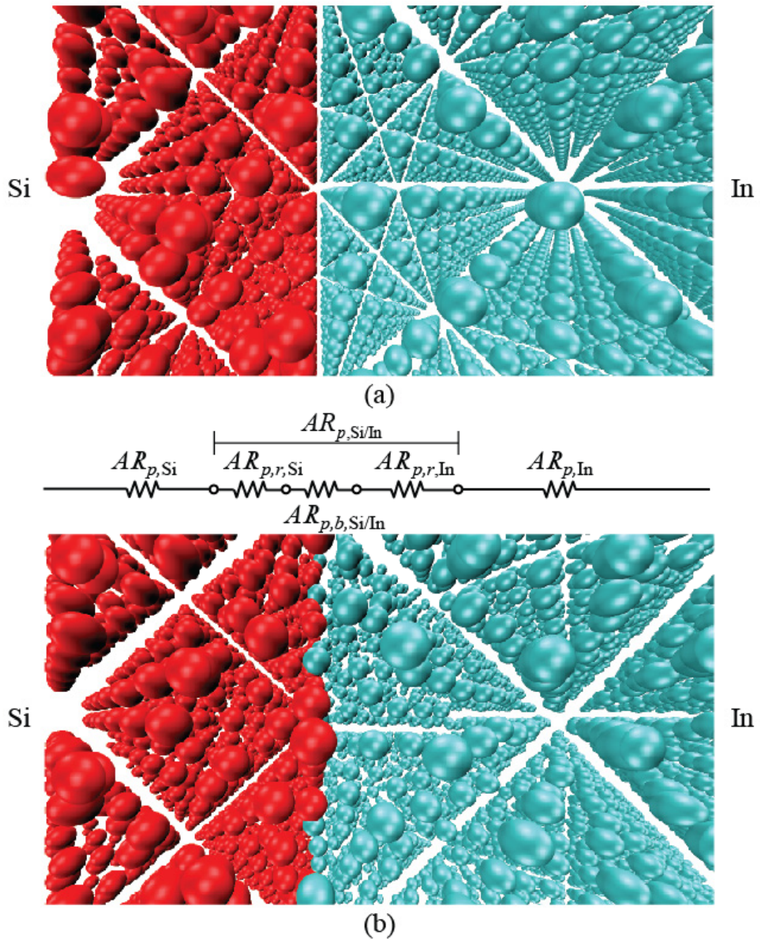
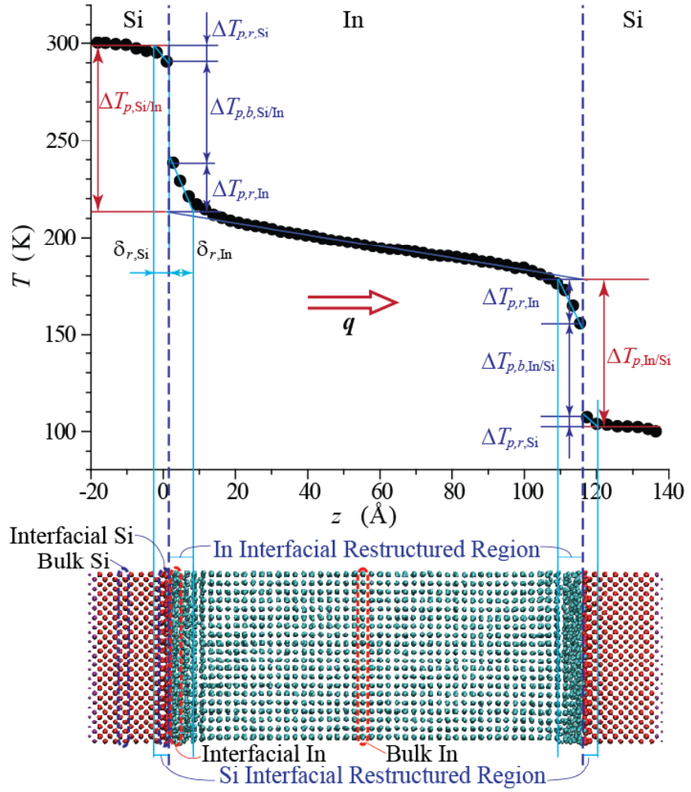
Atomic Restructuring in Interfacial Phonon Transport

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.

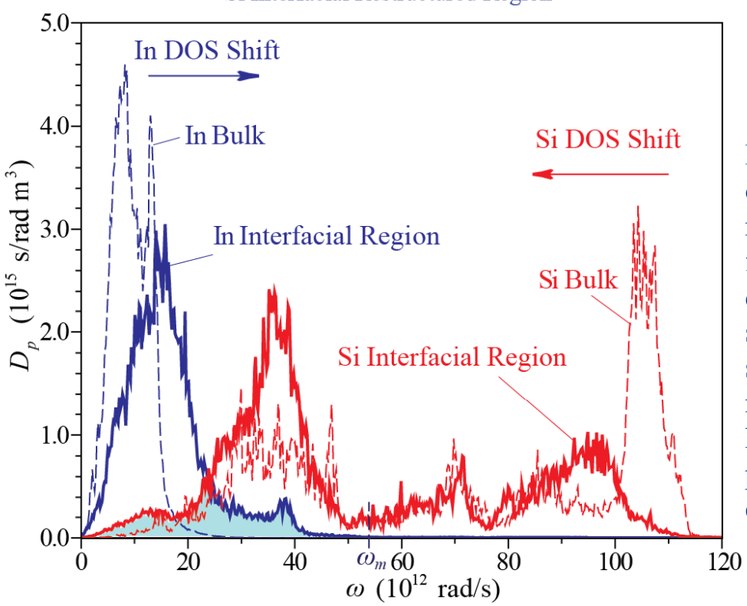


$$AR_{p,\mathrm{Si/In}} = AR_{p,b,\mathrm{Si/In}} + AR_{p,r,\mathrm{Si}} + AR_{p,r,\mathrm{In}}$$

(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 ($AR_{p,\mathrm{Si}}$ and $AR_{p,\mathrm{In}}$) and the total interfacial resistance ($AR_{p,\mathrm{Si/In}}$) [decomposed into the boundary ($AR_{p,b,\mathrm{Si/In}}$) and two interfacial region resistances ($AR_{p,r,\mathrm{Si}}$ and $AR_{p,r,\mathrm{In}}$)] 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_ps (solid lines) have more shared phonon states participating in the boundary transport, compare to the bulk D_ps (dashed lines).