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Thermal Transport in Silicon From Empirical Interatomic Potentials D. A. BROIDO, A. WARD, Department of Physics, Boston College, Chestnut Hill, MA 02467, N. MINGO, NASA-Ames Center for Nanotechnology, Moffet Field, CA 94035 — The accurate description of thermal transport of phonons in bulk and low-dimensional semiconductors is of central importance to the understanding of their thermoelectric properties. We present calculations of the lattice thermal conductivity of silicon based on several commonly used empirical models of the interatomic potential [1-3]. Second and third order force constants obtained from these potentials are used as inputs to an exact iterative solution to the phonon Boltzmann equation, which includes the anharmonic phonon-phonon scattering as well as isotopic defect and boundary scattering. Comparisons are made to available experimental data. The lattice thermal conductivity obtained from each model is not satisfactory, and suggestions for improvements are presented.

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David Broido
Department of Physics, Boston College, Chestnut Hill, MA 02467

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