Proceedings of CHT-15
ICHMT International Symposium on Advances in Computational Heat Transfer

May 25-29, 2015, Rutgers University, Piscataway, USA

CHT-15-081

# PARALLEL COMPUTATION OF THE PHONON BOLTZMANN TRANSPORT EQUATION FOR THE PREDICTION OF THERMAL TRNSPORT ACROSS SILICON/GERMANIUM INTERFACES

Syed Ashraf Ali, and Sandip Mazumder[§]
Department of Mechanical and Aerospace Engineering
The Ohio State University, Columbus, OH 43221, USA
[§]Correspondence author. Email: mazumder.2@osu.edu

**ABSTRACT** In this article, two models for phonon transmission across semiconductor interfaces are investigated and demonstrated in the context of large-scale spatially three-dimensional calculations of the phonon Boltzmann Transport Equation (BTE). These include two modified forms of the classical diffuse mismatch model: one, in which dispersion is accounted for, and another, in which energy transfer between longitudinal and transverse acoustic phonons is disallowed. As opposed to the vast majority of previous studies in which the interface is treated in isolation, and the thermal boundary conductance is calculated using closed-form analytical formulations, the present study also considers the interplay between the interface and intrinsic (volumetric) scattering of phonons. This is accomplished by incorporating the interface models into a parallel solver for the full seven-dimensional BTE for phonons. A verification study is conducted in which the thermal boundary resistance of a silicon/germanium interface is compared against previously reported results of molecular dynamics calculations. The BTE solutions overpredicted the interfacial resistance, and the reasons for this discrepancy are discussed. It is found that due to the interplay between intrinsic and interface scattering, the interfacial thermal resistance across a Si(hot)/Ge(cold) bilayer is different from that of a Si(cold)/Ge(hot) bilayer. Finally, the phonon BTE is solved for a nanoscale three-dimensional heterostructure, comprised of multiple blocks of silicon and germanium, and the time evolution of the temperature distribution is predicted, and compared against predictions using the Fourier law of heat conduction.