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A hybrid phonon Monte Carlo-diffusion method for ballistic-diffusive heat conduction in nano- and micro- structures

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ABSTRACT

The existing phonon Monte Carlo (MC) for ballistic-diffusive heat conduction are limited to small and simple structures owing to the huge time cost following with the increasing scale. This article presents a new hybrid phonon Monte Carlo-diffusion method for ballistic-diffusive heat conduction, which successfully characterizes the ballistic effect with significantly reducing the computational cost. Based on the idea that the phonon-boundary scattering mainly affects the regions adjacent to the boundaries when the system is considerably large, the whole system is divided into three zones: the boundary MC zone and the middle diffusion zone, between which is the overlap zone. By using an alternating method and setting virtual phonon bath or specular reflection as the boundary condition for the MC zones, the results of the phonon tracing MC and diffusion equation can be coupled and converge at the overlap zone. To verify, the cross-plane and in-plane film heat conduction, where slip boundary conditions are the major characteristics of the ballistic-diffusive regime, are simulated by the hybrid method as well as standard phonon tracing MC which works as a benchmark. It is found that the hybrid method can accurately predict the distributions of temperature and heat flux in the system with nearly the same precision as the phonon tracing MC while the computation time can reduce up to 90%, validating its potential use for larger and more complex structures.

1. Introduction

Thermal management is of critical importance for further miniaturization and integration of the next-generation electronic devices since the danger of overheating has emerged as a major concern in the design and operation of computing devices [1]. Local hot spots, which have much higher temperature than the average value of the die, reduce the lifetime of electronic devices remarkably. According to the data reported in 2006, more than 50% of integrated circuit (IC) failures are related to thermal issues [2], and the figure is supposed to be higher now as chips are more complex boasting larger number of transistors. Therefore, it is necessary to perform the thermal analyses of electronic devices for the improving designs aimed to eliminate hot spots.

Heat conduction in micro- and nano- electronic devices is a principle path of cooling and has attracted much attention. The classical Fourier's law, which considers heat is conducted diffusively with the thermal conductivity of bulk materials, is found to be only valid in macroscale. When the characteristic length of the structure reduces to micrometer and nanometer, a growing number of experimental measurements have observed the reduction of the thermal conductivity compared to the bulk value [3–10], indicating the failure of Fourier's law. Thus, great efforts have been devoted to investigating such non-Fourier heat conduction in the micro- and nano- scale in past decades. Theoretical models which could take the memory, non-local and nonlinear effect into consideration were proposed to modify Fourier's law [11–16]. These models have explained the major contributions to non-Fourier heat conduction well, but such analyses required a considerable amount of tedious mathematical derivations even for one-dimensional systems. It is nearly unachievable to establish the closed-formed expressions in theory to predict thermal properties when considering more dimensions and more complicated structural configuration. As a result, numerical methods were extensively developed to overcome the bottleneck by converting the difficulty of analyses to computation. First-principles calculation [17] is an atomic level approach and usually works as a preprocess to obtain key parameters for other numerical methods, such as, the potential function or atomic force constant. Molecular dynamics (MD) simulation [18] directly simulates the movement of a molecular system with the achievable maximum particle number of several million and is almost limited to the scale of tens of nanometers [19]. At a larger length scale, numerically solving

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phonon Boltzmann transport equation (BTE) is an active topic. Phonons, which represent the quantization of lattice vibration, are deemed to be the dominating heat carriers in semiconductors [20]. Spherical harmonic method [21], lattice Boltzmann method (LBM) [22] and Monte Carlo (MC) [23–35] are the commonly used numerical solutions of BTE. Spherical harmonic method is an approximate method, whose accuracy strongly depends on the approximation order. LBM is easy to deal with complicated structures, but it is limited by the grid model and can lose some details during the solving process. The MC method is especially flexible for use with complex geometric configurations and can readily include different scattering mechanisms. To explicitly study the non-Fourier heat conduction, phonon MC simulation is a worth recommending approach.

In general, two kinds of phonon MC methods are mostly adopted in related researches: (1) direct simulation Monte Carlo (DSMC), which is also called the ensemble MC [23–25], and (2) the phonon tracing MC [26–35]. DSMC, where the trajectories of phonons are simulated simultaneously at each time step, was first introduced by Peterson for phonon transport in a Debye crystal [23] and subsequently improved via considering the dispersion and polarization [24], as well as the contribution from optical phonons [25]. In contrast, the phonon tracing MC simulates phonon trajectories independently, bringing about a significant reduction of calculation costs compared to DSMC [26]. Klitsner et al. [27] employed the phonon tracing MC to study phonon surface scattering of silicon crystals under 100 K. Then, this method is more likely to be used for room temperature simulations with a wide range of structures, including nanofilms [28], nanowires [29], nanoporous materials [30] and nanomeshes [31], as well as transistors [32]. These work have proved that the results of the phonon tracing MC have a good agreement with existing models and experiments. Recently, Tang et al. [33–35] investigated the thermal wave effects in ballistic-diffusive regime using the phonon tracing MC. To sum up, the phonon tracing MC has a very good performance for problems of the complicated geometry and multi-scattering events, and can also handle the ultrafast transport processes.

