Thermal transport in disordered nanoporous Si geometries from large-scale molecular dynamics

Laura de Sousa Oliveira*, Vassilios Vargiamidis, and Neophytos Neophytou
School of Engineering, University of Warwick, Coventry, CV4 7AL, UK
* **L.de-Sousa-Oliveira@warwick.ac.uk**

Abstract

The introduction of nanopores has been known to drastically reduce a material's thermal conductivity, in some cases even below its amorphous limit. A clear and complete 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, as is needed to increase *ZT*. However, the effect of pore/void geometry and arrangement on thermal conductivity is complex, and a detailed understanding of the physical mechanisms that degrade the thermal conductivity in nanoporous materials has not yet been reached.

We report on a comprehensive atomistic-scale investigation of the effect of porosity on thermal transport in nanoporous bulk silicon, in what are some of the largest-scale (approximately 160,000 atoms) molecular dynamics (MD) simulations of nanoporous materials found in the literature. 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. Ultimately, the most significant result from this study is that even at the nanoscale, the intuitive particle picture of a reduced phonon *line-of-sight* comes to be the most important feature in understanding thermal conductivity in nanoporous materials, beyond other metrics such as porosity, surface/boundary scattering or coherence effects. Interestingly, we also observed geometry-dependent anticorrelation effects that can contribute to further reduce thermal conductivity. Finally, we combine non-equilibrium Greens functions electron transport calculations with our MD results to estimate the effect of nanoporosity in *ZT*.