Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First principles Theory of the Lattice Thermal Conductivity of Si and Ge D. A. BROIDO, Boston College, M. MALORNY, University of Regensburg, N. MINGO, CEA-Grenoble and University of California at Santa Cruz, D. A. STEWART, Cornell University — The room temperature lattice thermal conductivity of high quality crystalline semiconductors is limited by the scattering between phonons arising from the anharmonicity of the interatomic potential. We have calculated the lattice thermal conductivity of isotopically enriched silicon and germanium, combining a first principles approach to extract the harmonic and anharmonic interatomic force constants [1] with an iterative solution of the full Boltzmann-Peierls equation for phonon transport [2]. Our calculated lattice thermal conductivities for Si and Ge, obtained with no adjustable parameters, show very good agreement with measured values [3,4] and are a marked improvement to results obtained previously using empirical interatomic potentials [2]. [1] G. Deinzer, G. Birner, and D. Strauch, Physical Review B 67, 144304 (2003). [2] D. A. Broido, A. Ward, and N. Mingo, Physical Review B 72, 014308 (2005). [3] M. Asen-Palmer, et al, Physical Review B 56, 9431-9447 (1997). [4] T. Ruf, et al, Solid State Communications 115, 243-247 (2000).

David Broido
Boston College

Date submitted: 19 Nov 2006 Electronic form version 1.4