**Predicting the Thermal Conductivity of Defected Systems using the Spectral Energy Density**

Accurately predicting the thermal conductivity of a dielectric or semiconducting material requires the properties of phonons from the entire Brillouon zone. Of particular importance are the phonon lifetimes, which are not accessible in experiment. Common theoretical techniques (e.g., lattice dynamics calculations) require the use of a perfectly periodic crystal to predict the required phonon properties. These techniques, however, break down when the system’s periodicity is broken (e.g., through point defects or the presence of an external fluid). The spectral energy density technique, where the atomic velocities are projected onto traveling waves, can predict the phonon properties of systems with a small perturbation from periodicity. In this study, we demonstrate that the spectral energy density technique can be used to model A1-xBx Lennard-Jones alloys with mass and bond point defects up to concentrations of x=0.1. The phonon lifetimes of these defected systems show afourth-power scaling with the inverse of the phonon frequency, consistent with Rayleigh scattering theory. The phonon dispersion is found to agree with predictions from a virtual crystal approximation.