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Relative Contributions of Inelastic Phonon Scattering and Elastic Phonon Scattering to Thermal Boundary Conductance across Solid Interfaces

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ABSTRACT

The knowledge of inelastic phonon scattering is crucial for the understanding of thermal boundary conductance across solid interfaces. Several traditional theoretical models such as the acoustic mismatch model (AMM) and the diffuse mismatch model (DMM) assume that the elastic phonon scattering drives the thermal transport across the interface. But there are experiments indicating that the inelastic phonon scattering plays an important part in the interfacial thermal energy conduction as well. We use nonequilibrium molecular dynamics (NEMD) to predict the inelastic phonon conductance across Cu/Si interface. Temperature distribution across Cu/Si interface has been obtained from the simulation results, and a temperature drop across the interface is observed. The inelastic phonon scattering is compared to the elastic phonon scattering to demonstrate their relative contributions to the interfacial thermal conductance. The results show that at relatively high temperature, the inelastic phonon scattering can be comparable to elastic phonon scattering, providing an additional energy dissipation channel.

KEYWORDS

Inelastic phonon scattering, thermal conductance, molecular dynamics