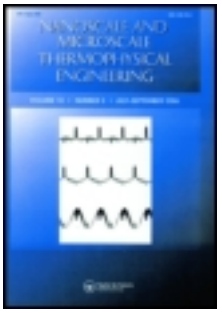

Nanoscale and Microscale Thermophysical Engineering

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/umte20

Effects of Joint Vibrational States on Thermal Boundary Conductance

Patrick E. Hopkins [a] & Pamela M. Norris [a]

[a] Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia, USA

Version of record first published: 28 Feb 2008.

To cite this article: Patrick E. Hopkins & Pamela M. Norris (2007): Effects of Joint Vibrational States on Thermal Boundary Conductance, Nanoscale and Microscale Thermophysical Engineering, 11:3-4, 247-257

To link to this article: http://dx.doi.org/10.1080/15567260701715297

Nanoscale and Microscale Thermophysical Engineering, 11: 247–257, 2007

ISSN: 1556-7265 print / 1556-7273 online
DOI: 10.1080/15567260701715297

EFFECTS OF JOINT VIBRATIONAL STATES ON THERMAL BOUNDARY CONDUCTANCE

Patrick E. Hopkins and Pamela M. Norris

Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia, USA

The accuracy of predictions of the thermal boundary conductance (h_{BD}) made using traditional models such as the diffuse mismatch model (DMM) varies depending on the types of material comprising the interface. At interfaces of materials with very different material properties, the discrepancy between the measured h_{BD} and the DMM results has been associated with inelastic scattering. In this study, a new model, the joint frequency diffuse mismatch model (JFDMM), is derived under the assumption that the phonon flux approaching the interface is altered by phonons vibrating at joint frequencies around the interface affected by phonons on both sides of the interface. This model yields improved h_{BD} predictions for a wide range of materials over a temperature range of several 100s of Kelvin, indicating that at these temperatures, substrate phonons are participating in interfacial thermal transport.

KEY WORDS: thermal boundary conductance, phonon, inelastic scattering, diffuse mismatch model, acoustic mismatch, Debye temperature

INTRODUCTION

An understanding of the basic energy transport mechanisms involved in interfacial thermal transport is critical for thermal management of nanostructured devices. As characteristic length scales decrease, heat transport away from the active regions in these devices is affected by the interfaces between the differing materials surrounding this region [1]. An ever increasing challenge in the development of these devices is successfully accounting for the temperature drop ΔT across the interface. This ΔT creates a heat flux across the interface $\dot{q}_{\text{int}}$ that differs from the flux in the materials on either side of the interface. The thermal transport across the interface is characterized by the thermal boundary conductance h_{BD}, which is the conductance per unit area that relates the heat flux to the temperature drop.

In an attempt to predict this thermal boundary conductance at low temperatures, Little proposed the acoustic mismatch model (AMM) to account for the specular scattering of phonons at an interface between two materials [2,3]. Although this has been shown to predict h_{BD} relatively well at low temperatures ($T < 7$ K) and at ideal interfaces where specular scattering is probable [4], this represents only a very limited population of interfaces in modern devices, which may operate at higher

Address correspondence to Pamela M. Norris, Department of Mechanical and Aerospace Engineering, P.O. Box 400746, University of Virginia, Charlottesville, VA, 22904-4746. E-mail: pamela@virginia.edu

NOMENCLATURE

D	= density of states, s m^{-3}	ζ	= weighting factor
h_{BD}	= thermal boundary conductance, W m^{-2} K^{-1}	θ_D	= Debye temperature, K
		ρ	= mass density, kg m^{-3}
M	= atomic weight, g mol^{-1}	ϕ	= angle of incidence
N	= density of oscillators, m^{-3}	ω	= frequency, s^{-1}
N_A	= Avagadro's number, mol^{-1}		
n	= Bose-Einstein distribution function	**Subscripts**	
		i	= side
$\dot{q}$	= heat flux, W m^{-2}	int	= interface
T	= temperature, K	j	= phonon modee
v	= phonon velocity, m s^{-1}	mod	= modified
Greek Symbols		**Superscripts**	
α	= transmission probability	c	= cutoff
Δ	= change in		

temperatures and have disordered regions near the interface that induce diffuse scattering.

