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Interfacial phonon transport with frequency-dependent transmissivity by Monte Carlo simulation

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ABSTRACT

Interfacial phonon transport widely exists in nanosystems, yet the physical mechanism has never been well understood. In this work, a numerical framework is developed for interfacial phonon transport between dissimilar materials with a frequency-dependent transmissivity by introducing the spectral diffuse mismatch model into an efficient kinetic-type Monte Carlo scheme. The numerical method is validated by modeling cross-plane phonon transport through several single-layer and bi-layer thin films, which shows good agreement with the discrete-ordinates solutions. Through mesoscopic modeling, the size effect of Kapitza conductance is found to be weak or vanishing when the equivalent equilibrium temperature or emitted phonon temperature is adopted for defining the interfacial temperature difference respectively. Furthermore, the effective Kapitza conductance decreases when interfacial roughness is introduced, which can be mainly ascribed to the increased interfacial area ratio by roughness. For engineering application, an empirical power law is proposed for the dependence of effective Kapitza conductance on interfacial area ratio. The present work will promote fundamental understanding and modeling capability of interfacial heat transport, as well as engineering design and optimization of interface in nano devices.

1. Introduction

In the past several decades, with the rapid developments of micro- and nano- manufacturing and nano-technology, there are increasing interests in nanoscale heat transport [1,2]. The thermal management of micro- and nano-electronics is pursuing thermal interfacial materials with high thermal conductivity [3]. The introduction of complex interfaces including dislocations, grain boundaries etc., is one of the main methods to improve the figure of merit of nanostructured thermoelectric material [4–6]. Both of the above two issues require a profound understanding of the physical mechanism in interfacial phonon transport. The classical Fourier's law, which is valid for heat transport in bulk material, becomes no longer available for this situation [1,7], where phonon-interface scattering is dominant over the intrinsic scattering. Therefore, it is essential to develop effective theories and methods for modeling interfacial phonon transport.

The interface between two dissimilar materials will cause a cross-plane thermal transport resistance comparable to the intrinsic thermal resistance of each material layer. There will be a temperature jump across the interface and the ratio of temperature jump to the heat flux across the interface is defined as Kapitza resistance or thermal boundary resistance. The Kapitza conductance or thermal boundary conductance is also often used as the inverse of the Kapitza resistance. There have been mainly two categories of approaches to predicting the thermal boundary conductance: (*i*) microscopic methods including molecular dynamics simulation [8–10], atomistic Green's function method [11–13], etc.; (*ii*) mesoscopic modeling based on the phonon Boltzmann equation [14]. The microscopic methods are usually situated for small nanostructures and simple interfaces due to an intensive consumption of computational time and resources. In contrast, the phonon Boltzmann modeling represents a feasible approach for much larger structures and more complex interfaces. The mesoscopic modeling requires an important physical parameter in determining the Kapitza conductance between a material pair: phonon transmission coefficient across the interface.

The classical models for phonon transmission coefficient include the acoustic mismatch model (AMM) [15] and the diffuse mismatch model (DMM) [16]. The AMM treats phonons as a kind of acoustic waves transmitting through the interface. The transmission coefficient is calculated from the acoustic impedance of materials that form the interface [15]. It provides an appreciably good prediction of Kapitza conductance at very low temperature

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where phonons are mainly populated at low frequency with wavelengths much larger than the size of interfacial asperity. In elevated temperature scope, the AMM becomes often overestimating the Kapitza resistance because of the stronger Rayleigh scattering of the phonon population when shifting to higher frequency scope with wavelengths comparable to or even smaller than the size of interface asperity [16,17]. The DMM was thus proposed, treating phonons as a kind of particles transmitting diffusely through the interface without keeping the information of the side they come from. The transmission coefficient is determined by the phonon dispersion relations of both materials. The DMM often works well at higher temperature such as around the room temperature [16]. Some mixed models have also been developed which consider partially specular and partially diffuse transmission through the interface, yet based on simplified gray Debye's approximation [14]. On the other hand, the portion of specular scattering at the interface, known as the interfacial specularity parameter, is difficult to specify in prior and has to be extracted from fitting the experimental results. Therefore, the DMM is currently the most popular one for describing interfacial phonon transport in realistic applications around room temperature inferred from some good agreements between Kapitza conductances measured by experiments and predicted by simulations for different material pairs [18–20].

Taking into account the aforementioned models for phonon transmission coefficient, people have paid much effort to study interfacial phonon transport by solving the phonon Boltzmann equation [14,21–25]. Two categories of numerical schemes are currently available for the solution of Boltzmann equation, including the deterministic method (discrete-ordinates method [14,25], finite volume method [21], lattice Boltzmann method [26] and so on) and the stochastic method (Monte Carlo method [22–24]). Monte Carlo method avoids directly solving the high-dimensional Boltzmann equation by tracking the phonon dynamics through the pseudo-particles. Therefore, the interface boundary treatment in Monte Carlo method is simpler with a clearer physical picture via mimicking the realistic phonon-interface scattering. As a result, the Monte Carlo method is a better choice compared with the deterministic methods for studying interfacial phonon transport with complex geometries. Jeng et al. [22] first used Monte Carlo method to model the thermal conductivity of nanoparticle composites based on the DMM under gray Debye's approximation. Huang et al. [23] presented an improved Monte Carlo scheme to simulate interfacial phonon transport based on the gray mixed interface model proposed in Ref. [14]. Recently, Péraud and Hadjiconstantinou [24] modeled the Al/Si interfacial heat transport in transient thermo-reflectance experiments using energy-based variance-reduced Monte Carlo formulations based on a semi-spectral interface model considering gray transmission coefficient for each individual frequency at mono-direction [27]. Besides, there are several Monte Carlo simulations of phonon transport through grain boundaries in polycrystalline nanostructures with empirical expressions for spectral transmission coefficient [28–30]. To sum up, the previous Monte Carlo simulations of interfacial phonon transport merely considered a constant gray transmissivity at one direction or at both directions between dissimilar materials, in spite of an empirical treatment of frequency-dependent transmissivity through grain boundary within a single material. It remains to carefully consider the strongly frequency-dependent interfacial phonon transmissivity between dissimilar materials, which has been demonstrated significant in both microscopic computation [13] and recent experimental measurement [31].

