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Mean free path dependent phonon contributions to interfacial thermal conductance

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ABSTRACT

Interfacial thermal conductance as an accumulation function of the phonon mean free path is rigorously derived from the thermal conductivity accumulation function. Based on our theoretical model, the interfacial thermal conductance accumulation function between Si/Ge is calculated. The results show that the range of mean free paths (MFPs) for phonons contributing to the interfacial thermal conductance is far narrower than that for phonons contributing to the thermal conductivity. The interfacial thermal conductance is mainly contributed by phonons with shorter MFPs, and the size effects can be observed only for an interface constructed by nanostructures with film thicknesses smaller than the MFPs of those phonons mainly contributing to the interfacial thermal conductance. This is why most experimental measurements cannot detect size effects on interfacial thermal conductance. A molecular dynamics simulation is employed to verify our proposed model.

1. Introduction

Heat transfer across the interface between two different materials has been studied for many years. In 1941, Kapitza first observed that when heat flows through two different materials [1], there is a temperature jump at the interface. The interfacial thermal conductance is used to measure the ability of heat to transfer across an interface, which is called Kapitza conductance. In 1989, Swartz et al. [2] reported a theoretical model to describe the interfacial thermal conductance, and this model is widely used to calculate the interfacial thermal conductance between two different bulk materials [3,4]. As described in Swartz's work [2], the interfacial thermal conductance across an interface depends only on the intrinsic properties of the two contacting materials, such as the density of phonon states and phonon group velocity, and has no dependence on the material size. If the sample size is large enough, interfacial thermal conductance can be considered an intrinsic property that depends only on the contacting conditions and materials, which is also the case for the material's thermal conductivity; this is consistent with the theoretical prediction. We know that thermal conductivity depends on sample size at the nanoscale, which is defined as the size effect. Therefore, if the sizes of two contacting samples are reduced to the nanoscale, is it possible to observe the size effects on interfacial thermal conductance? In a pump-probe experiment, it was reported that the thermal conductivity was dependent on the size of the heated region at low temperature, while the interfacial thermal conductance was independent of the heated region; thus, no size effect was observed on the interfacial thermal conductance [5]. Similarly, it was found that the interfacial thermal conductance across an epitaxial Bi film on a Si substrate is independent of film thickness [6,7], indicating that the size effects on the interfacial thermal conductance are not apparent. It seems that the classical theoretical model for interfacial thermal conductance is effective when the size of the samples is reduced to the nanoscale. However, recent reports [8–10] noted that obvious size effects have been observed on the interfacial thermal conductance of interfaces formed between nanoscale structures, and the theoretical model becomes invalid and even fails to explain the size effects. For instance, molecular dynamics (MD) simulations demonstrated that the interfacial thermal conductance varies with the system length, while the theoretical model only predicts a constant value that is independent of the system length [8]. The same method was used to demonstrate that the interfacial thermal conductance is independent of the cross-section area under periodic boundary conditions but is linearly proportional to the inverse of the system length [10]. Moreover, in a recent experiment, layer number dependent interfacial thermal conductance was observed between two multiwall carbon nanotubes [9], which manifested strong size effects.

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Therefore, whether the classical theoretical model is valid for the interfacial thermal conductance between nanostructures remains unclear.

Over the last decade, dramatic achievements have been made in exploring the thermal conductivity accumulation function [5,11–18]. Undoubtedly, these achievements have expanded our understanding of nanoscale thermal properties, especially when the sample size of a material is comparable to the phonon mean free paths (MFPs). Similar to the thermal conductivity accumulation function, the concept of the interfacial thermal conductance accumulation function that describes MFP-dependent contributions of phonons to the interface thermal conductance was also proposed [12], and it was revealed that the range of MFPs contributing to interfacial thermal conductance is far narrower than the range of those contributing to thermal conductivity. However, due to the assumption of a Debye dispersion and density of states as well as the high temperature occupancy limit, this model is coarse in that it can only give a rough trend of the interfacial thermal conductance accumulation function across two materials with different Debye temperatures. Keblinski et al. used a new theoretical model and MD simulations to investigate the size effects on the interfacial thermal conductance [19,20]. They found that, in the composite structure of a thin film contacting a substrate, the phonons transmitting from the substrate to the film can be reflected back to the substrate by the film surface when the thickness of the film is small enough, leading to the reduction of the effective phonon transmission coefficient. The results show that the size effects on the interfacial thermal conductance are the combined effects of boundary scattering and intrinsic phonon–phonon scattering. In a previous publication, it was suggested that the effect of film thickness on the thermal conductance can be predicted by considering the frequency dependence of the phonon MFPs [21]. However, the study did not give the explicit relationship between the thermal conductance and the phonon MFPs.