To account for this type of phonon scattering, Swartz and Pohl developed the diffuse mismatch model (DMM) to predict h_{BD} at more realistic interfaces [5]. The DMM theory assumes elastic scattering; that is, upon scattering a phonon forgets where it came from and thus the probability of reflection from one side equals the probability of transmission from the other. This model has been shown to predict the response of higher temperature interfaces ($T > 15$ K) relatively well [4,5]. However, at much higher temperatures, the DMM has been shown to do a poor job of predicting the value of h_{BD}, in some cases underpredicting [6] while in other cases overpredicting [6–9]. These inaccuracies at higher temperatures could be due to the assumptions made about elastic scattering of phonons across the interface.

This study examines the discrepancy between theoretical h_{BD} values calculated from the DMM and those measured at various metal/dielectric interfaces. The aim is to address the discrepancy that results specifically from the elastic scattering assumption. By introducing a simple correction to the DMM based on joint vibrations of the phonons near the interface, DMM predictions are shown to significantly improve when compared to recent data in systems where inelastic scattering is thought to dominate interfacial transport. In the following section, the DMM is reviewed and specific assumptions are readdressed. Previous experimental results are presented and compared with traditional DMM calculations and the discrepancies are discussed with reference to the DMM assumptions. Then, the effects of inelastic scattering on h_{BD} are qualitatively discussed followed by a presentation of improvements to the DMM and a comparison of calculations to previous experimental data.

DIFFUSE MISMATCH MODEL

A complete derivation of the DMM theory is outlined by Swartz and Pohl [5], and therefore only the critical points will be highlighted here. Consider a metal/dielectric system in which phonons are propagating toward an interface of the metal

(side 1) and the dielectric (side 2). In the following discussion, side 1 will refer to the side of the interface with the "softer" material and side 2 will refer to the side of the interface with the "stiffer" material. The net heat flux occurring from side 1 to side 2 can be calculated by

$$\dot{q} = h_{BD}\Delta T \tag{1}$$

Using the analogy between photons and phonons as wavepackets of energy, the intensity of phonons [10] is used to calculate the heat flux determined from the equation of phonon radiative transfer (EPRT) [11]. The heat flux is expressed as:

$$\dot{q} = \frac{1}{2}\int_0^{\pi/2}\int_0^{\omega_{1,j}^c} D_{1,j}(\omega)n(\omega,T)\hbar\omega v_{1,j}\alpha_{1,j}(\phi,\omega)\cos(\phi)\sin(\phi)d\omega d\phi = h_{BD}\Delta T \tag{2}$$

where ω^c is the cutoff frequency, $D(\omega)$ is the density of states, $n(\omega,T)$ is the Bose-Einstein phonon distribution function, ω is the phonon frequency, v is the phonon velocity, and $\alpha(\phi,\omega)$ is the phonon transmission probability. The subscripts *1* and *j* refer to the side and the phonon mode (longitudinal or transverse), respectively.

To apply the DMM in its simplest form, the following assumptions must be made [7]: (1) phonons are elastically scattered; i.e., a phonon from side 1 with frequency ω can only emit a phonon in side 2 with the same frequency ω; (2) phonon scattering is completely diffuse; i.e., a scattered phonon has no memory of the mode (longitudinal or transverse) or direction of the incident phonon; and (3) the materials on both sides of the interface are elastically isotropic; i.e., the longitudinal and transverse acoustic velocities are constant in all crystallographic directions. Assumption 3 relaxes the angle dependence in Eq. (2), which can be rearranged to calculate h_{BD} (this is the DMM):

$$h_{BD} = \frac{1}{4}\sum_j v_{1,j}\int_0^{\omega_{1,j}^c} \alpha_1(\omega)\hbar\omega D_{1,j}(\omega)\frac{\partial n(\omega,T)}{\partial T}d\omega \tag{3}$$

Since the goal of this study is to apply a simple correction to the DMM to account for discrepancies between calculations and experiments, the remainder of the discussion will assume the linear Debye approximation for the phonon dispersion. Although a more accurate density of states has been shown to increase DMM calculations by 2 or 3 times in the temperature range of the data referred to in this study [12], the focus of this work is to account for data that exceed calculations by almost an order of magnitude.

The cutoff frequency of each phonon mode *j* on side *1* can be calculated for the separate phonon modes. Assuming Debye dispersion, $\omega_{1,j}^c = v_{1,j}(6\pi^2 N_1)^{1/3}$, where N_1 is the total number of oscillators per until volume of side 1 [13]. In cubic structures (several metals), N_1 is simply the atomic density, calculated by $N_1 = \rho N_A/M$, where ρ is the mass density, N_A is Avagadro's number, and M is the atomic weight. However, in structures with more than one atomic basis (for example, diamond structures with diatomic basis such as Si), the number of primitive cells per unit volume must be divided by the number of atoms in the basis [14]. Therefore, for a diatomic basis, $N_1 = \rho N_A/(2M)$.