The aim of the present work is to develop a numerical framework for interfacial phonon transport between two material pairs by introducing the spectral diffuse mismatch model (SDMM) into an energy-based variance-reduced Monte Carlo scheme. Although the SDMM is still a crude approximation to the realistic situation in interfacial phonon transport [18], it is the most appropriate theoretical model available currently. In principle, when supplied with the detailed frequency-dependent phonon transmissivity from recent first-principle calculation [32,33], the phonon Boltzmann modeling can provide a more accurate description of interfacial heat transport. Yet for the convenience of development of numerical framework, we take the classical SDMM into account as a first step. The inclusion of *ab initio* frequency-dependent transmissivity into the present Monte Carlo scheme is straightforward and will be investigated in the future work. The remaining of this article is organized as below: a brief fundamental knowledge of the kinetic-type Monte Carlo method and a detailed introduction of the novel interface boundary treatment, are presented in Section 2. Section 3 gives the validation of our Monte Carlo framework by modeling cross-plane phonon transport through both single-layer and bi-layer thin films. Two pertinent applications are studied in Section 4: including the size effect and roughness effect on Kapitza conductance. Concluding remarks are finally made in Section 5.

2. Numerical method

Phonon Monte Carlo scheme is a kind of pseudo-particle method to solve the phonon Boltzmann equation [34], with its earlier counterpart in rarefied gas flow the direct simulation Monte Carlo (DSMC) [35–38]. It takes statistical samples (phonon energy packets in this work) to simulate phonon dynamics, where the drift process and scattering process take place separately. The required macroscopic information (temperature, heat flux, and so on) is then extracted by averaging over these statistical samples. The kinetic Monte Carlo scheme is adopted for solution of the energy-based deviational phonon Boltzmann equation [24,34,39]:

$$\frac{\partial e^{\mathrm{d}}}{\partial t}+\mathbf{v}_{\mathrm{g}}\cdot\nabla e^{\mathrm{d}}=-\frac{e^{\mathrm{d}}-(e^{\mathrm{eq}}_{\mathrm{loc}}-e^{\mathrm{eq}}_{T_{\mathrm{eq}}})}{\tau(\omega,\mathrm{p},T)}, \tag{1}$$

where $e^{\mathrm{d}}=\hbar\omega(f-f^{\mathrm{eq}}_{T_{\mathrm{eq}}})$ is the deviational energy distribution with the reduced Planck constant $\hbar$, phonon angular frequency ω, phonon distribution f and the Bose-Einstein distribution $f^{\mathrm{eq}}_{T_{\mathrm{eq}}}=[\exp(\hbar\omega/k_{\mathrm{B}}T_{\mathrm{eq}})-1]^{-1}$ at the referenced equilibrium temperature T_{eq}; $\mathbf{v}_{\mathrm{g}}$ is group velocity, $\tau(\omega,\mathrm{p},T)$ being the relaxation time for phonons with frequency ω, polarization p at a thermodynamic temperature T; $e^{\mathrm{eq}}_{\mathrm{loc}}=\hbar\omega f^{\mathrm{eq}}_{\mathrm{loc}}$ and $e^{\mathrm{eq}}_{T_{\mathrm{eq}}}=\hbar\omega f^{\mathrm{eq}}_{T_{\mathrm{eq}}}$ being the pseudo-equilibrium and equilibrium energy distributions at pseudo-equilibrium temperature T_{loc} and referenced equilibrium temperature T_{eq} respectively. The linearized version of Eq. (1) is actually solved under tiny temperature difference assumption in kinetic Monte Carlo scheme [34,39], with a more detailed introduction presented in Appendix A.

2.1. Interface treatment

The spectral diffuse mismatch model (SDMM) [40] is introduced into the kinetic Monte Carlo scheme considering only elastic phonon interfacial scattering without any polarization conversion. In other words, we do not consider the conversion of longitudinal acoustic phonon into transverse one or vice versa when the phonon scatters at the interface. The transmission coefficient is derived by applying the principle of detailed balance and the diffuse scattering assumption at interface. The phonon heat flux across the interface from side 1 to side 2 is expressed as [40]:

$$q_{1\to2}=2\pi\sum_{\mathrm{p}}\int_0^{\pi}\int_0^{\omega_{\mathrm{m}}}\cos\theta\sin\theta\hbar\omega f(\omega,T_{\mathrm{e1}})\alpha_{12}(\omega,\mathrm{p})D_1(\omega,\mathrm{p})\nu_{1\mathrm{g}}\mathrm{d}\omega\mathrm{d}\theta, \tag{2}$$