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Multi-Scale Phonon Transport Monte Carlo Simulations in Hierarchically Disordered Nanomaterials

Dhritiman Chakraborty[1,a], Samuel Foster[1,b], Neophytos Neophytou[1,c]

School of Engineering, University of Warwick, Coventry, CV4 7AL, U.K.

D.Chakraborty@warwick.ac.uk *(corresponding author),* S.Foster@warwick.ac.uk, N.Neophytou@warwick.ac.uk

Abstract

In nanostructures with feature sizes that could vary from a few up to hundreds of nanometers, phonon transport behaviour is distinctly different as compared to transport in bulk materials. As a result, materials with ultra-low thermal conductivities and enhanced thermoelectric performance can be realised. More specifically, some of the lower thermal conductivities in nanocrystalline materials have been achieved in materials that include hierarchical size of inclusions, at the atomic size, the nanoscale, and mesoscale, which can scatter phonons of various wavelengths and reduce phonon transport throughout the spectrum [1-2]. Another set of promising materials are nanoporous structures referred to as 'holey' materials, the most common of these are based on Silicon or SiGe [2-5]. The structure and porosity of these materials allows for ultralow thermal conductivity- even below the amorphous limit.

In this work, we describe the development of a large scale, comprehensive simulator to model thermal transport in nanostructured materials with a large and arbitrary degree of hierarchical disorder. Our simulations are based on the single phonon Monte Carlo (MC) algorithm to solve the Boltzmann transport Equation for phonons, which provides high computational efficiency, as well as accuracy [6]. Further, we discuss efforts to incorporate wave effects within the MC phonon transport algorithm, and how these influence heat transport. Geometry induced scattering of phonons on grain boundaries, surfaces, several defects, voids, and dislocations as in realistic nanocomposite materials (shown in **Fig. 1a**), which all contribute to reducing thermal conductivity, are examined; always while keeping in mind that significant degree of crystallinity should be allowed to keep the electronic conductivity high. Thermal conductivity reduction for a typical hierarchically nanostructured (but in ordered fashion) material is shown in the table of **Fig. 1b**. This work would be very useful in efforts to understand thermal conductivity in disordered materials, which are being heavily studied at the moment as efficient thermoelectric materials [2,5,8].

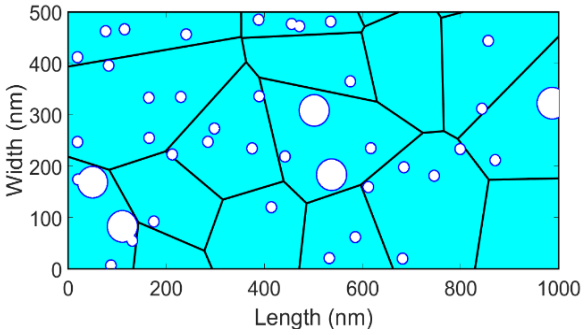

Figure 1a.: Geometry of simulation domain including defects, voids and grain boundaries.

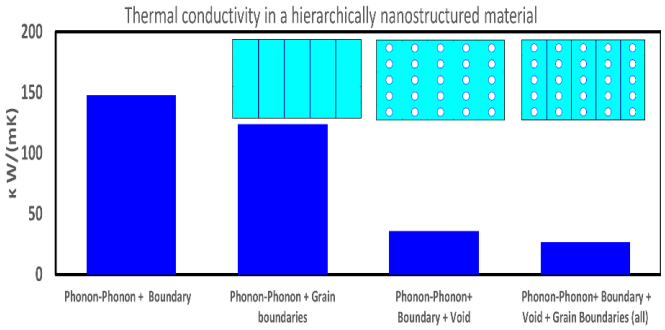

Figure 1b.: Thermal conductivity reduction for a typical hierarchically nanostructured material.

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