Due to the assumption of diffuse scattering, the probability of transmission from side 1 to side 2 is the same as the probability of reflection from side 2 to side 1, i.e., $\alpha_1(\omega) = 1 - \alpha_2(\omega)$. Therefore, according to the principle of detailed balance, the phonon transmission probability is calculated as [5]:

$$\alpha_1(\omega) = \frac{\sum_j v_{2,j} D_{2,j}(\omega)}{\sum_j v_{2,j} D_{2,j}(\omega) + \sum_j v_{1,j} D_{1,j}(\omega)} = \frac{\sum_j v_{2,j}^{-2}}{\sum_j v_{2,j}^{-2} + \sum_j v_{1,j}^{-2}} = \alpha_1 \tag{4}$$

This simplified transmission coefficient to the right of Eq. (4) is a result of assuming a Debye density of states and elastic scattering. However, the transmission probability calculated with the Debye density of states agrees well with the transmission calculated with a more realistic density of states and molecular dynamics simulations (MDS) [15, 16].

Calculations of the DMM for Au, Bi, Pb/diamond interfaces are shown in Figure 1 using elastic constants to calculate phonon velocities and material properties to calculate the cutoff frequencies [17]. Temperature-dependent h_{BD} measurements of Pb on diamond and Bi on hydrogen terminated diamond by Lyeo and Cahill [18] and Au on diamond by Stoner and Maris [9] are also represented in this figure. The DMM underestimates the data in these acoustically mismatched* material systems. The

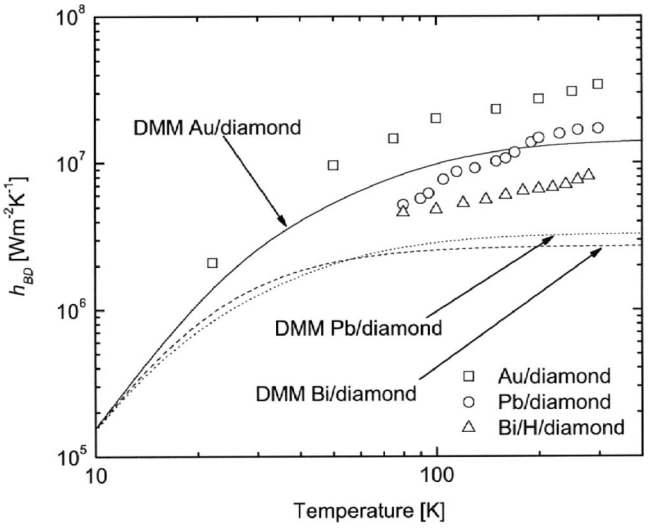

Figure 1. Temperature dependence of h_{BD} across several acoustically mismatched interfaces. The Pb and Bi on diamond measurements were taken from Lyeo and Cahill [18], and the Au on diamond measurements were taken from Stoner and Maris [9]. The discrepancy between the values and temperature trends of the measurements and the DMM could be evidence of inelastic scattering contributing to interfacial thermal transport, a transport mechanism that is not taken into account in the DMM.

*The term *acoustic mismatch* describes two materials that have significantly different acoustic velocities; the degree of the acoustic mismatch can be easily determined by comparing the material's Debye temperatures, θ_D.

discrepancy spans almost an order of magnitude in Pb on diamond. Huberman and Overhauser explained this discrepancy as electrons scattering at the film/substrate interface, thereby increasing the measured h_{BD} [19]. Lyeo and Cahill measured h_{BD} at various interfaces in addition to Pb and Bi on diamond, and the results and trends suggest that the discrepancies between the measurements and models are most likely due to inelastic phonon scattering, a transport mechanism that is not taken into account in the DMM.

EFFECTS OF INELASTIC SCATTERING ON h_{BD}

An underlying assumption governing the DMM is that a phonon transmits energy across an interface by emitting a phonon with the same frequency; i.e., the phonons are elastically scattered. Therefore, as the interface temperature is driven up above the Debye temperature of the softer material, h_{BD} is predicted to be relatively constant by the DMM (for example, Pb/diamond in Figure 1 where $\theta_{D\_Pb} = 105$ K and $\theta_{D\_diamond} = 2200$ K) [13]. This is a result of the change in phonon population with temperature predicted by the Bose-Einstein distribution function. At temperatures close to a material's Debye temperature, the change in phonon population with temperature becomes linear. The DMM is a function of the temperature derivative of the Bose-Einstein distribution, which results in the constant h_{BD} predicted at higher temperatures ($T > \theta_D$).

