Direct Atomistic Wave-packet Simulation of Coherent Phonon Transport in Superlattice Structures

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The molecular dynamics based phonon wave-packet method is a powerful tool for investigating how phonons defined from the dispersion of a bulk or functionalized material are scattered by some heterogeneous interface, amorphous layer, or other nanostructure. In this work, we conduct, to our knowledge, the first application of the wave-packet method to model phonons defined from the dispersion of the artificially periodic superlattice (SL) structure. The character of these "coherent phonons", which travel across the repeated interfaces of the SL without scattering, has previously been indirectly analyzed through macroscopic coefficients like thermal boundary conductance as a direct dissection of their transport behavior has been unavailable. We introduce the atomistic method and demonstrate an example application by a direct study of coherent phonon transmission through the aperiodic SL, also known as the random multilayer (RML). Our work offers important insights into the dynamics of coherent phonons in the RML and opens a new avenue for computational analysis of lattice thermal transport in artificially periodic structures.