To Symposium N: Nanostructures for Phononic Applications

Title

Phonon transport simulations in large scale hierarchically disordered nanostructures

Authors

Neophytos Neophytou, Dhritiman Chakraborty, Laura de Sousa Oliveira

Affiliations

School of Engineering, University of Warwick

Abstract (1500)

Nanostructuring is a promising approach for next generation thermoelectric materials yielding ultra-low thermal conductivities and enhanced thermoelectric performance. More specifically, some of the lower thermal conductivities in nanocrystalline materials have been achieved in materials that include hierarchically sized structures, at the atomic size, the nanoscale, and mesoscale, which can scatter phonons of various wavelengths and reduce phonon transport throughout the spectrum.

In this work, we describe the development of a large scale, comprehensive Monte Carlo simulator to model thermal transport in nanostructured materials with a large and arbitrary degree of hierarchical disorder. Geometry induced scattering of phonons on grain boundaries, surfaces, several defects, voids, and dislocations as in realistic nanocomposite which all contribute to reducing thermal conductivity, are investigated. Although this study focuses on Si-based materials, we discuss extensions of our simulator capabilities to other type of promising thermoelectric materials with various types of embedded nanoinclusions. For this, we discuss how we couple useful transport properties from molecular dynamics and ab initio calculations. We believe that this multi-physics/multi-scale approach could play a very useful part in optimizing thermal conductivity reductions not only in advanced new-generation thermoelectric materials.