Figure 2 shows the temperature derivative of the Bose-Einstein distribution as a function of temperature at two different frequencies, the cutoff frequency of Pb and cutoff frequency of diamond. The cutoff frequency is directly related to the Debye temperature by $\theta_D = \hbar\omega^c/k_B$. Figure 2 shows the derivative of the phonon population for two different frequencies at a range of temperatures. In this example, h_{BD} across a

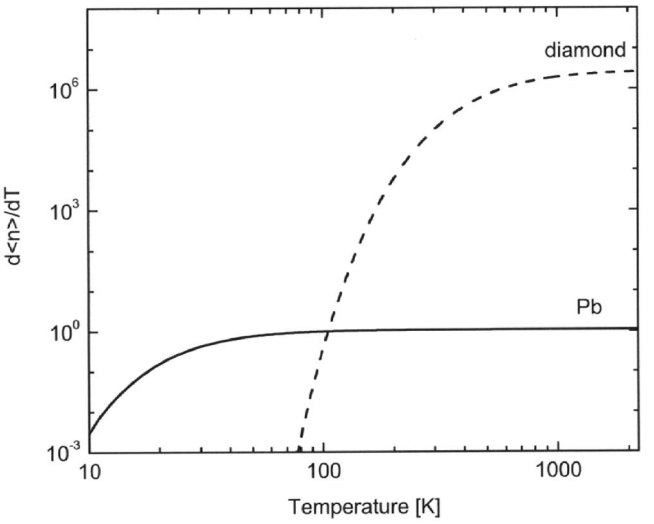

Figure 2. Temperature derivative of the Bose-Einstein phonon distribution function as a function of temperature shown for two different θ_Ds (i.e., cutoff frequencies), that of Pb and diamond. The calculations are normalized at the Debye temperature of Pb, 105 K [13].

Pb/diamond interface is considered. Assuming elastic scattering, the h_{BD} predictions would follow a trend relating to the change in the Pb phonon population with temperature. However, if inelastic phonon processes occur (i.e., several phonons scatter with frequency ω^c_{Pb} and emit a phonon with frequency $\omega^c_{diamond}$), then the change in h_{BD} with temperature would be related to the change in the diamond phonon population in addition to the Pb population. In this case, a fairly linear increase in h_{BD} should be observed at temperatures around and above θ_{D_Pb}. This linear trend with temperature was experimentally observed in the previous work presented in Figure 1.

A linear trend with temperature was also computationally observed with MDS. Chen *et al*. showed a linear increase in h_{BD} across a Kr/Ar nanowire with an increase in temperature from 35 to 55 K, which they ascribed to anharmonic processes [20]. Using MDS, Stevens *et al*. observed thermal transport across the interface of two FCC lattice systems with varying degrees of mass and lattice mismatch [15]. A linear increase in h_{BD} was observed through temperatures far above the Debye temperatures ($T >> \theta_D$), and the conclusion of inelastic scattering among the phonons in these systems was verified with a detailed wave packet analysis [21]. Kosevich considered the role of inelastic scattering on the phonon transmission probability [21]. With a multiharmonic model, Kosevich was able to show that inelastic scattering makes a greater contribution to h_{BD} than elastic scattering for interfaces with very different vibrational spectra (such as the materials shown in Figure 1); these calculations were not material specific. The results from this highly theoretical model in addition to the MD calculations are a product of extremely rigorous or computationally expensive calculations that may not be practical for many researchers studying interfacial transport. In addition, it is difficult to apply these works and techniques to specific material systems that may be of interest in thermal boundary conductance studies.

JOINT FREQUENCY DIFFUSE MISMATCH MODEL

To develop a model that accounts for inelastic scattering, ideally the transmission probability should be recalculated to account for one or more phonons in side 1 with frequency ω_1 emitting one or more phonons into side 2 with frequencies up to ω^c_2. This would require highly complicated theoretical calculations or time-consuming probabilistic simulations. In an effort to quickly and easily predict the effects that inelastic scattering may have on h_{BD}, the DMM is slightly modified to account for phonons in the softer material emitting phonons in the stiffer material with frequencies that are not available in the softer material.

