Analysis of Thermal Conductivity-A Reply

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The criticism of the assignment of a T^3 temperature dependence to the relaxation time due to longitudinal three-phonon interactions and the subsequent effect of this assignment on the temperature dependence of the lattice thermal conductivity of silicon, germanium, and gallium arsenide is considered. It is asserted that the reasons for the initial assignment have not been shown to be invalid, nor has a better assignment been established. However, the criticism of the statement that the transverse phonons can account for a majority of the heat flow is valid because this conclusion has not been adequately tested.

When "Analysis of Thermal Conductivity" was published,[1] there were two experimental facts which needed explanation. (i) For Si and Ge, and later for other III-V semiconductors,[2] the thermal conductivity κ varied as $\kappa \propto T^{-n}$ above the maximum and n was in each case greater than 1. (ii) The region over which the data were a straight line began well below the Debye temperature. The very dispersive nature of the transverse-phonon branches had recently been determined experimentally so that it appeared reasonable to try to explain the thermal conductivity data using the unusual properties of the transverse phonons in these semiconductors. The results of the analysis were that (a) a new expression for τ_{TU}^{-1} could be obtained for dispersive transverse phonons, and the heat flow could be readily separated into that due to longitudinal and transverse phonons. (b) The experimental data could be reasonably fitted from 2 °K to near the melting point for both Si and Ge. (c) The temperature dependence was $T^{-1.2}$ from well below the Debye temperature. (d) The transverse phonons seemed to be carrying a majority of the heat.

At that time it was clearly indicated that a more exact calculation would require a better description of the temperature and frequency dependence of the relaxation times. Of course it is possible to fit the thermal conductivity data using one average phonon mode and an expression of the form

$$\tau_U^{-1} = A\omega^p T^m ,$$

where p and m are both functions of T. However, such an approach is not physically justifiable. (Guthrie's[3] assertions that τ_U and τ_N have the same form, if based on his Eq. (9), does not seem to be well founded for the dispersive phonon spectra under consideration.[4])

The use of $\tau_{LN}^{-1} \propto T^3$ for the relaxation of longitudinal phonons does not seem to be a poor assignment. The contribution of κ_L to the total heat conductivity is only about 25% at 300 °K ($T = \frac{1}{2}\theta_D$) and even less at higher temperatures for Si. Further, depending on the frequency dependence, the low-frequency longitudinal phonons, with a frequency less than that corresponding to 190 °K ($T \sim 0.3\theta_D$) make a large contribution to κ_L at room temperature. According to Guthrie, $\tau_{LN}^{-1} \propto T^3$ is still reasonable at these frequencies in Si. Now if κ_L were adjusted to represent most of the heat conduction at $\frac{1}{2}\theta_D$, then it seems that the adjustment of τ_{LU}^{-1} from a $T^{1.1}$ to a T^3 dependence as the temperature was decreased would overestimate the heat conduction at temperatures just above the maximum. The same arguments hold for Ge and GaAs. Furthermore, the Guthrie calculations on the similarity of τ_U and τ_N and τ_L and τ_T are not at all definitive.

However, in agreement with Guthrie, the suggestion indicated in my analysis that the transverse phonons account for a majority of the heat flow cannot be regarded as conclusive. Further analysis and experimentation are necessary. For example, ultrasonic attenuation might eventually help clarify this point and help determine the frequency and temperature dependence of the various three-phonon scattering times.[5]

The original analysis was successful in fitting the thermal conductivity of Si and Ge over an extremely wide temperature range (2 to over 1000 °K) using essentially three parameters and a physically justifiable separation of integerals. The analysis has been equally successful for other III-V semiconductors[6] and has stimulated some thought concerning the role of transverse phonons in heat conduction. The validity and utility of the Guthrie calculations[3] of the relaxation times is still to be determined.

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[1] M. G. Holland, Phys. Rev. 132, 2461 (1963).
[2] M. G. Holland, Phys. Rev. 134, A971 (1964).
[3] G. L. Guthrie, Phys. Rev. 152, 801 (1966).
[4] See Ref. 1, Appendix A.
[5] M. G. Holland, IEEE Trans. Sonics Ultrasonics SU-15, 18 (1968).
[6] C. M. Bhandari and G. S. Verma, Phys. Rev. 140, A2101 (1965).