Predicting Thermal Transport in Nanostructured Materials using Multiscale Models (and *Ab-Initio* Calculations?)

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Controlling thermal transport is crucial for optimizing the performance, reliability, and lifetime of devices for electronic, optoelectonic, and energy conversion devices which commonly utilize semiconducting materials. Optimizing thermal transport in these devices and technologies offer the promise of reducing energy consumption at a national scale. Nanostructures (e.g., thin films, nanowires, superlattices) offer an intriguing opportunity to the tune thermal transport properties of the component materials, but multiscale models are necessary to provide the insight

Thermal transport in a semiconductor is controlled by phonons, quanta of energy associated with atomic vibrations. The properties of phonons are controlled at atomic-level length scales of 0.1-1 nm. Phonons themselves are non-localized vibrations which can extend over 100 nm – 10 microns in common semiconducting materials like silicon and germanium. A nanostructured material can be described by an effective thermal conductivity, which can be very different than the bulk values available in common references. The effective thermal conductivity of a nanostructure is lower than the bulk value due to the scattering of phonons with the system boundaries which have length scales of 10 nm – 100 microns. It is these boundary effects that provide the opportunity for controling thermal conductivity by engineering the device nanostructure. However, the relevant length scales involved span five order of magnitude.

Developing design strategies for controlling thermal conductivity through nanostructuring requires multiscale analysis. We present a multiscale model which can describe the thermal transport in nanostructures of arbitrary geometry. The required inputs are the nanostructure geometry, bulk phonon properties, and a boundary scattering model. The bulk phonon properties are obtained using *ab-initio* (from first-principles) calculations, which include quantum effects. *Ab-initio* methods, while computationally more demanding, are much more accurate than classical methods. The bulk phonon properties are inputs for a Monte Carlo sampling algorithm which accounts for the phonon-boundary scattering.

Thermal conductivities of nanostructures such as nanowires and nanoporous materials are predicted using the multiscale model and compared to experimental results. The results obtained provide insights to engineering novel nanostructures with tailored thermal conductivities. The work provides a compelling example of the necessity of mutilscale modeling.