To envision the interface between two materials as an abrupt junction of material properties is unphysical. The region around the interface, in reality, is comprised of a mixture of the two materials [23], which responds as a mixture of the materials' acoustic and thermal properties [24]. In fact, the atoms near the interface of two materials are coupled together into joint vibrational modes [19]. In well-matched material systems, the difference between the modes in the film and substrate are very small, so the joint vibrational modes near the interface are most likely present in both the film and substrate, making elastic scattering highly probable. However, in highly mismatched material systems, the frequencies of the atoms vibrating at the interface may not be available frequencies in the softer material. Therefore, by blending the vibrational spectra of the film and substrate materials, an approximation for the

contribution of these inelastic modes can be simply calculated with a diffuse scattering assumption with a joint frequency diffuse mismatch model (JFDMM).

Revisiting Eq. (3), the thermal boundary conductance can be redefined as:

$$h_{BD} = \frac{1}{4}\sum_{j} v_{\mathrm{mod},j} \int_{0}^{\omega^{c}_{\mathrm{mod},j}} \alpha_1(\omega)\hbar\omega D_{\mathrm{mod},j}(\omega)\frac{\partial n(\omega, T)}{\partial T}d\omega \tag{5}$$

where $v_{mod,j}$, $D_{mod,j}(\omega)$, and $\omega^{c}_{\mathrm{mod},j}$ are a modified velocity, density of states, and cutoff frequency, respectively, to account for joint modes around the interface. These modified acoustic properties, assuming a Debye density of states, can be approximated as:

$$D_{\mathrm{mod},j} = \frac{\omega^2}{2\pi^2 {v_{\mathrm{mod},j}}^3}, \omega \leq \omega^{c}_{\mathrm{mod},j} \tag{6}$$

$$\omega^{c}_{\mathrm{mod},j} = v_{\mathrm{mod},j}[6\pi^2(\xi_1 N_1 + \xi_2 N_2)]^{1/3} \tag{7}$$

$$v_{\mathrm{mod},j} = \xi_1 v_1 + \xi_2 v_2 \tag{8}$$

where the weighting factor ξ_i is simply a percentage of the composition of each material in the unit volume, mathematically expressed as:

$$\xi_i = \frac{\frac{N_i}{N_{3-i}} M_i}{\frac{N_i}{N_{3-i}} M_i + M_{3-i}} \tag{9}$$

where M_i is the atomic mass of side i. Since the DMM is calculated per unit volume, to better estimate the percentage composition of the joint vibrating atoms near the interface, the relative amount of each atom must be taken into account by including the number of oscillators per unit volume, N. This is similar to calculating the percent composition of atoms in any compound (for example, the %O in H_2O).

Conceptually, the JFDMM is a modification of the DMM to account for phonons of all frequencies in both materials that could participate in interfacial transport without explicitly examining the effects of inelastic scattering on phonon transmission probability. This correction is only a modification to the intensity of phonons approaching the interface, treating the side 1 phonons approaching the interface as the weighted average of all phonons in side 1 and side 2. The transmission of the incident phonon flux is calculated by Eq. (4), the same transmission that is used in the DMM. This ensures that the fundamental acoustic properties of the materials that determine phonon transmission are not lost. In a sense, the JFDMM still assumes elastic scattering (based on transmission calculations), but it assumes that the phonon flux across the interface from side 1 to 2 increases in a manner that is proportional to the density of phonons in side 2 in addition to side 1. Therefore, this accounts for an increase in h_{BD} that could be a result of inelastic scattering.

Figure 3 shows the temperature dependent predictions of h_{BD} from the JFDMM and DMM alongside the measured data presented in Figure 1. Lead on hydrogen terminated diamond data taken from Lyeo and Cahill are also shown [18]. The

