Full Band Monte Carlo Simulation of Phonon Transport in Semiconductor Nanostructures

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INTRODUCTION

Thermal dissipation in increasingly scaled MOS devices has prompted strong interest in both phonon emission and subsequent thermal transport in semiconductor nanostructures [1], [2]. New multi-gate device designs further exacerbate thermal issues by further localizing heat dissipation [3]. Simultaneously, dwindling energy resources have created renewed interests in thermoelectric (TE), or solid-state, energy conversion and refrigeration using semiconductor-based nanostructures, such as nanowires, nanoribbons, and superlattices [4]. TE cooling is also an attractive approach for targeted cooling of local hotspots inside integrated circuits due to inherently no moving parts, ease of miniaturization and on-chip integration, and the nanostructures enhanced TE conversion efficiency. In addition, thermoelectric power generation enables the reuse of waste heat in a variety of applications, but requires dramatic reduction of passive heat losses through phonon nanoengineering [5]. Consequently, a deeper understanding of nanoscale heat transfer, especially phonon transport and phonon interactions with each other, impurities, and nanoscale boundaries, is imperative.

PHONON MONTE CARLO ALGORITHM

In this paper, I will present numerical simulation and modeling of phonon transport based on solving the phonon Boltzmann transport equation using the established Monte Carlo method. Several groups reported progress on phonon Monte Carlo specifically targeted at silicon nanostructures [6], [7], [8], but typically lacked two key ingredients: phonon dispersion was given by an analytical and isotropic approximation, and phonon-phonon anharmonic scattering only conserved energy overall (typically over all the scattering events in one time step), but did not conseve energy and momentum at the level of each individual interaction. In this work, I add the full phonon dispersion computed from the Adiabatic Bond Charge model [9] and combine it with the iterative algorithm for anharmonic phonon-phonon scattering which is capable of conserving energy and momentum in each individual collision [10]. During the simulation, each simulated phonon goes through a sequence of states interrupted by scattering and sampled after scattering according to the individual transition probabilities between the initial and final state as given by perturbation theory. The resulting simulation is a continuous-time Markov Chain with a continuous state space.

DISCUSSION

The phonon Monte Carlo simulation is performed using a fixed number of phonons (typically 10^5 to obtain good averages), which helps reduce the computational cost. In the absence of external forces and gradients, the ensamble converges to the equilibrium distribution, as shown in Fig. 1. Both relative energy and number of phonons in each branch fluctuates, but converges to their equilibrium values after about 20 ns, as shown in Fig. 2 and 3. The thermal conductivity tensor is extracted using the Green-Kubo formula for heat flux autocorrelation function [11]

$$\kappa_{\alpha,\beta} = \frac{V}{k_B T^2} \int_0^{N\Delta t} \langle J_\alpha(t) \cdot J_\beta(0) \rangle dt \qquad (1)$$

where the bracket represents an ensamble average, N is the total number of time steps (typically 5×10^5) and Δt is the time step (typically 1 ps). A typical autocorrelation function (scaled by its initial value) is plotted in Fig. 4, where convergence of both the heat flux and velocity autocorrelation functions can be observed after around 50 ps, which is on the order of the phonon relaxation time.

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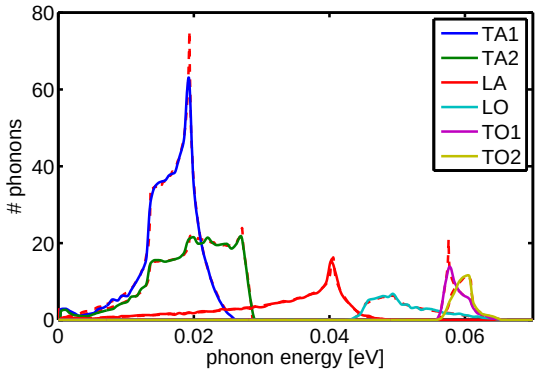

Fig. 1. Phonon energy histogram (solid line) and the equilibrium phonon distribution (dashed line) showing excellent agreement. In the absence of external gradients, the ensamble fluctuates around and converges to the equilibrium distribution.

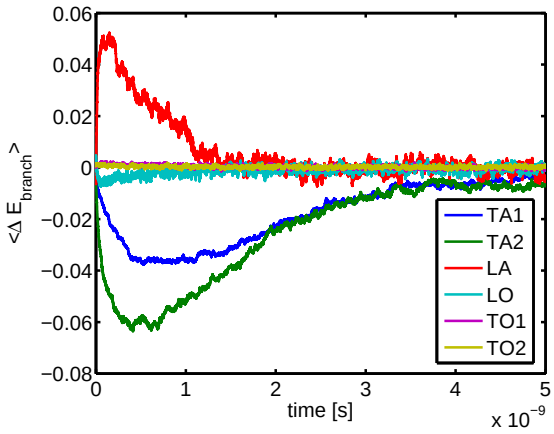

Fig. 2. Difference between average phonon energy and its equilibrium value for each phonon branch. The energy of phonons in each branch converges to the equilibrium value after 2-3 ns, much longer than the typical phonon relaxation time (≈ 50 ps)

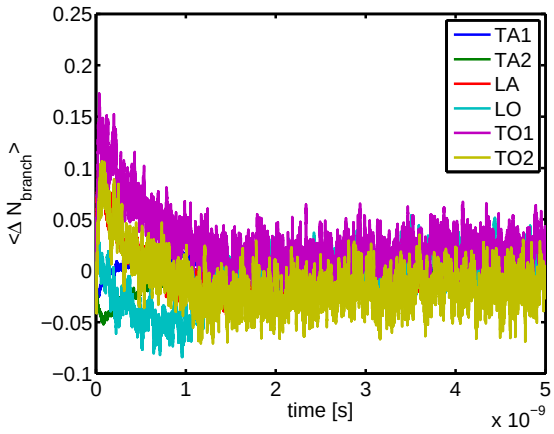

Fig. 3. Difference between the proportion of phonons in each branch and its equilibrium value, showing that phonons redistribute themselves according to the equilibrium distribution but undergo random thermal fluctuations due to scattering.

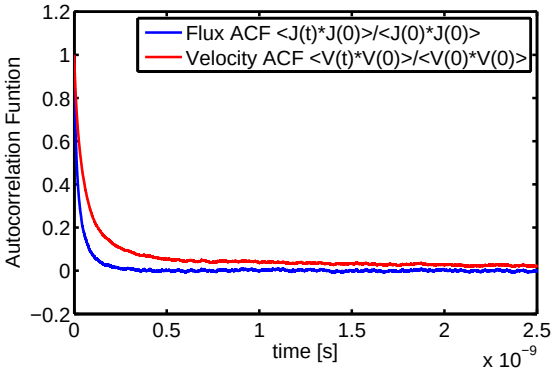

Fig. 4. Scaled heat flux (blue) and velocity (red) autocorrelation functions, showing rapid convergence after around 50 ps due to randomization of phonon direction during scattering.

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