On the Linear Temperature Dependence of Phonon Thermal Boundary Conductance in the Classical Limit

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John C. Duda
Department of Mechanical and Aerospace Engineering,
University of Virginia,
Charlottesville, VA 22904;
Sandia National Laboratories,
Albuquerque, NM 87185

Pamela M. Norris
Department of Mechanical and Aerospace Engineering,
University of Virginia,
Charlottesville, VA 22904

Patrick E. Hopkins
Sandia National Laboratories,
Albuquerque, NM 87185;
Department of Mechanical and Aerospace Engineering,
University of Virginia,
Charlottesville, VA 22904
e-mail: pehopki@sandia.gov

We present a new model for predicting thermal boundary conductance in the classical limit. This model takes a different form than those of the traditionally used mismatch theories in the fact that the temperature dependence of thermal boundary conductance is driven by the phononic scattering mechanisms of the materials comprising the interface as opposed to the heat capacities of those materials. The model developed in this work assumes that a phonon on one side of an interface may not scatter at the interface itself but instead scatter with phonons in the adjacent material via the scattering processes intrinsic in the adjacent material. We find that this model is in good agreement with classical molecular dynamics simulations of phonon transport across a Si/Ge interface. [DOI: 10.1115/1.4003575]

Keywords: thermal boundary conductance, phonon, classical limit, silicon, germanium, diffuse mismatch model, molecular dynamics

1 Introduction

The phonon thermal boundary conductance between two solids, h, has been an active area of research due to its implications on thermal management in nanosystems [1,2]. Various experimental [3–11], numerical [12–19], and theoretical [20–31] treatments have studied h for different material geometries and scenarios. In general, these studies rely on the acoustic [32] or diffuse [2] mismatch theories to explain phonon scattering processes at interfaces. Although these theories, or their variations, have proven successful in describing the phononic heat transfer between two solids in many cases, they fail to describe the observed temperature dependence of h in the classical limit, i.e., at temperatures above the Debye temperature, θ_D, of both solids comprising the interface. Through implementation of classical molecular dynamics simulations, several of the aforementioned numerical studies have found that h increases linearly with temperature [12,13,15]. These findings are in direct disagreement with the mismatch theories as the mismatch theories exhibit a temperature dependence that varies with the phononic heat capacity, thereby predicting a constant h in the classical limit.

This observed linear increase in h with temperature has been linked to multiple-phonon inelastic scattering events that occur at the interface itself; i.e., a phonon of frequency ω on side 1 will scatter at the interface and will emit multiple phonons of different frequencies on side 2. This aspect of interfacial phonon scattering has been used in conjunction with the mismatch theories to successfully explain the temperature dependence of h below the classical limit [21] but still predicts a constant h at temperatures above the classical limit and therefore lends no insight into the interfacial phonon scattering processes at high temperatures.

In this work, we develop a model for predicting h in the classical limit. This model takes a different form than that of the traditionally used mismatch theories in the fact that the temperature dependence of h is not driven by the heat capacities of the materials comprising the interface but rather is driven by their respective phononic scattering mechanisms. In brief, the model developed in this work assumes that a phonon of frequency ω in side 1 may not scatter at the interface itself but instead scatter in side 2 via the phononic scattering processes intrinsic to side 2. Where the mismatch theories assume that all phonons scatter at the interface, the theory developed in this work assumes that phonon scattering happens both at the interface and within some local area near the interface. This concept is similar to the idea of the transition layer described by Kosevich [31]. The theory developed in this work predicts a linear increase in h with temperature in the classical limit and is in good agreement with classical molecular dynamics simulations of thermal boundary conductance at a Si/Ge interface [13].

2 Traditional Diffuse Mismatch Model Predictions

From Refs. [2,13,33,34], we begin by considering the traditional formulation of thermal boundary conductance assuming that isotropic media comprise the interface. We refer to this quantity as h_{T}, where the subscript T indicates the “traditional” formulation, given by

$$h_{\mathrm{T}} = \frac{1}{8\pi^2}\sum_j \int_{k_1} \hbar\omega v_j k^2 \frac{\partial f}{\partial T}\zeta dk \tag{1}$$

where the subscript “1” refers to side 1 of the interface, j represents the phonon polarization, $\hbar$ is the reduced Planck constant, ω is the phonon angular frequency, v is the phonon group velocity, k is the wavevector, f is the Bose–Einstein distribution, T is the temperature, and ζ is the transmission probability. This formulation of h relies on the concept of defining a thermal flux in a material, q, as

