Abstract Submitted
for the DFD06 Meeting of
The American Physical Society

Modeling Thermal Transport in Two-dimensional Nanocomposites ARVIND PATTAMATTA, CYRUS MADNIA, University at Buffalo (SUNY) — The Boltzmann transport equation (BTE) for phonon intensity is numerically solved to study the thermal properties of nanocomposites. To establish the phonon particle model it is assumed that the phonon wave effect can be neglected and the frequency-dependent scattering rate in the bulk medium is approximated by the average phonon mean free path. Both Euler with first order Upwind and MacCormack with fourth order compact finite difference schemes are used to solve the BTE. The material considered in this study is composed of silicon (Si) nanowires embedded in the host semiconductor material of germanium (Ge). Due to the two-dimensionality of the nanocomposite the heat flow along the silicon wire is excluded, and therefore only the heat flow perpendicular to the wire is considered. In order to model the cell-cell interaction in the Si-Ge matrix, periodic boundary conditions are applied along the direction of heat flow. The interfaces between the host and nanowires are modeled as diffusely scattering. It is found that the thermal characteristics in the nanoscale composites are different from the macroscale composites. The resulting temperature profiles and effective thermal conductivity of the nanocomposites cannot be predicted accurately using the Fouriers heat conduction model. The dependence of thermal conductivity on the nanocomposite size has also been studied. The results of this study can be used to improve the efficiency of thermoelectric energy conversion materials.

Cyrus Madnia
University at Buffalo

Date submitted: 28 Jul 2006 Electronic form version 1.4