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THE EFFECT OF DISLOCATIONS ON THERMAL CONDUCTIVITY

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Abstract: Phonon scattering by the strain fields of deformed crystals is formulated in terms of the third order elastic constants. The thermal resistivity due to dislocations is calculated. Theory and experiment are in accord for Cu, Al, Ge and Si but not for LiF.

1. Aims: To formulate the problem of phonon scattering by the static strain fields of crystal defects in terms of the third order elastic (TOE) constants, and to calculate the thermal resistivity due to dislocations.

2. Formulation: A classical formulation of the equations of motion of a statically deformed continuum was presented by Kogure and Hikii. The system may be quantized to yield the Hamiltonian

\[ H = \sum_{k} \hbar \omega_{k} \left( a_{k}^{\dagger} a_{k} + \frac{1}{2} \right) + \frac{1}{V} \sum_{k} \left( h_{k k'}^{\alpha} a_{k}^{\dagger} a_{k'}^{\dagger} + h_{k k'}^{*} a_{k} a_{k'} \right) \]

where \( V \) is the volume of the deformed body and \( \alpha \equiv (j, k) \) = (polarization, wavevector). The operators \( a_{k} \) satisfy the usual commutation rules and

\[ a_{k}^{\dagger} = (\hbar/2\pi) \tilde{e}_{\alpha}(\kappa) e_{\alpha}(\kappa') + (k_{\kappa} k_{\kappa'})/\rho_{0} \omega_{\kappa} e_{\alpha}(\kappa) e_{\alpha}(\kappa') \tilde{N}_{\alpha\beta\gamma\delta} + C_{\alpha\beta\gamma\delta} \tilde{N}_{\xi\eta} \tilde{N}_{\xi\eta} \]

(1)

where repeated suffixes are summed. The \( e_{\alpha}(\kappa) \) are polarization vectors and \( \rho_{0} \) is the density of the undeformed crystal. The \( n_{ij}(\kappa - \kappa') \) and \( N_{ijkl} = -C_{ijklnpp} + C_{ijkp} n_{lp} + C_{ijkl} n_{kp} + C_{ijkl} n_{jp} + C_{ijkl} n_{lp}, \) respectively. The \( C_{ij} \) are the usual elastic moduli. Due to cancellation of cross-terms when (1) is squared we have, to a good approximation,

\[ |h_{kk'}^{\alpha}|^2 = \left( \hbar^2/16\rho_{0}^2 \omega^2 \right) k_{\alpha} k_{\alpha} e_{\alpha}^2(\kappa) e_{\alpha}^2(\kappa') \left[ \tilde{N}_{\alpha\beta\gamma\delta} + C_{\alpha\beta\gamma\delta} \tilde{N}_{\xi\eta} \tilde{N}_{\xi\eta} \right] + n_{11}^2 + n_{22}^2 + n_{33}^2 \leq 2 \rho_{0}^2 \omega^2 |n_{11}|^2 \leq 2 e_{\alpha}^2(\kappa) e_{\alpha}^2(\kappa') \]

(2)

The last term is negligibly small in practice and will be dropped. If we follow Klemens and set \[ e_{\alpha}(\kappa) = 1/\sqrt{3} = k_{\kappa}/k \] eqn. (2) becomes

\[ |h_{kk'}^{\alpha}|^2 = \left( \hbar^2 k_{\alpha} k_{\alpha}'^2/1296\rho_{0}^2 \omega^2 P \right) \]

where, for a cubic crystal

\[ P = A(\tilde{n}_{11}^2 + \tilde{n}_{22}^2 + \tilde{n}_{33}^2) + B(\tilde{n}_{12}^2 + \tilde{n}_{23}^2 + \tilde{n}_{31}^2) \]

\[ + C(\tilde{n}_{11}^* \tilde{n}_{22} + \tilde{n}_{22}^* \tilde{n}_{33} + \tilde{n}_{33}^* \tilde{n}_{11} + \text{complex conjugate}) \]

(3)
\( A = (c_{11} + 3c_{11})^2 + 4(c_{112} + c_{112})^2 + 2(c_{123} - c_{12})^2 + 2(c_{112} - c_{11})^2 \\
+ 8(c_{166} + c_{444})^2 + 4(c_{144} - c_{444})^2 \)

\( B = 8(2c_{166} + c_{11} + 2c_{444})^2 + 16(c_{144} + c_{12})^2 + 32(c_{65} + c_{444})^2 \)

\( C = (c_{111} + 3c_{111})(c_{112} - c_{111}) + 4(c_{112} + c_{12})^2 + 2(c_{123} - c_{12})^2(c_{112} + c_{12}) \\
+ 8(c_{166} + c_{444})^2 + 4(c_{144} + c_{444})(c_{144} - c_{444}) \)

The C's are the elastic constants in Voigt notation.

