Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Atomistic modeling of thermoelectric properties of Bi2Te3 and Sb2Te3[1] SEUNGWON LEE, PAUL VON ALLMEN, ABHIJIT SHEVADE, FABIANO OYAFUSO, Jet Propulsion Laboratory, California Institute of Technology — Low-dimensional structures with a high density of interfaces exhibit a large thermoelectric figure of merit. For example, a figure of merit ZT=2.5 was measured at 300 K in a Bi_2Te_3/Sb_2Te_3 superlattice. The design of thermoelectric materials with an even higher figure of merit is conceivable by exploiting the enhancement of the density of states in low dimensionality structures and optimizing the phonon scattering at interfaces to reduce the thermal conductivity. As a step toward modeling such structures, we have computed the thermoelectric properties of bulk Bi_2Te_3 and Sb_2Te_3 using an atomistic empirical tight-binding method and the Boltzmann transport equation. The tight-binding parameters for the materials are fitted to first-principle band structure calculations. Using the band structures obtained with the tight- binding model and the relaxation time approximation for the scattering, the Seebeck coefficient, the electrical conductivity and the electronic and lattice contribution to the thermal conductivity of bulk Bi_2Te_3 and Sb_2Te_3 are calculated. The lattice contribution to the thermal conductivity is obtained from a Monte Carlo solution to the Boltzmann equation for phonons.

[1]Funded by DARPA

Seungwon Lee
Jet Propulsion Laboratory, California Institute of Technology

Date submitted: 06 Dec 2004 Electronic form version 1.4