Longitudinal and Transverse Phonons in Lattice Thermal Conductivity

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Bhandari and Verma published "one[1]" of two articles to be commented on. The Bhandari-Verma paper[1] followed the analytical method given by Holland[2] in an earlier paper, giving due credit. The two papers[1,2] have been of considerable interest to other authors, leading in at least one case[3] to the unlikely conclusion that a $T^{1.1}$ to $T^{1.3}$ dependence of $1/\kappa_{\text{Lattice}}$ could be explained by separate considerations of longitudinal and transverse heat conduction, even though $1/\kappa_{\text{Lattice}}$ might be expected to possess a $T^{1.0}$ dependence in the case of a single mode considered separately. Recently, Bhandari and Verma published a brief erratum[4] correcting a minor error in their paper, thus giving the impression that there was little possibliity that any more serious difficulties existed.

Unfortunately, there is now reason[5] to believe that serious basic difficulties exist.

The Holland-Bhandari-Verma (H-B-V) calculations were based upon an assignment of a dependence of the type $\tau^{-1}_{3\text{-phonon}}$ (longitudinal) $\propto T^3$ for the relaxation of longitudinal-phonon populations via three-phonon processes at all temperatures. The results and conclusions of the H-B-V calculations rest on the correctness of this assignment. After the original H-B-V calculations and interpretations were published, theoretical limits were derived[5] for n in expressions of the type $\tau^{-1} \propto T^n$, and the longitudinal three-phonon value of 3.0 used in the H-B-V calculations appears to be well outside the expected limits in the high-temperature region of the H-B-V calculations.

The proper value for the exponent of T in the proportionality expression above depends upon the material and also on the temperature. In the expression above, the temperature exponent 3.0 is improper for InSb[5] if $T > 6.9$ °K, and is improper for GaAs[5] if $T > 108$ °K. At the highest temperatures (~ 300 °K) of the Bhandari-Verma calculation, the proper value[5] for the exponent of T in the expression above is approximately 1.1 ± 0.1 rather than 3.0. Corresponding information on the temperature dependence of $\tau^{-1}_{3\text{-phonon}}$ (longitudinal) for Si and Ge may be found in Ref. 5.

If an attempt were made to repair the H-B-V calculations in the light of present knowledge, it is possible to assign a functional dependence $f(T)$ to $\tau^{-1}_{3\text{-phonon}}$ (longitudinal) which would stay inside the theoretically derived[5] limits for n, while adding no new computer-adjusted parameters to the H-B-V procedure. If the H-B-V work were recalculated using new functional dependences consistent with Ref. 5, it is obvious that the outcome would be qualitatively different from the original results, due to the drastic change required in the $\tau^{-1}_{3\text{-phonon}}$ (longitudinal) input function. However, a new difficulty might well arise in the computation. In choosing the functional representations of $\tau^{-1}_{3\text{-phonon}}$ (longitudinal) and $\tau^{-1}_{3\text{-phonon}}$ (transverse), there would be no justification for using two functions whose temperature dependences differ greatly from each other over the major part of the temperature range of the H-B-V work. In fact, it appears that the functions representing these quantities should be quite similar, except at low temperatures, where the Herring[6] relations apply. Consequently, it is likely that an attempt to modify the work of Refs. 1 and 2 to conform to the now-apparent limitations of temperature dependence of the separate relaxation times would be largely unsuccessful. This is so because an attempted calculation, using currently available[5] knowledge, could be expected to lead to a practical computation difficulty arising from the necessity to distinguish between two overly similar functions.

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