3. Dislocation Thermal Resistivity: In cases where the frequencies \( \omega_j = \nu_j k \) are not degenerate and the dislocations not all parallel it is necessary to use the variational formula:

\[ \omega_{\text{dis}} = \left( \frac{\nu}{2k_B T^2} \right) \sum_{\kappa \kappa'} \left( \phi_{\kappa} - \phi_{\kappa'} \right)^2 P_{\kappa \kappa'} / \left[ \sum_{\kappa \kappa'} \phi_{\kappa} \phi_{\kappa'} \frac{d\phi_{\kappa}}{dT} \right]^2, \]

\[ P_{\kappa \kappa'} = \sum_d \left( \frac{8\pi}{h^2 T^2} \right) \left| h_{\kappa \kappa'}^{d} \right|^2 \frac{n_0 (1 + n_0)}{3} \delta(\omega_{\kappa} - \omega_{\kappa'}), \]

where \( k_B \) is Boltzmann's constant. The sum in (5) is over all dislocations in the crystal, which are assumed straight but of random orientation and arbitrary character. When the resistivity tensor is isotropic, we expect the standard trial function \( \phi_\kappa = k_\nu VT \) to furnish a good approximation, particularly since it removes the singularity from the forward scattering amplitude for each dislocation. It yields in (4):

\[ \omega_{\text{dis}} \lesssim \frac{\pi^2 h^2 b^2}{2Z p^2 k_B T^2} \frac{I_5}{I_4} \frac{S_4 S_5}{S_3} \frac{L e + L s}{V} \frac{L f_s + L s_f_s}{V} \sum_{j=1}^3 \frac{1}{S_n}, \]

where \( L e, L s \) are the total lengths of edge and screw dislocation, respectively, \( f_s = B/4, f_e = (1-\nu)^{-2} \left[ A(\nu^2 - \nu + 3/8) + B/16 + 2C(\nu^2 - \nu/2 + 1/16) \right] \)
in a crystal of (average) Poisson's ratio \( \nu \), and \( I_n = \int_0^\infty x e^{x}(e^x - 1)^{-2} dx = 26.0, 124 \) for \( n = 4,5 \) respectively.

We have followed previous authors in averaging (3) over directions in the plane normal to each dislocation. The corresponding relaxation rate for a density \( N \) (length/volume) of randomly oriented dislocations is \( \Gamma_j^{-1} = \Gamma_j N w \) where \( \Gamma_j = \hbar^2 (f_s + 2f_e)/1296 \rho^2 \equiv \Gamma_j \), independent of \( j \)

\[ \Gamma_j = \hbar^2 (f_s + 2f_e)/1296 \rho^2 \equiv \Gamma_j \]

For random characters we take \( L e = 2L/3 = 2L s \) in (6) for a total length \( L \) of dislocation line. The elastic constants of \( 17-101 \) were adopted. The sums \( S_n \) were evaluated for the [100], [110] and [111] directions and the arithmetic mean was taken. The results are shown in the table. To check the reliability of the trial function we repeated the calculation for the case of parallel dislocations and degenerate polarization branches, a case which leads to a tractable Boltzmann
equation. The results suggest that the upper bound (6) overestimates the true resistivity by a factor 4/3 when either dislocation scattering or electron-phonon scattering dominate, and is exact if boundary scattering dominates. On the other hand the proportion of edge dislocations in deformed crystals is normally much greater than 2/3 of the total so this overestimation will be largely compensated.

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$\mu \equiv \left[ L/V \right] \left( T_{\text{dis}}^{2w} \right)^{-1}$</th>
<th>$\Gamma \left( 10^{-16} \text{ cm}^2 \right)$</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>\begin{align*} &amp;\text{Eqn. (6)} \quad \text{Experiment*} \ \text{Cu} &amp; 2.1 \quad 2.5 \pm 0.3 \ \text{Al} &amp; 3.8 \quad 4.0 \quad 39 \quad 1.9 \ \text{Si} &amp; 8.9 \quad 8 \pm 2 \quad 11 \quad 0.24 \ \text{Ge} &amp; 10.6 \quad 8.4 \quad 15 \quad 0.26 \ \text{LiF} &amp; 6.2 \quad 0.14 \pm 1.2 \quad 14 \quad 0.59 \end{align*}</td>
<td></td>
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* We have doubled etch-pit counts to get length per unit volume.

A detailed discussion of the data will be given elsewhere.

4. Conclusion: The theory is in agreement with data for Cu, Al, Si and Ge. For LiF the theory underestimates the resistivity by a factor of 5 (data of /11/) or 40 (data of /12/; a similar discrepancy appears for other alkali halides /13/).

References:

/10/ J.F. Thomas, Phys. Rev. 175, 955 (1968).