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PHONON CONDUCTIVITY DUE TO NONDIAGONAL ENERGY-FLUX OPERATOR

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Abstract. Using the Zwanzig-Mori projection operator method we present calculations of renormalised phonons and their contribution to the thermal conductivity of Ge from the nondiagonal part of the heat-flux operator given by Hardy.

Recently we\(^1\) have used the Zwanzig-Mori projection operator method to obtain expressions for the lattice thermal conductivity of an anharmonic crystal from the diagonal and nondiagonal parts of the heat-flux operator given by Hardy\(^2\). In the van Hove limit the diagonal contribution is the well known single-mode relaxation time result\(^3\), in which only the true phonon frequency appears. But the nondiagonal contribution includes renormalised phonons, with shifted frequencies. Here we present results of our calculations of renormalised phonons and their contribution to the thermal conductivity of Ge from the nondiagonal part of the heat-flux operator.

In the notation of Ref. \(^1\) the expressions for the diagonal and nondiagonal contributions to the lattice thermal conductivity are as follows

\[ \kappa_d = \frac{\kappa^2 B^2 k_B}{3N_0 \Omega} \sum_i \omega_i c_i^2 \frac{N_i}{N_i + 1} \tau_i \]

(1)

\[ \kappa_{nd} = \frac{\kappa^2 B^2 k_B}{3N_0 \Omega} \sum_{ij} \omega_i \omega_j c_{ij}^2 \frac{N_j}{N_j + 1} \left( \frac{N_j}{N_j + 1} \right) \left( \frac{N_j}{N_j + 1} \right) \left( \frac{N_j}{N_j + 1} \right) \frac{\tau_{ij}}{\tau_{ij}^2 + (\omega_{ij} + \Delta_{ij})^2} \]

(2)
Here \( i \equiv (q,s) \), \( j \equiv (q',s') \), \( \omega_{i+j} = \omega_i + \omega_j \), \( \Delta_{ij} = \text{Im}(\delta_i) - \text{Im}(\delta_j) = \Delta_i - \Delta_j \)

\[
\tau_{ij}^{-1} \equiv \text{Re}(\delta_i) + \text{Re}(\delta_j) = \frac{1}{2}(\tau_i^{-1} + \tau_j^{-1}),
\]

and \( \hat{c}_{ij} \equiv \hat{c}_{qss'} \) is a generalised group velocity. \( \Delta_i \) and \( \tau_i^{-1} \) are the frequency shift and the inverse relaxation time of a phonon in mode \( i \) and are, respectively, calculated from the imaginary and real parts of \( \delta_i \) where

\[
\delta_i = \frac{-1}{i\hbar} \int_0^\infty dt \langle [\Gamma_i(t),\Gamma_i^\dagger] \rangle_0 e^{i\omega t}, \tag{3}
\]

with \( \Gamma_i \) as a measure of cubic anharmonicity: \( H = H_{\text{harm}} + \sum_i \Gamma_i A_i \). As in our previous paper in these proceedings we express \( \Gamma_i \) in terms of the Grüneisen constant of the material

\[
\Gamma_i \equiv \Gamma q = \frac{|\hbar|^2}{3! \sqrt{2\rho N_0 \Omega}} \sum q' q'' q''' \frac{\psi_{q'+q''} q''' A_q A_{q'} A_{q''}}{\omega_{q'+q''} \delta_{q'+q''}}, \tag{4}
\]

\( q \equiv (q,s) \). With this then

\[
\langle [\Gamma_q(t),\Gamma_q^\dagger] \rangle_0 = \sum_{q' q'' q'''} |\phi_{q' q'' q'''}|^2 \langle [A_q(t), A_{q'} A_{q''}] \rangle_0, \tag{5}
\]

where

\[
|\phi_{q' q'' q'''}|^2 = \frac{\hbar^3 \gamma^2}{2\rho c^2 N_0 \Omega} \frac{\omega_{q'+q''} \delta_{q'+q''}}{\omega_{q' q''} \delta_{q'+q''}}, \tag{6}
\]

With equations (4-6) and a little bit of algebra, we can express \( \delta_i \) for three phonon processes as

\[
\delta_q = \frac{-1}{i\hbar^2} \sum_{q' q''} |\phi_{q' q''}|^2 \int_0^\infty dt \{ (\hat{N}' - \hat{N}'') e^{i(\omega_{q'+q''})t} \}
+ \frac{1}{2} (1 + \hat{N}' + \hat{N}'') e^{i(\omega_{q' q''})t}\}
\]

From this \( \Delta_q \) and \( \tau_q^{-1} \) can be evaluated using the relation

\[
\int_0^\infty dt e^{i(\omega \pm \omega')t} = \pi \delta(\omega \pm \omega') - i P \left( \frac{1}{\omega \pm \omega'} \right), \tag{8}
\]

With equations (4-6) and a little bit of algebra, we can express \( \delta_i \) for three phonon processes as
where P denotes the principal part. It is interesting to note that 
\( \tau_{q}^{-1} \) calculated in this way is the same as the result obtained using 
the first order perturbation method\(^3,4\).

In Fig. 1 we have plotted \( \Delta_{q} \) and \( \tau_{q}^{-1} \) for the longitudinal mode at 
300 K. Although \( \tau_{q}^{-1} \) is an increasing function of frequency, \( \Delta_{q} \) shows 
a pronounced structure at \( \omega \approx 25 \times 10^{12} \text{ s}^{-1} \). We find that in general 
\( \Delta_{q} > \tau_{q}^{-1} \) and \( (\omega_{q} + \Delta_{q}) > \tau_{q}^{-1} \), implying that a pseudoharmonic model\(^5\) is 
a good description for phonons in Ge. Furthermore, our calculations 
show that \( \kappa_{nd} \) is negligibly small in comparison to \( \kappa_{d} \) in the tempera-
ture range 10-900 K. A similar conclusion was reached by Hardy\(^2\), and 
Semwal and Sharma\(^6\) using qualitative arguments.

Fig. 1: The inverse relaxation time \((\tau^{-1})\) and frequency shift \((\Delta)\) 
for the longitudinal acoustic phonon mode in Ge at 300 K as a function 
of frequency \((\omega)\).

References