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Full Band Monte Carlo Simulation of Phonon Transport in Semiconductor Nanostructures

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In this paper, a numerical simulation of thermal transport at the nanoscale is developed by solving the phonon Boltzmann transport equation by the Monte Carlo method. A full phonon dispersion is used to determine accurately the vibrational frequencies and group velocities of all phonon modes. Simultaneous conservation of energy and momentum in anharmonic phonon-phonon scattering events in enabled by a novel algorithm developed in this work. The inclusion of rough boundaries and the treatment of their impact on phonon transport is also discussed. The results demonstrate the convergence, accuracy, and efficiency of the proposed simulation.