Phonon relaxation times extracted from first principles thermal conductivity calculations\textsuperscript{1} D. A. BROIDO, A. WARD, Department of Physics, Boston College, Chestnut Hill, MA 02467 — The lattice thermal conductivity of semiconductors, \(\kappa_L\), is a key component in assessing a material’s utility for thermoelectric applications. Calculations of \(\kappa_L\) commonly employ phonon relaxation times, \(\tau_{ph}\). Over the past few decades, a variety of mathematical forms have been used for these \(\tau_{ph}\) to represent the phonon-phonon scattering \cite{1}, which dominates the behavior of \(\kappa_L\) 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 \(\kappa_L\) using no adjustable parameters \cite{2}. In this presentation, we use our \textit{ab initio} results for Si, Ge and diamond to examine the accuracy of the different models for \(\tau_{ph}\), and we identify alternative models. \cite{1} See for example, M. Asen-Palmer et al., Phys. Rev. B 56, 9431 (1997), and references therein. \cite{2} D. A. Broido, M. Malorny, G. Birner, N. Mingo and D. A. Stewart, Appl. Phys. Lett. 91, 231922 (2007).

\textsuperscript{1}(Supported by NSF)

David Broido
Boston College

Date submitted: 20 Nov 2008