The effect of geometry on thermal transport in nanoporous Si from large-scale molecular dynamics

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Abstract

Nanoporous materials are of broad interest for various applications, in particular advanced thermoelectric materials. The introduction of nanopores, even at modest levels, has been known to drastically reduce a material's thermal conductivity, in some cases even below its amorphous limit [1]. The effect of pore/void geometry and arrangement on thermal conductivity is complex. While several computational studies have addressed various geometrical aspects of porosity (e.g. pore surface area, number, size, shape, distance, roughness), a clear and complete understanding of the physical mechanisms that degrade the thermal conductivity has not yet been reached. Yet, a detailed understanding of the effect of pore configuration on thermal transport is key to engineering porosity to optimally reduce lattice thermal conductivity without significant detriment to electronic transport.

In this work [2], we perform an exhaustive atomistic-scale investigation of the effect of porosity on thermal transport in nanoporous bulk silicon using large-scale equilibrium molecular dynamics (of approximately 160,000 atoms). Upwards of 50 different geometries are considered, spanning a large number of geometrical degrees of freedom, such as (cylindrical) pores and (spherical) voids, different porosities, diameters, neck sizes, pore/void numbers, and surface-to-volume ratios, placed in ordered fashion, or fully disordered. We quantify and compare a number of important parameters that determine the thermal conductivity reductions in nanoporous materials. The main results are highlighted in this talk, including the effects of clustering and staggering, and geometry-dependent anticorrelation effects. Ultimately, the main result from this study is that even down to the nanoscale, the intuitive *line-of-sight* argument comes to be maybe the most important feature in understanding thermal conductivity in nanoporous materials, beyond other metrics such as porosity and surface/boundary scattering.

[1] Tang, J., *et* al. "Holey silicon as an efficient thermoelectric material." Nano letters, 10(10), 4279-4283.
[2] de Sousa Oliveira, L., Neophytou, N. (2019) "Large-scale molecular dynamics investigation of geometrical features in nanoporous Si" (under review at Physical Review B