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BOLTZMANN-BGK-BASED MONTE-CARLO SIMULATION OF PHONON FLOW

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A Monte-Carlo simulation solver was developed for solving the phonon Boltzmann-BGK equation in order to explore the phonon behavior within nanostructured materials and predict the associated thermal conductivity. To reduce the computational amount, the grey medium approximation was adopted and thus only the nanostructures at a scale comparable to or smaller than the phonon mean free path were targeted. The solver was developed based on unstructured grids due to the randomness of nanostructures. Phonon bundles are first displaced at their group velocities and then possibly suffer intrinsic scattering; the scattering probability is determined by the phonon relaxation time. Phonon bundles are either transmitted through or reflected from boundaries or embedded interfaces; the inelastic acoustic mismatch and diffuse mismatch model are employed for specular and diffuse interfaces/boundaries respectively. Frequency and group velocity are reset according to the local temperature and the moving direction is randomly distributed whenever a phonon suffer scattering. Energy conservation needs special attention though when scattering occurs. Energy counters were employed to monitor the energy imbalance within each grid. Additional phonons must be generated or existing phonons must be eliminated whenever necessary.

Nanostructures investigated include superlattice thin films, nanowire-embedded-in-host materials, compact nanowire composites, compact nanoparticle composites, and nanocanyons assembled porous thin films. The thermal boundary resistance caused by the embedded interfaces was of particular interest. Size effect on the phonon motion and consequently on the effective thermal conductivity was explored and used to verify the effective medium approximation models.

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