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Molecular dynamics simulations to understand phonon transport in nanoporous materials

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Abstract

Nanoscale pores and voids have been found to significantly decrease the thermal conductivity of thermoelectric materials. Recent works on Si-based nanoporous materials have reported thermal conductivities at, or even below the amorphous limit [1,2]. However, understanding the microscopic details of phonon scattering on pores and voids of various sizes and configurations, from a few to several nanometers and from ordered to disordered, also accounting for possible coherent effects, is far from complete. Although a large number of theoretical investigations concerning rough surfaces and boundary scattering can be found, studies on nanoporous materials are less common.

In this work, we present thermal conductivity results for bulk crystalline Si with (spherical) nanovoids and (cylindrical) nanopores, computed with equilibrium molecular dynamics (MD) using the Green–Kubo formalism. We perform an exhaustive investigation on how void/pore size, concentration and distribution affect thermal conductivity. To comprehend the full picture of the phonon transport physics in these geometries, we further perform a qualitative analysis of how individual acoustic and optical modes are scattered, by means of a wavepacket approach. This approach can visually show how the phonon modes interact with voids/pores as they pass through them; moreover, it can be generalized to boundaries and interfaces, which are similarly used to achieve drastic reductions in thermal conductivity. Finally, we discuss how the knowledge acquired with MD can be used in tandem with large-scale Monte Carlo simulations, which can help to bridge the gap between nano- and mesoscale transport for better predictions of thermal conductivity in highly disordered materials.

References:

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