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A Modification of the Generalized Callaway Thermal Conductivity Equation to Allow for Phonon Dispersion

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The convenient approximation $\vec{q}\cdot\vec{v} = \omega$ is often used in the formulation of the thermal conductivity integrals, which is in fact far from reality. In experimental dispersion curves $\vec{q}$ and ω do not obey a linear relation. ω is generally a function of the magnitude and direction of the wave vector $\vec{q}$. But for convenience of calculation $\vec{q}$ can be assumed a function of ω. Joshi and Verma (1) suggested that $\vec{q}$ is a quadratic function of ω. Later on it was modified by Sharma et al. (2) considering that $\vec{q}$ is a cubic function of ω. Thus according to Sharma et al.

$$\vec{q}\cdot\vec{v} = \omega_s(1 + \nu_s\omega_s^2) , \tag{1}$$

where ν_s is a constant and is calculated from experimental data of the dispersion curve with the help of the following relation:

$$\nu_s = \frac{1}{\omega_s^2}\left(\frac{\vec{q}\cdot\vec{v}_s}{\omega_s} - 1\right).$$

Recently Kosarev et al. (3) published a generalization of the Callaway (4) thermal conductivity equation to calculate the contribution of different polarization branches. Unfortunately their results are incorrect. Later on it was corrected by Parrott (5), Kosarev et al. (6) have also published its correct form in the Erratum. Both of them have used $\vec{q}\cdot\vec{v} = \omega$ and do not differentiate between phonon group velocity and phase velocity. In the present note, Parrott's result is modified by using a better dispersion relation $\vec{q}\cdot\vec{v}_s = \omega_s(1 + \nu_s\omega^2)$ as stated in equation (1). The difference between phonon group velocity and phase velocity is also made. Inserting into equation (1), one has

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$$\text{group velocity} \qquad \vec{v}_{g,s} = \frac{\vec{v}_s}{1 + 3r_s\omega_s^2} ,$$

$$\text{phase velocity} \qquad \vec{v}_{p,s} = \frac{\vec{v}_s}{1 + \gamma_s\omega_s^2} . \tag{2}$$

According to Parrott, the expression for the lattice thermal conductivity is given by (see equation (4) of Parrott's paper)

$$K = \frac{k_o}{(2\pi)^3}\left(\frac{\hbar}{k_oT}\right)^2\left\{\sum_s\int C_s^2\omega_s^2\mu^2\left(\frac{\tau_N^s\tau_R^s}{\tau_N^s+\tau_R}\right)\tilde{N}(\tilde{N}+1)d^3q + \right.$$

$$\left. + \frac{\left[\sum_s\int C_s\omega_s\mu^2q\left(\frac{\tau_R^s}{\tau_N^s+\tau_R^s}\right)\tilde{N}(\tilde{N}+1)\,d^3q\right]^2}{\sum_s\int\mu^2q^2\left(\frac{1}{\tau_N^s+\tau_R^s}\right)\tilde{N}(\tilde{N}+1)\,d^3q}\right\} , \tag{3}$$

where k_o is the Boltzmann constant, $\hbar$ is the Planck constant divided by 2π , C_s is the group velocity, μ is the cosine factor, ω_s is the phonon frequency, τ_N^s is the relaxation time of the three-phonon normal processes, τ_R^s is the relaxation time of those processes which do not conserve momentum, the polarisation branch is labelled by the suffix s. $\tilde{N}$ is Planck's distribution function. Inserting equations (1) and (2), and on further simplification of equation (3), one gets the following expression for the thermal conductivity:

$$K = \frac{k_o}{6\pi^2}\left(\frac{k_oT}{\hbar}\right)^3\left\{\sum_s\frac{1}{v_s}\int_0^{\theta_s/T}\left(\frac{\tau_N^s\tau_R^s}{\tau_N^s+\tau_R^s}\right)\frac{(1+R_sx^2)^2}{(1+3R_sx^2)}\frac{x^4e^x}{(e^x-1)^2}dx + \right.$$

$$\left. + \frac{\left[\sum_s\frac{1}{v_s^3}\int_0^{\theta_s/T}\left(\frac{\tau_R^s}{\tau_N^s+\tau_R^s}\right)(1+R_sx^2)^3\frac{x^4e^x}{(e^x-1)^2}\,dx\right]^2}{\sum_s\frac{1}{v_s^5}\int_0^{\theta_s/T}\left(\frac{1}{\tau_N^s+\tau_R^s}\right)(1+R_sx^2)^4(1+3R_sx^2)\frac{x^4e^x}{(e^x-1)^2}\,dx}\right\} \tag{4}$$

where $R_s = r_s(k_oT/\hbar)^2$ and $x = \hbar\omega_s/k_oT$.

If γ_s is assumed to be zero, i.e. the phonon dispersion curve is straight-line, equation (4) reduces to

$$K = \frac{k_o}{6\pi^2}\left(\frac{k_oT}{\hbar}\right)^3 \left\{ \sum_s \frac{1}{v_s} \int_0^{\theta_s/T} \left(\frac{\tau_N^s \tau_R^s}{\tau_N^s + \tau_R^s}\right) \frac{x^4 e^x}{(e^x-1)^2}\,dx + \frac{\left[\sum_s \frac{1}{v_s^3} \int_0^{\theta_s/T} \left(\frac{\tau_R^s}{\tau_N^s + \tau_R^s}\right) \frac{x^4 e^x}{(e^x-1)^2}\,dx\right]^2}{\sum_s \frac{1}{v_s^5} \int^{\theta_s/T} \left(\frac{1}{\tau_N^s + \tau_R^s}\right) \frac{x^4 e^x}{(e^x-1)^2}\,dx} \right\}$$

which is same as is given by Parrott.

If one neglects the correction term due to three-phonon normal processes, equation (4) reduces to

$$K = \frac{k_o}{6\pi^2}\left(\frac{k_oT}{\hbar}\right)^3 \sum_s \int_0^{\theta_s/T} \left(\frac{\tau_N^s \tau_R^s}{\tau_N^s + \tau_R^s}\right) \frac{x^4 e^x}{(e^x-1)^2}\, \frac{(1+R_s x^2)^2}{(1+3R_s x^2)}\,dx$$

which is similar to the modified form of the Holland (7) equation as modified by Sharma et al. (2).

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