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Phonon relaxation times extracted from first principles thermal conductivity calculations[1] D. A. BROIDO, A. WARD, Department of Physics, Boston College, Chestnut Hill, MA 02467 — The lattice thermal conductivity of semiconductors, κ_L, is a key component in assessing a material's utility for thermoelectric applications. Calculations of κ_L commonly employ phonon relaxation times, τ_{ph}. Over the past few decades, a variety of mathematical forms have been used for theseτ_{ph}s to represent the phonon-phonon scattering [1], which dominates the behavior of κ_L around and above room temperature. However, these forms have typically been obtained in a low frequency/low temperature approximation where umklapp scattering is weak and outside the thermal regime of interest for thermoelectrics. Recently we have developed a first principles approach that accurately calculates κ_L using no adjustable parameters [2]. In this presentation, we use our *ab initio* results for Si, Ge and diamond to examine the accuracy of the different models for τ_{ph}, and we identify alternative models. [1] See for example, M. Asen-Palmer et al., Phys. Rev. B 56, 9431 (1997), and references therein. [2] D. A. Broido, M. Malorny, G. Birner, N. Mingo and D. A. Stewart, Appl. Phys. Lett. 91, 231922 (2007).

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