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Full-Band Particle-Based Monte-Carlo Simulation with Anharmonic Corrections for Phonon Transport in III-N Nanostructures[1] SASI SUNDARESAN, Department of Electrical and Computer Engineering, Southern Illinois University, Carbondale, IL, THUSHARI JAYASEKERA, Department of Physics, Southern Illinois University, Carbondale, IL, SHAIKH AHMED, Department of Electrical and Computer Engineering, Southern Illinois University, Carbondale, IL — Monte Carlo based statistical approach to solve Boltzmann Transport Equation (BTE) has become a norm to investigate heat transport in semiconductors at sub-micron regime, owing to its ability to characterize realistically sized device geometries qualitatively. One weakness of this technique is that the approach predominantly uses empirically fitted phonon dispersion relation as input to determine the properties of phonons and predict the thermal conductivity for a specified material geometry. The empirically fitted dispersion relations assume harmonic approximation, thereby failing to account for thermal expansion, effects of strain on spring stiffness, and accurate phonon-phonon interactions. To account for the anharmonic contributions in the calculation of thermal conductivity, in this work, we employ a coupled molecular mechanics-Monte Carlo (MM-MC) approach. The atomistically-resolved non-deterministic approach adopted in this work is found to produce satisfactory results on heat transport and thermal conductivity in both ballistic and diffusive regimes for III-N nanostructures.

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