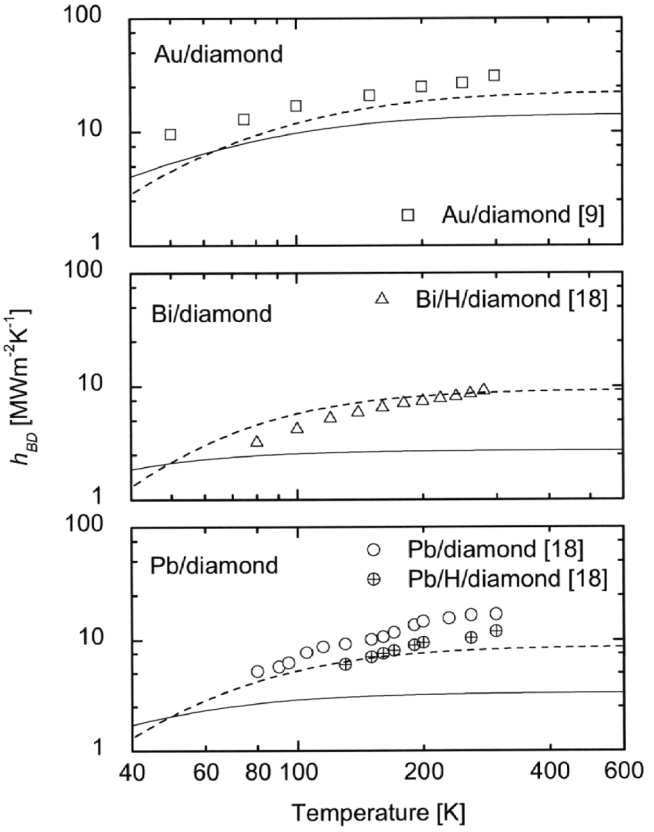

Figure 3. Measurements of h_{BD} at various temperatures compared with the DMM and JFDMM. The solid lines represent the DMM and dashed lines represent the JFDMM. The Au/diamond data were taken from Stoner and Maris [9] and the Bi and Pb on diamond data were taken from Lyeo and Cahill [18]. The JFDMM shows an improvement from the DMM in both value and trend compared to the experimental data. These materials form a highly mismatched interface and the agreement between the JFDMM and the data are much better than the DMM at temperatures above the film's Debye temperature.

JFDMM predicts h_{BD} values and trends that are closer to the measured data than the DMM for temperatures above the softer material's Debye temperature ($\theta_{D\_Au} = 165$ K, $\theta_{D\_Bi} = 119$ K, and $\theta_{D\_Pb} = 105$ K). Excellent agreement is shown between the data taken on Bi and Pb on hydrogen terminated diamond and the JFDMM. The prediction of the JFDMM is much better for the hydrogen terminated samples than the non-hydrogen terminated samples. The hydrogen termination substrate preparation could have reduced the amount of film/substrate mixing during deposition [25], which can change the thermal boundary conductance and affect the accuracy of the predictions of the DMM and JFDMM, since interfacial mixing is not taken into account in these models [23, 26]. The small amount of mixing that occurs around these interfaces can cause an increase in phonon scattering events, which increases h_{BD} in these acoustically mismatched samples [5], explaining the close agreement between the JFDMM and the hydrogen terminated data and the slight underprediction of the JFDMM compared to the non-hydrogen terminated data.

Figure 4 shows the JFDMM and DMM h_{BD} calculations with high-temperature data from Hopkins et al. [27]. The three data sets shown are shown are for Pt/AIN, Pt/Al_2O_3, and Al/Al_2O_3. These data were taken at temperatures well above θ_{D_Pt} (240 K) and around θ_{D_Al} (428 K). In all cases, a better agreement in trend is achieved with the JFDMM. At the higher temperatures, the JFDMM predicts h_{BD} relatively well. In the case of Al/Al_2O_3, the JFDMM predicts values less than the DMM. This material system is better matched then the other material systems in this study. Only in heavily mismatched material systems are inelastic scattering or increased scattering events theorized to improve h_{BD} [5, 22]. Since the JFDMM does not explicitly consider inelastic scattering, but considers changes in phonon fluxes due to substrate phonons,[†] the Al/Al_2O_3 data may be in a temperature regime where multiple phonon scattering is decreasing h_{BD} more so than inelastic phonon scattering is increasing it. In either case, the increase in the experimental data over this temperature range suggests that Al_2O_3 phonons are involved in interfacial thermal transport.

