Comparison of spectral energy density and normal mode decomposition methods for predicting phonon properties

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To predict the thermal conductivity of a dielectric or insulating material requires the phonon frequencies and lifetimes. Numerous techniques for predicting these quantities have been proposed based in molecular dynamics simulation and lattice dynamics calculations. Here, the spectral energy density and normal mode decomposition techniques are described and applied to three test systems: Lennard-Jones argon, Stillinger-Weber silicon, and carbon nanotubes modeled with the REBO potential. We find that while the spectral energy density technique can be used to predict the phonon frequencies without the need for lattice dynamics calculations, it is not generally able to predict the lifetimes due to terms omitted in the original derivation.