. The exact $I(x)$ periodically decreases to zero; however this is due to the idealized model employed. The collision frequency τ^{-1} is never equal to zero. Other processes, the fact that dislocations will never be perfectly straight, etc. all combine to smooth out the curve near its minima. Thus we take

$$I(x) = 2/x^2. \tag{44}$$

Then Eq. (38) becomes

$$\tau(\mathbf{q})^{-1} = Gq|\cos\theta|; \tag{45}$$

$$G \equiv [gb\alpha \ln(R/r_0)]^2/(\rho^2 R^2 48\pi c^3). \tag{46}$$

It is worthwhile to consider the meaning of the quantities entering into Eq. (46). First consider the logarithmic dependence on the size of the domain.[19] (We set the core radius equal to b.) This term arises from the Fourier transform of the strain field displacement. Next note the factor of R^{-2} in the denominator. This is just the area of the cross section perpendicular to the dislocation.[20] That is, the frequency τ^{-1} of scattering decreases as the area increases. This is understandable from the following considerations.

Equation (46) was calculated with the assumption that somewhere in the volume Ω there was a phonon incident perpendicular to the dislocation.[21] Thus the z direction will not enter.

R^{-2} is just proportional to the probability of finding a (localized) wave packet,[22] in some given region. If the scattering field were localized, the probability of scattering would thus vary like R^{-2}. The factor $[\ln(R/b)]^2$ counterbalancing the R^{-2} just reflects the long range nature of the strain field. It is evident from the translational invariance of the Hamiltonian in the z direction that the argument also holds for dislocations not incident perpendicular to the dislocation.

The appearance of R^{-2} is made even more perspicuous by considering the modification of Eq. (46) when there are n parallel dislocations in the crystal. This is made a reasonable picture of reality: for instance, consider a series of concentric loops from a Frank-Read source; we have seen that the screw components of the loops do not scatter much, so that effectively the scattering is done by a line of roughly parallel edge dislocations. Further suppose that n is small enough so that the effective phonon wave length is less than the inter-dislocation spacing.[23] Then the scattering probability is just proportional to n. (Cf. the previous discussion.) R is given by $nR^{-2} = \sigma =$ dislocation density; we have[24]:

$$G(n) = \sigma[gb\alpha \ln(R/b)]^2/(48\pi\rho^2 c^3). \tag{47}$$

Now it is necessary to make some estimate of the anharmonicity term g. In order to compare expression Eq. (47) directly with that of Klemens[2] it is necessary to relate g to Grüneisen's γ, using the results of Klemens' analysis.[4] Examining Eq. (35) and transforming Klemens' expression (5.20) in reference 4 to our notation (putting the lattice constant $a = b$), we find

$$gb^3 \cong 24M\gamma c^2/N, \tag{48}$$

or

$$g \cong 24\rho\gamma c^2. \tag{49}$$

In finding this approximate[25] result each angular factor in (32) has been replaced by $1/\sqrt{2}$; the sum over nearest neighbors is replaced by a typical number, 8. [If this should overestimate Eq. (32), as is possible, then the anharmonicity g will in fact be underestimated; Eq. (48) is a rough lower bound on g.] Further, in Eq. (47), replace the factors $(2\alpha)^2 = (1-2\nu)^2/(1-\nu)^2$ by the typical value $\frac{1}{2}$. For the present argument we replace $\cos\theta$ by $1/\sqrt{2}$. Then

$$\tau(\mathbf{q})^{-1} \cong \tfrac{1}{3}\sigma b^2\gamma^2 c[\ln(R/b)]^2 q. \tag{50}$$

It must be emphasized that the present crude arguments are necessary only to compare our formula Eq. (47) more directly with that of Klemens.[2] Formula (47) already includes the effect of the angular factors, etc. which were averaged over in deriving Eq. (49). Modifying Eq. 5.25 of reference (4) to describe an edge dislocation (a factor of about 1.1) and multiplying by a factor of ≈ 15 as indicated in reference 9, Klemens' theory gives the result[26]

$$\tau_K(q)^{-1} \cong \sigma b^2\gamma^2 cq. \tag{51}$$

The ratio β of (50) to (51) is

$$\beta = \tfrac{1}{3}[\ln(R/b)]^2. \tag{52}$$

This equation says that the present theory predicts the

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[19] Note that the elastic strain energy in a crystal due to a dislocation is proportional to $\ln(R/r_0)$.

[20] Recall the integration over q_z in obtaining (38).

[21] $p_z \approx$ const, $\Delta z \approx R$.

[22] See reference 16 for a justification of substituting wave packets for plane wave phonons.

[23] See Appendix 1.

[24] This R is essentially a geometrical factor; the R in the logarithm represents the range of the strain field and must be estimated separately [see Eqs. (53) and (54)].

[25] It should be evident that (59) is only valid as to order of magnitude.

[26] Both (50) and (51) have assumed the temperature gradient to be perpendicular to the dislocation line. Klemens[1] has shown the effect of randomness in orientation may be accounted for by a factor of about $\frac{1}{2}$ in (51). It is easily seen that essentially the same factor is correct in (47).

thermal resistivity of edge dislocations to be greater than that of Klemens by the factor β.

In estimating R two cases must be considered. However, due to the slow variation of the logarithm there is little numerical difference between the two cases. For a random array of dislocations

$$R \cong \sigma^{-\frac{1}{2}}, \tag{53}$$

σ being the dislocation density. If n dislocations are lying in the same slip plane, the appropriate choice is[27]

$$R \cong n\sigma^{-\frac{1}{2}}. \tag{54}$$

Since $\sigma^{-\frac{1}{2}} \ll b$ in general, and since n is typically 30 to 1000, the order of magnitude of β is usually given by Eq. (53). [However, systematic experiments might be able to check Eq. (54).]