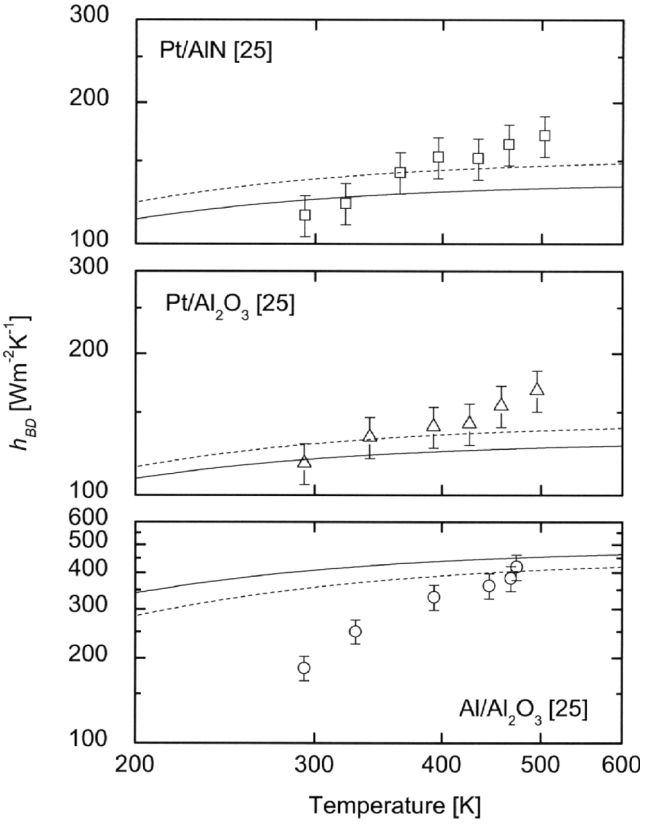

Figure 4. JFDMM and DMM compared to high-temperature h_{BD} data across interfaces of material systems that are better matched then those in Figure 3. The JFDMM gives a better prediction than the DMM in the data at temperature above the film's Debye temperature.

[†]Which in heavily mismatched material systems has been associated with inelastic scattering.

CONCLUSIONS

The accuracy of h_{BD} predictions made using DMM varies depending on the types of materials comprising the interface. The underlying assumptions made when applying the DMM may not be valid in certain material systems at temperatures characteristic in modern devices. It is apparent from the values and trends in experimental data presented in Figures 3 and 4 that additional transport mechanisms, such as inelastic scattering, are involved in interfacial thermal transport that are not taken into account in the DMM. In this study, a new model, the JFDMM, is derived under the assumption that the phonon flux approaching the interface in side 1 is altered by phonons vibrating at joint frequencies around the interface affected by phonons on both side 1 and side 2. This model yields improved h_{BD} predictions for several material systems over a temperature range of several 100s of Kelvin, indicating that over these temperatures, substrate phonons are participating in interfacial thermal transport. In highly mismatched materials, this has been associated with inelastic scattering. The JFDMM involves a simple correction to the DMM that does not involve highly theoretical or computationally expensive simulations and is ideal for simple calculations of h_{BD} at interfaces where the assumptions of the DMM may prevent accurate predictions. Although the JFDMM provides a simple approximation of the effects of joint vibrational modes on h_{BD} using a Debye approximation, more rigorous calculations would truly elucidate the effects of these joint modes in specific material systems. In many material systems, certain vibrational states may have a larger role in h_{BD} than others, which is not taken into account in the JFDMM. A realistic density of states and probabilistic phonon Monte Carlo simulations would give more insight. In addition, MD simulations using potentials that are more appropriate for specific materials systems would tremendously advance the current knowledge of the effects of various transport mechanisms on interfacial thermal transport.

REFERENCES

1. D.G. Cahill, W.K. Ford, K.E. Goodson, G.D. Mahan, A. Majumdar, H.J. Maris, R. Merlin, and S.R. Phillpot, Nanoscale Thermal Transport, *Journal of Applied Physics*, vol. **93**, pp. 793–818, 2003.
2. J.D.N. Cheeke, H. Ettinger, and B. Hebral, Analysis of Heat Transfer between Solids at Low Temperatures, *Canadian Journal of Physics*, vol. **54**, p. 1749, 1976.
3. W.A. Little, The Transport of Heat between Dissimilar Solids at Low Temperatures, *Canadian Journal of Physics*, vol. **37**, pp. 334–349, 1959.
4. E.T. Swartz, and R.O. Pohl, Thermal Resistances at Interfaces, *Applied Physics Letters*, vol. **51**, pp. 2200–2202, 1987.
5. E.T. Swartz, and R.O. Pohl, Thermal Boundary Resistance, *Reviews of Modern Physics*, vol. **61**, pp. 605–668, 1989.
6. R.J. Stevens, A.N. Smith, and P.M. Norris, Measurement of Thermal Boundary Conductance of a Series of Metal-Dielectric Interfaces by the Transient Thermoreflectance Technique, *Journal of Heat Transfer*, vol. **127**, pp. 315–322, 2005.
7. D.G. Cahill, A. Bullen, and S.-M. Lee, Interface Thermal Conductance and the Thermal Conductivity of Multilayer Thin Films, *High Temperature-High Pressures*, vol. **32**, pp. 135–142, 2000.
8. R.M. Costescu, M.A. Wall, and D.G. Cahill, Thermal Conductance of Epitaxial Interfaces, *Physical Review B*, vol. **67**, p. 054302, 2003.