$$q = \frac{1}{8\pi^2}\sum_j \int_{k_1} \hbar\omega k^2 v_j f dk \tag{2}$$

and then projecting this flux across the interface by calculating ζ. In the classical limit, the Bose–Einstein distribution reduces to $f = k_{\mathrm{B}}T/(\hbar\omega)$, and therefore, its temperature derivative, which dictates the temperature dependence of thermal boundary conductance in the framework outlined in Eq. (1), is independent of temperature. In addition, calculations involving ζ also rely on this flux concept and are therefore also independent of temperature when both materials comprising the interface are in the classical limit [27,34]. This flux concept, which is the kernel for nearly all models of h, inherently limits the study of phonon interfacial processes to those temperatures below the classical limit. Equally as

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Contributed by the Heat Transfer Division of ASME for publication in the JOURNAL OF HEAT TRANSFER. Manuscript received October 11, 2010; final manuscript received January 26, 2011; published online April 4, 2011. Assoc. Editor: Robert D. Tzou.

important, it prevents further insight into many of the aforementioned molecular dynamics results that show a linear trend in h with temperature.

The present work will address a major assumption of the various models that implement Eq. (1), namely, that all phonons must scatter at the interface. In this assumption, at a perfect interface (i.e., atomically flat), it may not be physical to assume that all phonons will scatter as a result of the mismatch between the materials comprising sides 1 and 2. Instead, due to phonon wavelength and mean free path considerations, many phonons may not "see" the interface and, subsequently, may not scatter until they traverse a certain distance into the material comprising side 2 of the interface. Consequently, the total thermal boundary conductance will be the sum of two individual components, one accounting for phonons that scatter at the interface as described by the traditional mismatch theories and the second accounting for phonons that do not see the interface but instead scatter once they have propagated into side 2.

3 Thermal Boundary Conductance in the Classical Limit

To model the component of h that accounts for those phonons that propagate some distance into side 2 from side 1 before scattering, first consider the internal energy of phonons originating in side 1 that propagate into side 2, $U_{1\to 2}$, given by

$$U_{1\to 2}=\frac{1}{8\pi^2}\sum_j \int_{k_1} \hbar\omega k^2 f dk \tag{3}$$

The differences between the atomic mass, interatomic potential, and interatomic spacing of the crystalline lattice in side 2 and those in side 1 will immediately cause the propagating phonons to scatter at some rate, τ_2^{-1}, where τ_2 is the intrinsic relaxation time of phonons in side 2. Since the mean free path of a phonon originating in side 1 and now traveling in side 2 is an undefined concept due to the change in material properties, the distance that the side 1 phonon will propagate before experiencing a scattering event is taken as the phonon wavelength, λ. Our reason for choosing λ as the characteristic length is as follows: From the viewpoint of phonons originating in the material comprising side 1 of the interface, the material comprising side 2 of the interface appears as an impurity-rich amorphous material despite its crystalline nature. This is due to the fact that, as mentioned above, the material on side 2 of the interface differs from that on side 1 in terms of atomic mass, interatomic potential, and interatomic spacing. Following suit, we turn to the description of the phonon mean free path utilized in models describing phonon scattering in amorphous and heavily disordered materials; i.e., the mean free path is equal to the wavelength [35,36]. With the mean free path of a phonon from side 1 traveling into side 2 established, the internal energy of phonons that will propagate from side 1 into side 2 will do so with a velocity of λ/τ_2. Thus, the interfacial phonon flux of those phonons that propagate some distance into side 2 from side 1 before scattering is given as

$$q=\frac{1}{8\pi^2}\sum_j \int_{k_1} \beta\hbar\omega k^2 f\frac{\lambda}{\tau_2} dk \tag{4}$$

where $\beta=[1-H(\omega_1(k)-\omega_{2,\max})]$ and H is the Heaviside function. This β term ensures that phonons that exist on side 1 at frequencies greater than the maximum frequency allowed on side 2 do not contribute to this channel of energy transport, consistent with the behavior of phonon wave-packets traversing an interface, as observed via classical molecular dynamics simulations [19,37]. The corresponding component of thermal boundary conductance, h_{S}, where the subscript S indicates this new "scattering" formulation, is then given by

$$h_{\mathrm{S}}=\frac{1}{8\pi^2}\sum_j \int_{k_1} \beta\hbar\omega k^2 \frac{\partial f}{\partial T}\frac{\lambda}{\tau_2} dk \tag{5}$$

Now, as suggested above, this work proposes that h is a measurement of phonons both scattering at the interface between sides 1 and 2 described by h_{T}, as well as phonons traversing the interface and scattering in side 2 described by h_{S}. Thus, this new formulation of h must include contributions from both Eqs. (1) and (5).