Referring to earlier studies on MFP range and size effects on interfacial thermal conductance, a new theoretical model is put forward to describe the accumulation function that describes the MFP-dependent phonon contributions to interfacial thermal conductance. Compared to the previous publication [12], this model is more rigorous, with fewer assumptions, which gives more accurate predictions of the interfacial thermal conductance accumulation function. In addition, the relationship between the interfacial thermal conductance and thermal conductivity can be derived from our model. Based on the derived model, the interfacial thermal conductance accumulation function for the Si/Ge interface is calculated using the density functional theory [22] (DFT) and the Boltzmann transport equation [23] (BTE) methods. With the help of the model, it is possible to determine the size effects on the interfacial thermal conductance across a nanostructure contacting a substrate. A MD simulation [24] is performed to verify the theoretical model. This study is expected to provide a new insight into the size effects on interfacial thermal conductance.

2. Theoretical model

To derive the interfacial thermal conductance accumulation function, we begin with the theoretical model of interfacial thermal conductance given by Swartz et al. [2], which can be derived from the principle of detailed balance [4,25]:

$$\frac{\dot{Q}^{gross}_{1\to 2}(T)}{A} = \frac{1}{2}\sum_j \int_0^{\frac{\pi}{2}}\int_0^{\infty} N_{1,j}(\omega,T)\hbar\omega v_{1,j}\gamma_{1\to 2}(\theta,j,\omega) \times \cos(\theta)\sin(\theta)d\theta d\omega \quad (1)$$

where the subscripts 1 and 2 correspond to the materials on side 1 and side 2, respectively, $\dot{Q}^{gross}_{1\to 2}(T)$ is the gross heat current from side 1 to side 2, A is the cross-sectional area, j is the phonon mode, ω is the phonon frequency in side 1, $v_{1,j}$ is the phonon group velocity, $\gamma_{1\to 2}(\theta,j,\omega)$ is the phonon transmission probability, and T is the temperature. $N_{1,j}(\omega,T)$ is the product of the density of phonon states $D_{1,j}(\omega)$ times the Bose occupation factor g_{BE}, which can be expanded as follows:

$$N_{1,j}(\omega,T) = D_{1,j}(\omega)g_{BE} \quad (2)$$

The interfacial thermal conductance equals the derivative of the gross heat current per area. Using Eq. (2), the interfacial thermal conductance across two isotropic bulk materials can be written as:

$$G_{bulk} = \frac{\partial \dot{Q}^{gross}_{1\to 2}(T)}{A\partial T} = \frac{1}{2}\sum_j \int_0^{\frac{\pi}{2}}\int_0^{\infty} D_{1,j}(\omega)\frac{\partial g_{BE}}{\partial T}\hbar\omega v_{1,j}\gamma_{1\to 2}(\theta,j,\omega) \times \cos(\theta)\sin(\theta)d\theta d\omega \quad (3)$$

Here, the volumetric specific heat capacity per unit frequency can be written as:

$$C_{1,j}(\omega) = D_{1,j}(\omega)\frac{\partial g_{BE}}{\partial T}\hbar\omega \quad (4)$$

Using Eq. (4), Eq. (3) can be simplified as follows:

$$G_{bulk} = \frac{1}{2}\sum_j \int_0^{\frac{\pi}{2}}\int_0^{\infty} C_{1,j}(\omega)v_{1,j}\gamma_{1\to 2}(\theta,j,\omega)\cos(\theta)\sin(\theta)d\theta d\omega \quad (5)$$

To derive the interfacial thermal conductance accumulation function of bulk materials, we change the integration variable from ω to Λ_{bulk}, where Λ_{bulk} represents the bulk MFP, and then transform the form of Eq. (5):

$$G_{bulk} = \frac{3}{2}\sum_j \int_0^{\frac{\pi}{2}}\int_0^{\infty} -\frac{1}{3}C_{1,j}(\Lambda_{bulk})v_{1,j}\Lambda_{bulk}\frac{d\omega}{d\Lambda_{bulk}}\frac{1}{\Lambda_{bulk}} \times \gamma_{1\to 2}(\theta,j,\Lambda_{bulk})\cos(\theta)\sin(\theta)d\theta d\Lambda_{bulk} \quad (6)$$

The negative sign is derived from swapping the limits of integration, because Λ_{bulk} monotonously decreases with the increasing phonon frequency ω. According to the work of C. Dames et al. [11], the thermal conductivity per MFP can be written as:

$$k_1(\Lambda_{bulk}) = -\frac{1}{3}\sum_j C_{1,j}(\Lambda_{bulk})v_{1,j}\Lambda_{bulk}\frac{d\omega}{d\Lambda_{bulk}} \quad (7)$$

Here, the sign of summation is removed and the thermal conductivity per MFP with different phonon modes is defined as follows:

$$k_{1,j}(\Lambda_{bulk}) = -\frac{1}{3}C_{1,j}(\Lambda_{bulk})v_{1,j}\Lambda_{bulk}\frac{d\omega}{d\Lambda_{bulk}} \quad (8)$$

Using Eq. (8), Eq. (5) can be simplified and transformed as follows:

$$G_{bulk} = \sum_j \int_0^{\infty} k_{1,j}(\Lambda_{bulk})d\Lambda_{bulk} \times \int_0^{\frac{\pi}{2}} \frac{3}{2}\frac{1}{\Lambda_{bulk}}\gamma_{1\to 2}(\theta,j,\Lambda_{bulk})\cos(\theta)\sin(\theta)d\theta \quad (9)$$

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