Ordered and Disordered Contributions to Lattice Thermal Conductivity

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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 that transport energy over distances much larger than the atomic spacing. For disordered materials (e.g., alloys, amorphous phases), with the exception of very long wavelength modes, the vibrational modes are localized and do not propagate like phonons. The Einstein model assumes that the mean free path of these localized vibrations is the average interatomic distance and that their group velocity is equal to the speed of sound. The Cahill-Pohl model assumes that the mean free path of the localized modes is equal to half of their wavelength.[1] While these approaches can be used to estimate a lower limit to the thermal conductivity of disordered systems, they only provide a qualitative description of the vibrations that contribute to the lattice thermal conductivity.

Using lattice dynamics calculations and molecular dynamics simulations on Lennard-Jones crystalline, alloy, and amorphous systems, we predict and characterize the contributions from phonons and localized vibrations to lattice thermal conductivity. The results are used to motivate simple and computationally cheap models to predict the lattice thermal conductivity of a range of disordered materials.

[1]D. G. Cahill, S. K. Watson, and R. O. Pohl, “Lower limit to the thermal conductivity of disordered crystals”, *Phys. Rev. B* **46**, 6131 (1992).