Phonon transport in hierarchically disordered silicon nanostructures: Monte Carlo to wave-informed Monte Carlo using multi-physics.

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Hierarchical nanostructuring can significantly reduce thermal conductivity due to phonon scattering at various wavelengths, reducing phonon transport throughout the spectrum, thus yielding high values of *ZT*. Such materials have experimentally demonstrated ultra-low thermal conductivities, even below the amorphous limit, and are excellent candidates for next generation thermoelectric applications [1, 2]. However, a comprehensive qualitative and quantitative theoretical understanding of heat transport in such materials requires large scale simulations that bridge across various length scales (atomic, nano, macro scales), which are dictated by different physics.

In this work, we consider the thermal conductivity in large scale highly disordered silicon-based hierarchical nanomaterials coupling features and insight extracted from Non-Equilibrium Green's Functions (NEGF) and Molecular Dynamics (MD) into Monte Carlo simulations. NEGF easily provides information about wave effects [3]. MD provides insight into atomistic effects, including anharmonicity among others [4] but both are limited by domain size. MC allows larger domain sizes and treatment of complex geometries. However, MC is stretched when incorporating minute feature sizes where wave effects and anharmonicity play a significant role. We first examine hierarchical nanoporous nanocrystalline structures with MC to arrive at analytical models that effectively describe hierarchical structures with a high degree of disorder [5,6]. We then adopt mode specific information extracted from NEGF and MD to get better accuracy for length scales where MC is limited. By incorporating wave effects and scale specific physics phonon transport can be treated more accurately in hierarchically disordered nanomaterials across length scales.

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