Stochastic Thermodynamics of Silicon Nanostructures

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Nanoscale thermal transport is a growing area of research due to its implications to a wide range of applications, from thermal cooling of electronic devices to thermoelectrics. In crystals, the transport is influenced by the interaction of phonons with nanoscale structural constraints, such as boundaries [1,2] and periodic features [3]. On the one hand, the analysis of the thermal conductivity provides insights into the different scattering mechanisms limiting heat conduction. On the other hand, the phonon band structures extracted from lattice dynamics or molecular dynamics (MD) simulations inform on the prevalence of wave-like mechanisms underlying the transport [4]. However, the non-equilibrium behavior of nanostructured crystalline systems is not completely illuminated using these traditional analysis frameworks.

Here, we present a methodology to characterize a number of microscopic mechanisms that affect the thermodynamical response in crystalline nanostructures at room-temperature, using both equilibrium and nonequilibrium MD simulations. We reveal that phonon mechanisms triggered by the atomic-scale nanostructures fundamentally modify the anharmonic phase-space for phonon interactions, with implications for thermal control and manipulation in semiconductors and a wider range of condensed matter systems.

References

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