Phonons 2012 Topics:

Lattice Dynamics
Phonons in glasses and disordered materials

Quantification of Ordered and Disordered Contributions to Lattice Thermal Conductivity

Understanding thermal transport in crystalline systems requires detailed knowledge of phonons, which are the quanta of energy associated with atomic vibrations. By definition, phonons are non-localized vibrations which transport quickly over distances much larger than the atomic spacings. For amorphous and disordered materials, the vibrations in the system are not completely characterized by phonons. With the exception of very long wavelength modes, the vibrational modes are localized and do not propagate like phonons in a crystal (see Section ). Commons models assume the mean free path of these localized vibrations is given by the average interatomic distance, while the group velocity for all the modes is equal to the speed of sound. While this approach can be used to estimate a lower limit to the thermal conductivity in amorphous and disordered systems, this approach can give only a qualitative description of the vibrations which contribute to the lattice thermal conductivity in disordered systems. Using Lattice and Molecular Dynamics calculations and Lennard-Jones model crystalline, alloy, and amorphous systems, we quantify and characterize the contribution from phonons and localized vibrations to the lattice thermal conductivity. The results are used to motivate simple and computationally cheap models which can predict the lattice thermal conductivity of a range of disordered materials.