The phonon tracing MC has demonstrated that the size effect of effective thermal conductivity observed in micro- and nano- scale experiments can be explained by phonon ballistic-diffusive heat conduction, since the calculated effective thermal conductivity agrees well with experiment measurements [28,29,36]. The Knudsen number which describes the strength of the size effect is defined as $Kn = l_{MFP}/L$, where l_{MFP} denotes the phonon mean-free-path (MFP) and L denotes the characteristic length of the system. For the acoustic thick limit ($Kn \to 0$), the phonon–phonon scattering is sufficient and all phonons travel diffusively, as a result of which Fourier's law is valid. For the acoustic thin limit ($Kn \to \infty$), the phonon-boundary scattering dominates the transport process and phonon travels directly from one boundary to the other without scattering, resulting in the ballistic transport. For a middle Kn, the corresponding regime is called the ballistic-diffusive heat conduction [37]. As the physical and ubiquitous features of the boundary-driven steady state non-Fourier heat conduction, the boundary temperature jump and heat flux slip have been substantially investigated. Figs. 1 and 2 show the boundary temperature jump and boundary heat flux slip observed in the cross-plane and in-plane heat conduction in a nanofilm, respectively. The

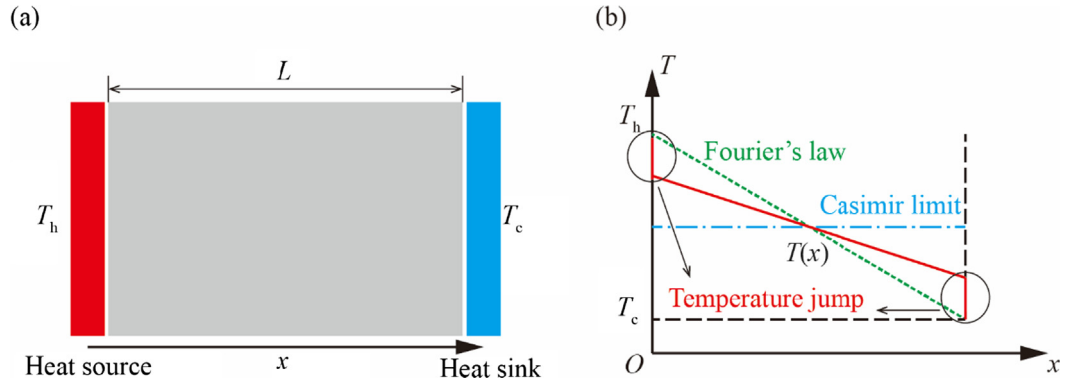

Fig. 1. (a) Schematic diagram of the cross-plane heat conduction in a film: a nanofilm with a characteristic length of L, in contact with two phonon baths of temperature T_h and T_c. (b) Temperature jumps, δT_h and δT_c, occur at the boundaries, but the temperature distribution is still linear in the middle region.

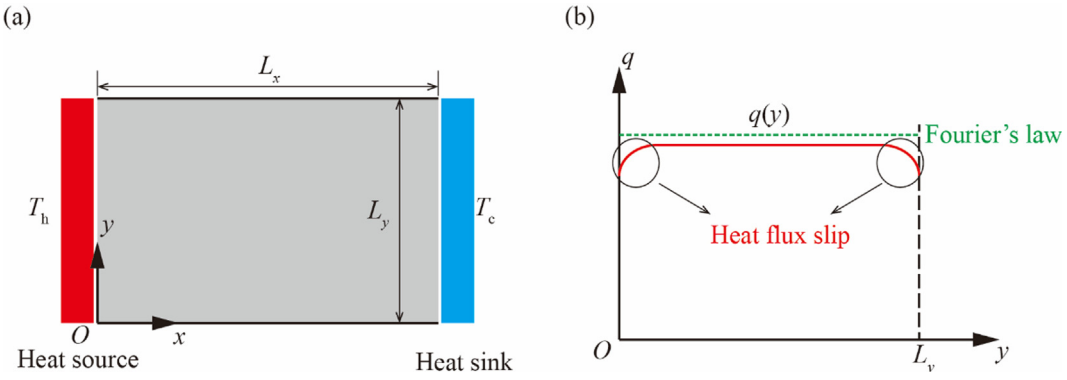

Fig. 2. (a) Schematic diagram of the in-plane heat conduction in a film: a nanofilm with the x-directional length of L_x and y-directional thickness of L_y. Two phonon baths of temperature T_h and T_c are placed in the x-direction, and two adiabatic boundaries are set in the y-direction. (b) The heat flux slip occurs at regions adjacent to the boundaries, but $q(y)$ is nearly uniform in the middle region.