Atomic Restructuring in Interfacial Phonon Transport

Using *ab initio* calculations, and using molecular dynamics simulation and the diffuse mismatch model for Si/In as example, we decompose phonon interfacial resistance into boundary and interfacial-region resistances. These show that the interfacial atomic restructuring as well as the cross-boundary interactions reduce the phonon boundary resistance by providing additional transport channels altering their phonon density of states, and cause extra interfacial-region resistances due to additional phonon scattering.

\[
AR_{p,\text{Si/In}} = AR_{p,b,\text{Si/In}} + AR_{p,\text{Si}} + AR_{p,\text{In}}
\]

(a) Interfacial Si and In atomic structures without interactions (initial equilibrium condition), and (b) with interactions and restructuring obtained from the MD simulations at 300 K. The bulk resistances \(AR_{p,b,\text{Si/In}}\) and the total interfacial resistance \(AR_{p,\text{Si/In}}\) [decomposed into the boundary \(AR_{p,b,\text{Si/In}}\) and two interfacial region resistances \(AR_{p,\text{Si}}\) and \(AR_{p,\text{In}}\)] are shown through the thermal circuit diagram.

Temperature distribution with heat flowing along direction \(z\) (cold thermostat at 100 K and hot at 300 K).

MD phonon density of states (p-DOS, \(D_p\)) of Si and In, in the bulk and the interfacial regions. Due to the interpenetration of force fields and atomic restructuring, \(D_p\) is distorted in the interfacial region. The blue shaded region represents shared phonon states between Si and In in the interfacial region. The interfacial \(D_p\) (solid lines) have more shared phonon states participating in the boundary transport, compare to the bulk \(D_p\) (dashed lines).