

Abstract Submitted
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Thermal boundary resistance of closely-spaced Si/Ge interfaces from lattice dynamics calculations ERIC LANDRY, ALAN MCGAUGHEY, Carnegie Mellon University — An ability to accurately predict the thermal boundary resistance (TBR) of closely-spaced semiconductor interfaces will allow the design of superlattices with high values of the thermoelectric figure-of-merit. Here, the TBR and phonon transmission coefficients of closely-spaced Si/Ge interfaces are predicted using harmonic lattice dynamics calculations and the scattering boundary method. The atomic interactions are modeled using the Stillinger-Weber potential. The computational domain contains a thin germanium layer sandwiched between two semi-infinite extents of silicon, forming two closely-spaced interfaces. We also consider the opposite situation, where a silicon layer is placed between two large extents of germanium. Due to the harmonic approximation, the calculations are only valid when the phonon scattering is elastic. To examine the assumption of elastic scattering, we compare the lattice dynamics predictions to those obtained using molecular dynamics simulations and the direct method, which require no assumptions about the nature of the phonon transport. We conclude by discussing how the atomic force constants needed in the lattice dynamics calculations can be calculated from density functional theory. This novel approach will allow for the prediction of TBR for interfaces between semiconductors for which a suitable interatomic potential does not exist.

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