Dressed and Intrinsic Thermal Boundary Conductance across Interfaces from a Nonequilibrium Landauer Approach

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Abstract

Thermal boundary conductance (TBC) is critical in thermal management of modern electronic devices. However, a decades-old puzzle has been that many of the measured TBCs, such as those well characterized across Al/Si and ZnO/GaN interfaces, significantly exceed theoretical results or even the theoretical limit called the “radiation limit”. Here, we identify that a commonly used assumption that phonons are in local thermal equilibrium at the interface is generally invalid. The measurable temperature for each individual mode is not the emitting temperature but the modal equivalent equilibrium temperature. Due to the wide range of transmission functions, different phonon modes are driven into strong thermal non-equilibrium with their respective equivalent equilibrium temperatures. We develop a ”nonequilibrium Landauer approach” to capture such nonequilibrium effect, and define the ”dressed” and ”intrinsic” interface thermal conductances assuming same modal emitted temperatures and same local equivalent equilibrium temperatures respectively. Using our approach on the Al/Si and ZnO/GaN interfaces doubles the TBC and can even surprisingly exceed the original radiation limit. Our predictions can now well explain the experimental results.
As modern electronic devices shrink in size, heat dissipation is increasingly limited by thermal resistances across interfaces [1, 2]. For example, the thermal boundary resistance (TBR) at the CNT-graphene junction is comparable to the resistance of a 200 nm long pure CNT [3, 4]. Hence, understanding thermal interfacial transport and designing interfaces with high thermal boundary conductance (TBC) are urgent problems to study. The Landauer approach [5–16], as shown below in Eq. (1), has been widely used to predict the thermal boundary conductance $G$:

$$G = \sum_p \int_0^{+\infty} \frac{1}{4} D v_g \tau h \omega (f(T_e1) - f(T_e2)) d\omega \frac{1}{T_e1 - T_e2} = \sum_p \int_0^{+\infty} \frac{1}{4} D v_g \tau h \omega \frac{df(T)}{dT} d\omega,$$

where the $p$-sum is over all the incident phonon branches, $\hbar$ is the reduced Planck constant, $\omega$ is the phonon angular frequency, $D$ is the phonon density of states, $v_g$ is the modal phonon group velocity, $\tau$ is the modal transmission coefficient at the interface from one material to the other, $f(T)$ is the carrier statistics at a certain temperature $T$ (the Bose Einstein distribution function is used for phonons), and $T_{e1}$ and $T_{e2}$ are the emitted phonon temperatures from two reservoirs.

However, experimental and molecular dynamics simulation results [15, 17, 18] often exceed the TBC predicted from the Landauer formula Eq. (1) and even the radiation limit (when the transmission coefficients are set as 1 in Eq. (1)) [7, 8, 19], which is usually considered as the upper limit of the thermal boundary conductance. Two possible mechanisms have been proposed in the literature, including inelastic scattering at the interface [20, 21] and cross-interface electron-phonon inelastic coupling [22–26]. However, before involving these mechanisms, we can examine whether Eq. (1) itself is a sound representation of the elastic conductance. In fact, Eq. (1) is clearly based on an important assumption that an interface is a local thermal equilibrium system, where the measurable temperatures of all phonon modes are the emitted phonon temperature $T_e$. Such an assumption may be reasonable for electron and photon interfacial transport, for which the Landauer approach was originally developed, since the temperature reservoirs can be held right adjacent to the interface or surface, and the local temperature near the interface is not affected by the transmitted photons or electrons. However, it is questionable for phonons, since in standard measurements of interfacial thermal conductance such as the two-bar method [27], the reservoirs are placed far away from the interface. It was pointed out in previous works by Simons [28],
and Zeng and Chen [29] that on the left side of the interface (as shown in FIG. 1) there are three groups of phonons: incident phonons traveling toward the interface with $T_{e1}$, reflected phonons with $T_{e1}$, and transmitted phonons from the right-side with $T_{e2}$. Clearly the incident, reflected, and transmitted phonons are not in equilibrium, and the measurable temperature near the interface should be affected by the transmitted phonons from the other side and different from the emitted phonon temperature $T_e$. A local equivalent equilibrium temperature was defined in Zeng and Chen’s work [29], and it correctly predicts a zero resistance for an imaginary interface in a pure material (the transmission coefficients $\tau_{1\rightarrow2}$ and $\tau_{2\rightarrow1}$ are both 1) rather than a finite resistance that would be predicted by Eq. (1).

However, the model was a gray approach so it did not consider different phonon modes and the consequences of their varied transmission coefficients. Recently, a modal nonequilibrium molecular dynamics approach [30] has been developed and the results show that different phonon modes are in strong nonequilibrium near an interface. Such nonequilibrium effect needs to be incorporated in the Landauer approach.