The factor Eq. (52) is sufficient to explain the observations of Sproull *et al.*[7] mentioned in the introduction. In these experiments $\sigma \approx 10^7$ cm^{-2}; for LiF $b \cong 4$Å. For random dislocations this gives $\beta = 28$. If there are $n = 50$ (500) dislocations in an average slip plane then the resistivity is doubled (quadrupled): $\beta = 60$ (120). Recalling that the experiments were compared to Eq. (51) *before* it had been multiplied by 15, we see that indeed the factor of 10^3 is accounted for, if it is assumed that the dislocations lie in slip planes in groups of about 50 or more. This number is reasonable from the results of the careful investigation of Gilman and Johnston.[28]

For screw dislocations it is evident that the present theory gives roughly the same resistivity as Klemens formula.[2] This follows from comparison of Eq. (25) and Eq. (28) and the final result, Eq. (50). The angular factors in $C_{qq'}$ will probably make the numerical coefficient slightly different.

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APPENDIX 1. EFFECT OF A VOLUME DISTRIBUTION OF SCATTERERS

The displacement of the point $\mathbf{m}$ is the sum of the displacements due to the various imperfections at positions $\mathbf{n}_\alpha$:

$$\mathbf{v}'(\mathbf{m}) = \sum\nolimits_{\mathbf{n}_\alpha} \mathbf{v}_\alpha(\mathbf{m} - \mathbf{n}_\alpha). \tag{A-1}$$

The index α in $\mathbf{v}_\alpha$ indicates that $\mathbf{v}_\alpha(\mathbf{m}-\mathbf{n}_\alpha)$ may depend on the orientation of α. Expanding (20) in Fourier series:

$$\sum\nolimits_{\mathbf{q}} \mathbf{v}_{\mathbf{q}}' \exp(i\mathbf{q}\cdot\mathbf{m}) = \sum\nolimits_{\mathbf{q}} \{ \sum\nolimits_{\mathbf{n}_\alpha} \mathbf{v}_\alpha(\mathbf{q}) \exp(i\mathbf{q}\cdot\mathbf{n}_\alpha) \} \exp(i\mathbf{q}\cdot\mathbf{m}). \tag{A-2}$$

In the latter expression one must be careful in defining $\mathbf{v}(\mathbf{m})$ as a periodic function of $R = (\Omega)^{\frac{1}{3}}$, since a change of variable has occurred in evaluating the right-hand side. On the other hand, if the strain field is short-range (e.g., as for point defects but *not* for dislocations) then this restriction may be neglected. For the important special cases of isotropic strain fields, and parallel straight dislocations with Burgers' vectors in the same direction (21) reduces to

$$\mathbf{v}_{\mathbf{q}}' = \mathbf{v}_{\mathbf{q}} \sum\nolimits_{\mathbf{n}_\alpha} \exp(i\mathbf{q}\cdot\mathbf{n}_\alpha), \tag{A-2$'$}$$

so that (19) is changed by the insertion of a factor

$$h(\mathbf{q}' - \mathbf{q}) = \left| \sum\nolimits_{\mathbf{n}_\alpha} \exp[i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{n}_\alpha] \right|^2 \tag{A-3}$$

under the integral sign in (19).

In particular, for an array of straight parallel equidistant dislocations lying in the same slip plane (a crude model of the distribution of dislocations in many crystals) then one has a diffraction grating for phonons, which will be effective for phonons of wavelength comparable with the distance between dislocations. If the density of dislocations in a substance is such that the average spacing between dislocations in a slip plane is less than the effective wavelength of the phonons involved in heat transport, then one can expect such effects to be important. Thus the longest wavelength phonons see essentially the total Burgers vector of the array. The importance of such effects must be evaluated separately for each experimental situation.

APPENDIX 2. FORM OF THE COEFFICEINTS $b_{ijk}^{(1)}(q,q',q'-q)$

Using the definition (7) one finds that (8a) can be written as

$$b_{ijk}^{(1)}(\mathbf{q},\mathbf{q}',\mathbf{q}'-\mathbf{q}) = 2i \sum\nolimits_{\mathbf{mn}} B_{\mathbf{mn}}^{ijk} \{ \sin[\mathbf{q}'\cdot(\mathbf{m}-\mathbf{n})] - \sin[\mathbf{q}\cdot(\mathbf{m}-\mathbf{n})] - \sin[(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{m}-\mathbf{n})] \}. \tag{A-4}$$

$B_{\mathbf{mn}}^{ijk}$ will be large only for $|\mathbf{m}-\mathbf{n}| \sim a$, where a is the lattice constant. For the temperatures of interest $qa \ll 1$ so that it is a very good approximation to expand the sines. The terms linear in q cancel; collecting terms in the next higher order gives

$$b_{ijk}^{(1)}(\mathbf{q},\mathbf{q}',\mathbf{q}'-\mathbf{q}) = i \sum\nolimits_{\mathbf{mn}} B_{\mathbf{mn}}^{ijk} \mathbf{q}\cdot(\mathbf{m}-\mathbf{n}) \times \mathbf{q}'\cdot(\mathbf{m}-\mathbf{n})(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{m}-\mathbf{n}). \tag{A-5}$$

This is accurate to terms of order $(qa)^5$.

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[27] *Note added in proof.*—A better value of R is probably $R \cong (n_p n/\sigma)^{\frac{1}{2}}$, where n_p is the number of slip planes per cm.

[28] J. J. Gilman and W. C. Johnston, in *Dislocations and Mechanical Properties of Crystals* (John Wiley and Sons, Inc., New York, 1957), p. 116.