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Atomistic simulations of heat transport in nanostructures

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Engineering materials at the nanoscale allows for tuning several of their properties over a broad range. These holds particularly for thermoelectric performances of group IV semiconductors, such as silicon and germanium. Experiments [1,2] suggest that improvements of the thermoelectric figure of merit in nanostructured silicon are mostly related to a drop in the thermal conductivity of about two orders of magnitude with respect to the bulk. In spite of success of macroscopic empirical approaches, we argue that atomistic simulations are necessary to provide the correct physical behavior and achieve significant understanding of a complex phenomenon such as thermal transport at the nanoscale ($\sim$ 10nm). By means of atomistic simulation methods, we address the issue of lattice thermal transport in silicon and SiGe nanostructures and nanostructured materials, e.g. nanowires, nanoporous and amorphous silicon thin films. We have reviewed and compared several simulation approaches (equilibrium and non-equilibrium molecular dynamics and anharmonic lattice dynamics), and developed a new method for large scale simulations, based on the scattering approach. We have identified strength, weaknesses and possible artifacts for each method, and established reliable simulation procedures to compute thermal transport properties. Our results shed light on the cooperative effects of dimensionality reduction, nanostructuring and disorder, in reducing the thermal conductivity of silicon-based nanostructured materials, stemming from prominent changes of lattice vibrational properties and enhancement of phonon scattering [3].

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