Contribution of coherent and incoherent phonons to heat conduction

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Knowledge on characteristic lengths for phonons such as coherence length and mean free path is indispensable for thermal conductivity manipulation by structural control. While recent anharmonic phonon calculations have quantitatively revealed order of phonon mean free path, investigations on coherence length, being a length scale for wave nature of phonon, are still limited.

In this work, by performing molecular dynamics simulations to Lennard-Jones superlattices, we have calculated frequency-dependent coherence length of phonon at given temperature. Furthermore, from the obtained knowledge on coherence length, we have separately evaluated contributions of coherent and incoherent phonons to overall thermal conductivity in frequency space, which facilitates understanding of heat conduction in phononic crystal exploiting wave nature of phonon and leads to design low-coherence-loss phononic crystal.