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Analytical models for thermal conductivity in highly disordered nanostructures

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Abstract

Nanostructuring is a promising approach for next generation thermoelectric materials yielding ultra-low thermal conductivities and enhanced thermoelectric performance by scattering phonons of various wavelengths and reducing phonon transport throughout the spectrum. Despite intense theoretical and simulation works to investigate the effect of disorder on the atomistic scale using molecular dynamics and ab initio methods, accurate compact models, that can give first order prediction about the thermal conductivity of disordered materials do not yet exist.

In this work, we first solve the Boltzmann transport equation for phonons using the Monte Carlo method in Si-based nanostructures with large degree of disorder and then provide simplified models that accurately describe the effects of disorder at the nanoscale. We examine thermal conductivity in nanocrystalline structures which also include nanopores, both in an ordered and highly randomized fashion. Such materials have recently demonstrated experimentally ultra-low thermal conductivities, even below the amorphous limit [1, 2]. We also show quantitatively 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. We extract analytical models that capture quantitatively the thermal conductivity in nanostructures that include a combination of nanograins and nanopores, as in hierarchically disordered nanostructures [3]. Finally, we compare our models with predictions by Mattheissen's rule and find good agreement.

References:

[1] J. A. P.-Taborda, M. M.-Rojo, J. Maiz, N. Neophytou, M. M. González, *Nature Sci. Rep*., 6, 32778, 2016.
[2] J. Tang, H. T. Wang, D. H.Lee, M. Fardy, Z. Huo., T.P. Russell.,P. Yang. *Nano Letters*, 10(10), 4279-4283. 2010.
[3] D. Chakraborty, S. Foster, and N. Neophytou, *Phys. Rev. B* 98, 115435 (2018).