UC RIVERSIDE UNIVERSITY OF CALIFORNIA | Mechanical Engineering

ME 250 SEMINAR

Engineering Phonon Transport in Nanoparticle-in-Alloy Semiconductor Composites

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. 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 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 a wide range of wavelengths, and their subsequent use in Boltzmann transport models of thermal transport and (2) the development of a frequency-domain atomistic numerical approach to simulate scattering from nanoparticles of arbitrary complexity in a mode-resolved manner across the entire Brillouin zone. The efficiency and scalability of the approach allow for extremely large system sizes size to be studied, including systems that incorporate thousands of nanoparticles to understand multiple scattering effects including phonon localization.

THURSDAY, April 15, 2021 | **ZOOM** | **11:00 AM - 11:50 AM**

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