Modal Phonon Transport across Interfaces
by Non-Equilibrium Molecular Dynamics Simulation

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ABSTRACT

Phonons represent the quantization of lattice vibration, responsible for heat transfer in semiconductors and dielectrics. Phonon heat conduction across interfaces is crucially important for the thermal management of real-life devices such as smartphones, electric vehicles, and satellites. Although recent studies have broadly investigated spectral phonon contribution to lattice thermal conductivity, the mechanism of phonon modal transport across interfaces is still not well-understood. Previous models, including the acoustic mismatch model (AMM) and diffuse mismatch model (DMM), only consider elastic process while neglecting inelastic phonon contributions. Herein, we employ spectral Non-Equilibrium Molecular Dynamics Simulation (NEMD) to probe the temperature and heat flux of each phonon mode, particularly resolving phonon information near the interface constructed by silicon (Si) and germanium (Ge). We impose a heat flux across the interfaces and observe a temperature profile. After exactly mapping the phonon modal transmission from Si to Ge, we find that all the acoustic-acoustic transmission is elastic and optical phonons contribute almost 50% of the heat flux. Surprisingly, inelastic phonon transmission contributes 43% to interfacial conductance, all by TO-TO and LO-LO transmissions. Besides, there exists nearly 20% mode conversion, i.e., TA-LA and LA-LO conversions, where T, L, O, and A denotes transverse, longitudinal, optical and acoustic, respectively. The results show significant non-equilibrium between different phonon modes at the interface. Also, low-energy phonons carry a large amount of heat with small temperature drops. The modal phonon heat flux corroborates that the thermal transport across interfaces is contributed by both elastic and inelastic phonon transmission.

KEYWORDS

Nanoscale heat transfer, inelastic phonon transport, molecular dynamics