9. R.J. Stoner, and H.J. Maris, Kapitza Conductance and Heat Flow between Solids at Temperatures from 50 to 300 K, *Physical Review B*, vol. **48**, pp. 16373–16387, 1993.
10. W.G. Vincenti, and C.H. Kruger, *Introduction to Physical Gas Dynamics*, Krieger Publishing Company, Malabar, FL., 2002.
11. A. Majumdar, Microscale Heat Conduction in Dielectric Thin Films, *Journal of Heat Transfer*, vol. **115**, pp. 7–16, 1993.
12. P. Reddy, K. Castelino, and A. Majumdar, Diffuse Mismatch Model of Thermal Boundary Conductance Using Exact Phonon Dispersion, *Applied Physics Letters*, vol. **87**, p. 211908, 2005.
13. C. Kittel, *Introduction to Solid State Physics*, John Wiley and Sons, New York., 1996.
14. C. Dames, and G. Chen, Theoretical Phonon Thermal Conductivity of Si/Ge Superlattice Nanowires, *Journal of Applied Physics*, vol. **95**, pp. 682–693, 2004.
15. R.J. Stevens, P.M. Norris, and L.V. Zhigilei, Molecular-Dynamics Study of Thermal Boundary Resistance: Evidence of Strong Inelastic Scattering Transport Channels, Proceedings of the 2004 ASME International Mechanical Engineering Congress, Anaheim, CA, **IMECE2004**, 60334.
16. P.K. Schelling, S.R. Phillpot, and P. Keblinski, Phonon Wave-Packet Dynamics at Semiconductor Interfaces by Molecular Dynamics Simulation, *Applied Physics Letters*, vol. **80**, pp. 2484–2486, 2002.
17. D.E. Gray, *American Institute of Physics Handbook*, McGraw Hill, New York., 1972.
18. H.-K. Lyeo, and D.G. Cahill, Thermal Conductance of Interfaces between Highly Dissimilar Materials, *Physical Review B*, vol. **73**, p. 144301, 2006.
19. M.L. Huberman, and A.W. Overhauser, Electronic Kapitza Conductance at a Diamond-Pb Interface, *Physical Review B*, vol. **50**, pp. 2865–2873, 1994.
20. Y. Chen, D. Li, J. Yang, Y. Wu, J. Lukes, and A. Majumdar, Molecular Dynamics study of the Lattice Thermal Conductivity of Kr/Ar Superlattice Nanowires, *Physica B*, vol. **349**, pp. 270–280, 2004.
21. P.K. Schelling, S.R. Phillpot, and P. Keblinski, Comparison of Atomic-Level Simulation Methods for Computing Thermal Conductivity, *Physical Review B*, vol. **65**, p. 114306, 2002.
22. Y.A. Kosevich, Fluctuation Subharmonic and Multiharmonic Phonon Transmission and Kapitza Conductance between Crystals with Very Different Vibrational Spectra, *Physical Review B*, vol. **52**, pp. 1017–1024, 1995.
23. P.E. Hopkins, and P.M. Norris, Thermal Boundary Conductance Response to a Change in Cr/Si Interfacial Properties, *Applied Physics Letters*, vol. **89**, pp. 131909, 2006.
24. B. Abeles, Lattice Thermal Conductivity of Disordered Semiconductor Alloys at High Temperatures, *Physical Review*, vol. **131**, pp. 1906–1911, 1963.
25. K. Oura, V.G. Lifshits, A.A. Saranin, A.V. Zotov, and M. Katayama, Hydrogen Interaction with Clean and Modified Silicon Surfaces, *Surface Science Reports*, vol. **35**, pp. 1–69, 1999.
26. T. Beechem, and S. Graham, Estimating the Effects of Interface Disorder on the Thermal Boundary Resistance Using a Virtual Crystal Approximation, Proceedings of the 2006 ASME International Mechanical Engineering Congress, Anaheim, CA, **IMECE2006**, 14161.
27. P.E. Hopkins, R.J. Stevens, and P.M. Norris, Influence of Inelastic Seattering at Metal-Dielectric Interfaces, *Journal of Heat Transfer*.