Phonon Transmission across Lattice-Mismatched Dissimilar Material Interfaces

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Phonon transmission in lattice-matched system has been studied a lot in recent years with an atomistic Green's function (AGF) approach. However in real materials, interfaces are usually lattice-mismatched. With lattice mismatch, atoms at the interface could reconstruct, which could results in different phonon scattering from the lattice-matched interfaces. Due to lattice constant difference and the asymmetric feature of a lattice mismatched system, relatively large material sizes need to be considered, and phonon transmission across lattice-mismatched dissimilar interfaces has not been investigated. An integrated molecular dynamics (MD) and AGF approach is developed to study the frequency-dependent phonon transmission across lattice-mismatched interfaces. In our simulation, the structure reconstruction of the lattice-mismatched interfaces is captured through MD simulations, and a recursive AGF approach is used to solve the numerical challenge in phonon transmission calculation. Three types of interfaces are studied considering the lattice mismatch and the structures which usually occur at the interface: (1) Si/Ge-like interfaces formed from two bulk materials (2) interfaces with defects (3) alloyed interfaces. The results show that lattice mismatch is important for phonon transmission across dissimilar material interfaces: the larger the lattice mismatch, the lower the average phonon transmission. For interfaces with defects, low frequency phonons can be scattered more with increasing defect size. Across alloyed interfaces, phonon transmission of high frequency phonons can be brought down to a very low value (<0.1), and phonon transmission is also insensitive to the phonon spectral.