

MAR16-2015-030144

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Mode resolved modeling of phonon-structure interactions in semiconductor nanocomposites

JOSEPH FESER, University of Delaware

Introducing nanoscale inhomogeneities into semiconductor alloys is a known route to enhance the scattering of long wavelength phonons and to subsequently reduce thermal conductivity. For key applications such as thermoelectric energy conversion materials, this must be done efficiently to avoid harming electronic functionality. Thus, key questions arise such as what type (i.e. contrast mechanisms), shape, size, and number density of particles should be used. This talk presents two new theoretical developments in this area from our group: (1) The use of continuum mechanics to analytically calculate exact phonon scattering cross sections of cylindrical and spherical shaped elastic discontinuities across the Mie regime, and their subsequent use in Boltzmann transport models of thermal transport and (2) the development of a new frequency-domain atomistic approach to simulate the scattering cross section of nanoparticles of arbitrary complexity for wavevectors spanning the entire Brillouin zone, and which can accommodate very large atomistic systems. Its advantages compared to Atomistic Green's functions and molecular dynamics will be discussed.