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Large scale atomistic approaches to thermal transport and phonon scattering in nanostructured materials[1]

IVANA SAVIC, Department of Chemistry, University of California at Davis, Davis, California, USA

Decreasing the thermal conductivity of bulk materials by nanostructuring and dimensionality reduction, or by introducing some amount of disorder represents a promising strategy in the search for efficient thermoelectric materials [1]. For example, considerable improvements of the thermoelectric efficiency in nanowires with surface roughness [2], superlattices [3] and nanocomposites [4] have been attributed to a significantly reduced thermal conductivity. In order to accurately describe thermal transport processes in complex nanostructured materials and directly compare with experiments, the development of theoretical and computational approaches that can account for both anharmonic and disorder effects in large samples is highly desirable. We will first summarize the strengths and weaknesses of the standard atomistic approaches to thermal transport (molecular dynamics [5], Boltzmann transport equation [6] and Green's function approach [7]) . We will then focus on the methods based on the solution of the Boltzmann transport equation, that are computationally too demanding, at present, to treat large scale systems and thus to investigate realistic materials. We will present a Monte Carlo method [8] to solve the Boltzmann transport equation in the relaxation time approximation [9], that enables computation of the thermal conductivity of ordered and disordered systems with a number of atoms up to an order of magnitude larger than feasible with straightforward integration. We will present a comparison between exact and Monte Carlo Boltzmann transport results for small SiGe nanostructures and then use the Monte Carlo method to analyze the thermal properties of realistic SiGe nanostructured materials. This work is done in collaboration with Davide Donadio, Francois Gygi, and Giulia Galli from UC Davis.

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[5] See e.g. Y. He, D. Donadio, and G. Galli, Nano Lett. 11, 3608 (2011).
[6] See e.g. A. Ward and D. A. Broido, Phys. Rev. B 81, 085205 (2010).
[7] See e.g. I. Savic, N. Mingo, and D. A. Stewart, Phys. Rev. Lett. 101, 165502 (2008).
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[9] See e.g. J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, Phys. Rev. B, 79, 064301 (2009).

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