

Prediction of thermal conductivity in highly disordered nanocomposite structures: From large-scale Monte Carlo simulations to simple analytical models.

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Abstract

Nanostructuring is a promising approach for next generation thermoelectric materials yielding ultra-low thermal conductivities and enhanced thermoelectric performance. Some of the lower thermal conductivities in nanocrystalline materials have been achieved in materials that include hierarchically sized features, at the atomic size, the nanoscale, and the mesoscale. These can scatter phonons of various wavelengths and reduce phonon transport throughout the spectrum. However, understanding qualitatively, but more importantly quantitatively how hierarchical disorder reduces thermal conductivity in nanostructured materials, is still far from clear.

In this work, we solve the Boltzmann transport equation for phonons using the Monte Carlo method in Si-based nanostructures with a large degree of disorder. We examine thermal conductivity in structures with nanocrystalline grain boundaries, in addition to nanopores in both an ordered and highly randomized fashion. Such materials have recently demonstrated experimentally ultra-low thermal conductivities, even below the amorphous limit [1, 2]. We find that the influence of nanocrystallinity by itself on the thermal conductivity becomes dominant when the grain sizes become smaller than the average mean free path of phonons. We also show that the reduction in thermal conductivity in porous structures is significantly higher when the pores are randomized in terms of size and position, compared to when they are placed in an orderly fashion. Finally, we extract simple, analytical models that accurately captures the thermal conductivity in nanostructures which include a combination of nanograins and nanopores, either in ordered, or randomized fashions.

References:

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