Title:

Ultra-low thermal conductivity due to geometry dependent specular scattering in nanoporous Si

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Abstract:

Nanostructuring has been shown to substantially decrease the thermal conductivity of semiconducting materials thereby improving their thermoelectric efficiency. Current strategies focus on increasing scattering and reducing the mean-free-path of phonons across the spectrum. Whether coherence effects too can significantly affect thermal transport remains an open-ended question. We identify an unusual anticorrelated specular phonon scattering effect yielding an additional 80% decrease in the thermal conductivity of specific porous geometries. Specular scattering is a necessary requirement for coherence effects, and our simulations suggest that such effects can occur at room temperature. Large-scale equilibrium molecular dynamics (MD) simulations performed for nanoporous Si show the presence of negatively correlated (anticorrelated) heat flux. We further demonstrate with MD how the pore size-to-neck ratio and periodicity can be manipulated to control the strength and duration of the reflections. These results are corroborated by wave-packet simulations which show how heat becomes trapped between pores with narrow necks. The amount of heat trapped between the pores is wave-vector dependent, which could have widespread applications in heat guidance and phonon (frequency) filtering. Finally, we develop a simple analytical ray-tracing model to illustrate how specular scattering can give rise to anticorrelated heat flux, and reproduce the behavior observed in the MD simulations.