Lattice Thermal Conductivity of Embedded Nanoparticle Composites: The Role of Particle Size Distribution

Theodore Maranets[1, C] and Yan Wang[1, S, C]

[1]*Mechanical Engineering, University of Nevada, Reno, Reno, NV, U.S.A.*
tmaranets@nevada.unr.edu

Nanoparticles embedded within a crystalline solid serve as impurity phonon scattering centers that reduce lattice thermal conductivity, a desirable result for thermoelectric applications. Most studies of thermal transport in nanoparticle-laden composite materials have assumed the nanoparticles to possess a single size. If there is a distribution of nanoparticle sizes, how is thermal conductivity affected? Moreover, is there a best nanoparticle size distribution to minimize thermal conductivity? In this work, we study the thermal conductivity of nanoparticle-laden composites through a molecular dynamics approach which naturally captures phonon scattering processes more rigorously than previously used analytical theories. From thermal transport simulations of a systematic variety of nanoparticle configurations, we empirically formulate how nanoparticle size distribution, particle number density, and volume fraction affect the lattice thermal conductivity. We find at volume fractions below 10%, the particle number density is by far the most impactful factor on thermal conductivity and at fractions above 10%, the effect of the size distribution and number density is minimal compared to the volume fraction. In fact, upon comparisons of configurations with the same particle number density and volume fractions, the lattice thermal conductivity of a single nanoparticle size can be lower than that of a size distribution which contradicts intuitions that a single size would attenuate phonon transport less than a spectrum of sizes. The random alloy, which can be considered as a single size configuration of maximum particle number density where the nanoparticle size is equal to the lattice constant, is the most performant in thermal conductivity reduction at volume fractions below 10%. We conclude that nanoparticle size distribution only plays a minor role in affecting lattice thermal conductivity with the particle number density and volume fraction being the more significant factors that should be considered in fabrication of nanoparticle-laden composites for potential improved thermoelectric performance.