Formulation of Phonon Spectral Energy Density for Measuring Frequencies

We present a formulation for the phonon spectral energy density which can predict phonon properties using *only* the velocities obtained from molecular dynamics simulations. This formulation of the phonon spectral energy requires no knowledge of the phonon properties *a priori*. Using this formulation, we calculate the spectral energy density of 3 systems; Lennard-Jones argon, bulk (Stilinger-Weber?) silicon, and carbon nanotubes (CNTs). Using this formulation, phonon properties (frequencies, group velocities, and relaxation times) are measured and compared to anharmonic lattice dynamics (ALD) and normal mode decomposition (NMD). The phonon frequencies are well characterized by this formulation, while the relaxation times show agreement with ALD and NMD only under certain conditions.