Integrating Eq. (5) over the entire side 1 Brillouin zone assumes that all phonons are scattered by processes in side 2 and that there is no scattering event at the interface itself. Similarly, integrating Eq. (1) over the entire side 1 Brillouin zone assumes that all phonons are scattered at the interface. Clearly, taking either extreme is not physical; the longer wavelength phonons will be more likely to propagate across the interface and scatter in side 2, and the shorter wavelength phonons will be more likely to scatter at the interface. Therefore, h is a combination of Eqs. (1) and (5), given by

$$h=\frac{1}{8\pi^2}\left[\sum_j \int_{k_1\le k_{\mathrm{trans}}} \beta\hbar\omega k^2 \frac{\partial f}{\partial T}\frac{\lambda}{\tau_2} dk + \sum_j \int_{k_1> k_{\mathrm{trans}}} \hbar\omega v_j k^2 \frac{\partial f}{\partial T}\zeta dk\right] \tag{6}$$

Here, k_{trans} is the transition wave vector separating the long wavelength phonons that propagate into side 2 and short wavelength phonons that scatter at the interface. Note that in the case that no phonons propagate into side 2, $k_{\mathrm{trans}}=0$ and Eq. (6) reduces to Eq. (1). When $k_{\mathrm{trans}}=k_{1,\max}$ (the maximum wave vector in side 1), no phonons see the interface and all phonons are scattered at a distance equal to their wavelength into side 2; in this case, h is driven by the intrinsic scattering processes in side 2 and Eq. (6) reduces to Eq. (5). At this point, we will refer to the two components of Eq. (6) as h_{S}' and h_{T}', where the primes indicate the unique integration limits imposed (compared with the related expressions given by Eqs. (1) and (5)). That is, $h=h_{\mathrm{S}}'+h_{\mathrm{T}}'$.

4 Results Compared With Molecular Dynamics Simulations

Figure 1 shows calculations of Eq. (6) for a Si/Ge interface compared with molecular dynamics results by Landry and McGaughey [13]. When calculating the component of h corresponding to those phonons that scatter at the interface (h_{T}'), the wave-vector-space diffuse mismatch model approach discussed by Duda et al. [38] is implemented. We take the phonon dispersion of Stillinger–Weber (SW) Si and Ge in the [100] direction from Ref. [39] such that the dispersion calculations and the molecular dynamics simulations utilize the same values when parametrizing the SW potential for describing Si and Ge. The lattice constants of Si and Ge are taken as 0.531830 nm and 0.573527 nm, respectively, from the cross plane lattice constants used in the molecular dynamics work [13]. In addition, as per Beechem et al. [40], optical phonons are included. Since the focus of these calculations is inelastic scattering, the right expression in Eq. (6) is calculated, assuming the "maximum transmission model" for interface transmission, as discussed by Dames and Chen [41]. This model is explicitly formulated in the wave-vector space in Eq. 3 of Ref. [38], although the bounds on the integral over side 1 are adjusted to account for k_{trans}. For the calculations of side 1 phonons (Si) propagating across the interface and scattering in side 2 (Ge) (h_{S}'), we again use the SW Si dispersion, and we take the three-phonon relaxation times (Umklapp and normal) of the form given by Ward and Broido [42] in which U- and N-process scattering rates are given by $\tau_{\mathrm{U},j}^{-1}=A_j\omega^4 T[1-\exp(-3T/\theta_D)]$ and $\tau_{\mathrm{N},j}^{-1}=A_j\omega^2 T[1-\exp(-3T/\theta_D)]$, respectively. In the classical limit, these simplify to $\tau_{\mathrm{U},j}^{-1}=A_j\omega^4 T$ and $\tau_{\mathrm{N},j}^{-1}=A_j\omega^2 T$. The coefficients A_j are deter-

