

## MULTISCALE SIMULATION OF PHONON-MEDIATED THERMAL TRANSPORT

**SCIENTIFIC ACHIEVEMENT:** Heat is transported by phonons in electrical insulators and semiconductors. We have performed atomic-level simulations to determine the interfacial (Kapitza) resistance of carefully selected grain boundaries in silicon. We find that the Kapitza resistance is generally higher for grain boundaries that are more structurally disordered, i.e., have higher energies. Such simulations do not, however, provide microscopic information on the phonon-interface interactions themselves. To obtain such atomic-level information, we have developed a simulation technique by which a wave packet of phonons of a single branch and well-defined frequency and polarization is launched at an interface. The resulting transmitted and reflected waves are characterized in detail. We have applied this method to both coherent semiconductor interfaces and to semiconductor grain boundaries. We find that in the low-frequency limit the transmission coefficients of both longitudinal and transverse acoustic phonons agree well with those predicted by the continuum-based acoustic-mismatch model. However, the transmission coefficients rapidly decrease close to the cutoff frequency, a result that for the coherent interfaces, can be understood within a simple one-dimensional discrete atomic-chain model. We also find that the transmission coefficient for transverse acoustic phonons depends strongly on the polarization. For scattering from grain boundaries we find that there is a considerable amount of mode mixing with, e.g., an incident longitudinal acoustic wave packet being scattered into transverse and optical modes.

We have constructed a particle-based mesoscale model for phonon transport and the scattering of phonon wave packets at interfaces. The model, which incorporates the critical interference effects associated with the wave nature of phonons, is parameterized with frequency-dependent scattering rates obtained from the molecular-dynamics simulations of the interaction of phonon wave packets with a single interface. In simulations of scattering of phonon wave packets from superlattices, we find that when the interference effects are included there is quantitative agreement between the molecular-dynamics and the mesoscale simulations. Moreover, we show that such interference effects tend to increase the amount of energy being transmitted through a superlattice.

**SIGNIFICANCE:** The relentless decrease in the size of nanostructures places ever-increasing demands on heat management systems. As the system sizes approach and even become less than the phonon mean free path, the interaction of phonons with interfaces begin to dominate thermal transport. Our simulation studies are providing the first microscopic information on interfacial thermal conductivity and on phonon-interface interactions. Such information is essential input into mesoscale models of thermal transport in device structures, which are usually based on the Boltzmann Transport Equation.

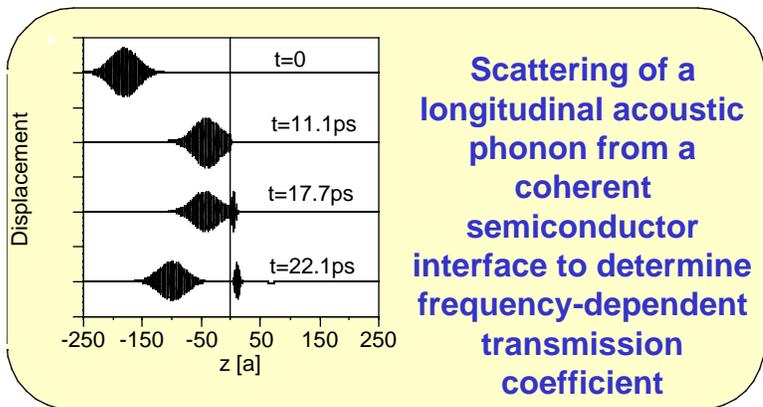
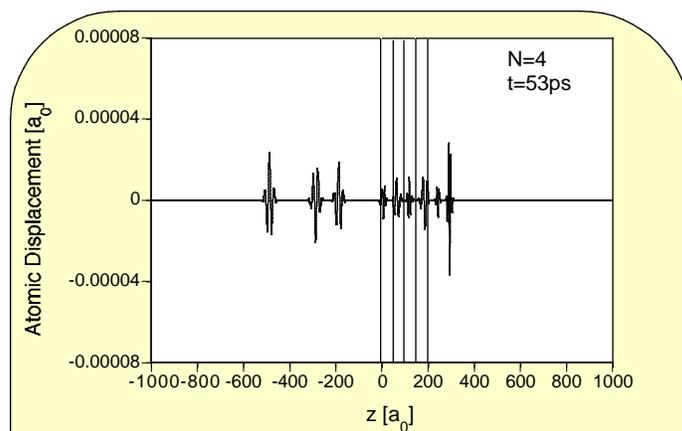
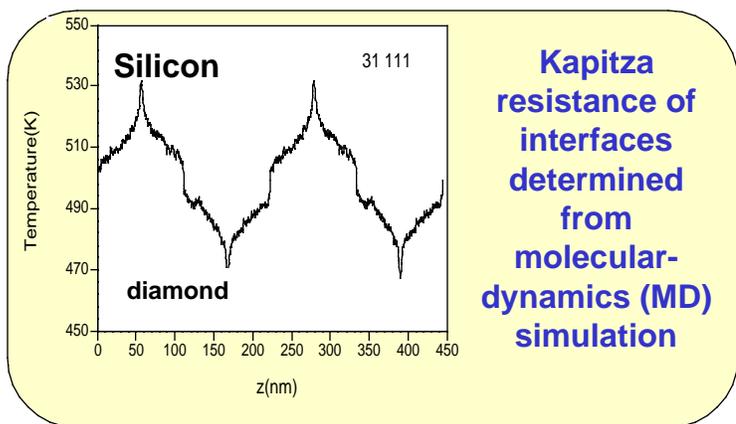
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**PERFORMERS:** P K. Schelling and S. R. Phillpot, Materials Science Division, Argonne National Laboratory

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# Multiscale Simulation of Phonon-Mediated Thermal Transport



**MD simulation of scattering of phonon wave packet incident from left from a superlattice of coherent interfaces. Mesoscale particle model quantitatively reproduces MD results**

**P. K. Schelling, S. R. Phillpot (ANL)**