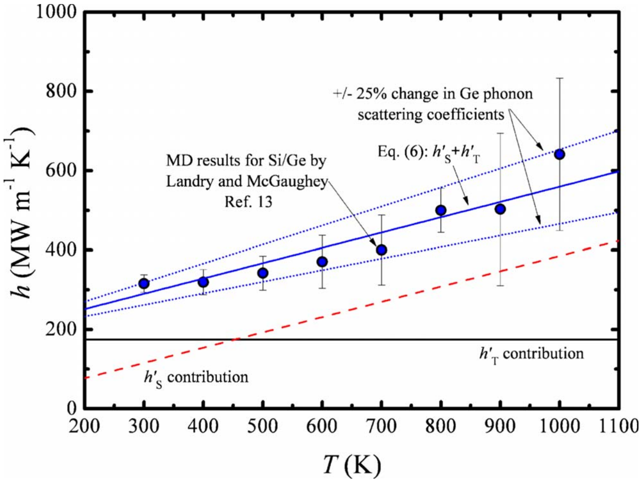

Fig. 1 Calculations of Eq. (6) in the classical limit compared with predicted thermal boundary conductance at a Si/Ge interface via classical molecular dynamics simulations [13]. The contributions from the various phonon scattering mechanisms are shown, where the Eq. (1) contribution assumes a fraction of phonon scatter at the interface due to the change in material properties and the Eq. (5) contribution assumes that phonons will propagate into side 2 and scatter based on the three-phonon scattering rates of Ge. The dotted lines on either side of the calculations of Eq. (6) indicate the sensitivity of the model to changes in the scattering coefficients taken from Ref. [42].

mined from the ab initio calculations by Ward and Broido and are tabulated in their work [42], and the total relaxation time used in Eq. (6) is determined through Matthiessen's rule. While these coefficients were not fit for SW Ge, we believe that due to the similarity between the SW dispersion curves and those determined via ab initio calculations, the use of those coefficients is a reasonable approximation. To determine the sensitivity of Eq. (6) to this assumption, we varied the coefficients by ±25%. It is found that the model is not particularly sensitive to these changes, as shown in Fig. 1. Optical phonons are not included in the calculation of the left integral expression of Eq. (6), although the effects of the optical phonons on three-phonon scattering are included in the acoustic phonon scattering rates [42]. Ward and Broido discussed the contribution of optical phonons and determined that their role is most important in acoustic phonon scattering and will only contribute less than 10% to the thermal flux.

Finally, we take k_{trans} as the limiting maximum wave vector of the materials comprising the interface, i.e., $k_{\mathrm{trans}}=2\pi/a_{\mathrm{Ge}}$, where a_{Ge} is the lattice constant of Ge. This selection of k_{trans} suggests that Si phonons that exist at wave vectors greater than the maximum allowable wave vector of Ge must scatter at the interface. This is consistent with the fact that interfacial scattering processes as described by the mismatch theories are not required to conserve crystal momentum. On the other hand, those processes described by h_S can conserve crystal momentum as they are subject to the intrinsic scattering processes of the material on side 2 (Ge).

With the three-phonon relaxation times discussed above, the thermal boundary conductance model given in this work takes the form of $h=b+cT$ in the classical limit, as has been phenomenologically theorized [12,27]. The contributions of both h'_S and h'_T to the total h are also shown in Fig. 1, indicating that the temperature trends in h in the classical limit are driven by phonons in side 1, experiencing three-phonon scattering events in side 2. These temperature trends and this conclusion have not been quantified previously as, until this work, no theoretical model existed to quantify the temperature trends in h in the classical limit.

5 Conclusion

In conclusion, we have described the linear temperature dependence of thermal boundary conductance in the classical limit through a formalism for interfacial phonon transport based on the intrinsic phonon scattering rates of the materials comprising an interface. Where mismatch theories assume that all phonons must scatter at an infinitesimally thin interfacial plane (i.e., all phonons scatter due to the change in the material properties at the interface), the model derived in this work assumes that some fraction of phonons can propagate into side 2 before scattering. The predictions of this model are in excellent agreement with classical molecular dynamics simulations. Additionally, they show that the linear temperature dependence of thermal boundary conductance observed in the classical limit is due to three-phonon scattering events in which phonons propagating across the interface interact with phonons on the other side of the interface.

Acknowledgment

J.C.D. is appreciative of funding from the National Science Foundation Graduate Research Fellowship Program. P.E.H. is appreciative of funding from the LDRD program office through the Sandia National Laboratories Harry S. Truman Fellowship Program. Sandia is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

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