In this work, we first apply the original Landauer method Eq. (1) to the Al/Si interface, because the TBC of the Al/Si interface has been measured by several groups [31–33]. However, we show that both literature and our calculated results from the original Landauer formula underestimates the TBC by over 25%. For the ZnO/GaN interface, the underestimation is as high as 56% [15], which means the experimental TBC results are higher than twice the predictions from Landauer approach. We identify the underestimation to come from the assumption that all phonon modes are at equilibrium and the local temperature $T$ is the same as the emitted temperature $T_e$ near the interface. Then we define the modal equivalent equilibrium temperature $T_\lambda$ of the corresponding phonon mode $\lambda$, and develop the nonequilibrium Landauer approach with $T_\lambda$ for the Al/Si interface. We then calculate the modal conductance and define the ”dressed” and ”intrinsic” interfacial conductances $G_{\text{dressed}}$ and $G_{\text{intrinsic}}$. It should be noted that these two types of conductances can only be distinguished using our modal approach while not in the gray approach in Refs. [28-29]. The results from our approach can now well explain the experimental results for both Al/Si and ZnO/GaN interfaces.

We begin with the original Landauer approach, and the TBC at the interface is calculated from the net heat flow rate $q$, cross-sectional area $A_c$ of the interface, and emitted phonon
FIG. 1. The general structure of thermal transport considered in Landauer approach.

Temperatures $T_{e1}$ and $T_{e2}$ as shown in the following equation:

$$G = \frac{q}{A_c \Delta T} = \frac{q}{A_c (T_{e1} - T_{e2})},$$  \hspace{1cm} (2)

The net heat flow rate $q$ as shown in FIG. 1 usually takes the following form [6, 10]:

$$q = \sum_p \int_0^{+\infty} \frac{1}{2\pi} M(\omega) \tau(\omega) h \omega [f(T_{e1}) - f(T_{e2})] d\omega,$$  \hspace{1cm} (3)

where $M(\omega)$ is the phonon number of modes of material 1 at a given frequency $\omega$. The detailed derivation of Landauer formula can be found in the supplemental material. For the interface between three dimensional (3D) materials, the number of modes is:

$$M_{3D} = \frac{A_c k(\omega)^2}{4\pi},$$  \hspace{1cm} (4)

where $k(\omega)$ is the wave number at a certain frequency $\omega$. The $q$ expression with number of modes is equivalent to the $q$ expression with density of states, which is the numerator in Eq. (1) (the proof of the equivalence can be found in the supplemental material). The number of modes expression is used here to simplify the derivation of transmission function later. It should be noted that only the phonon properties of material 1 is needed here because of the constraint from detailed balance, that the net heat flow rate is 0 when $T_{e1} = T_{e2}$, and the information of material 2 is included in the transmission coefficient $\tau$. The related proof can be found in Supplemental Material. Moreover, the Eq. (3) is for interfaces with transmission coefficients independent of phonon incident angle, or at least one of material 1 and 2 is one dimensional (1D). Here the diffuse mismatch model (DMM) [7] is applied to calculate the transmission coefficient, and this approximation is valid as the transmission from DMM
does not depend on the angle of incidence. The DMM is used here but not other methods like acoustic mismatch model (AMM) because in our work the Landauer approach is applied to compare with experiments. The AMM usually works well for transmission process at low temperature across smooth interface, because materials are considered as continua without lattice structures, which might work for long wavelength but not short wavelength phonons. However, in experiments, there are usually defects at interfaces, and DMM has better agreement with experiments at room temperature, because of its assumption that all the phonons are diffusely scattered at the interface. Therefore, the DMM is selected to calculate the transmission coefficients. From the DMM model, the transmission coefficient is defined as:

$$\tau_{1\rightarrow2}(\omega) = 1 - \frac{\sum_p M_2}{\sum_p M_1 + \sum_p M_2}.$$ (5)

The detailed balance of Landauer formula with transmission function from DMM is automatically satisfied because of the definition, and a proof can be found in the supplemental material. The phonon properties of both Al and Si are obtained from ab initio calculations within the framework of density-functional theory (DFT), as implemented in the Vienna Ab initio Simulation Package (VASP), and the dispersion curves are shown in FIG. 2. Because all the incident modes lose their memory during transmission process, the transmission coefficients of DMM only depend on the frequency but not polarization unlike AMM, which is another widely used model for transmission prediction. Both DMM and AMM assume elastic transmission process without the change of phonon frequency.

With all the information, $G_{\text{original}}$ from the original Landauer approach at the Al/Si interface can be calculated as:

$$G_{\text{original}} = \sum_p \frac{\int_0^{+\infty} \frac{1}{8\pi^2} k(\omega)^2 \tau(\omega) h\omega \left[f(T_{e1}) - f(T_{e2})\right] d\omega}{T_{e1} - T_{e2}}.$$ (6)

The calculated spectral transmission coefficients $\tau$ from DMM can be found in the supplemental material. The modal interface conductance and spectral conductance accumulation at room temperature 300K are shown in supplemental material as well. The temperature dependant original Landauer approach results are then compared to the TBC results from the experiments as shown in FIG. 3. The radiation limit, which is usually considered as the upper limit of the TBC because of the assumption of unity transmission, is
FIG. 2. The phonon dispersion relation of Al and Si calculated from first principles method.

also calculated and plotted in FIG. 3. It is clear the original Landauer approach generally underestimates the TBC at Al/Si interface, and we suspect that the underestimation comes from the local nonequilibrium near the interface.

Hence, we closely examine the phonon nonequilibrium at the interface as shown in FIG. 4. For each incident phonon mode, the transmitted phonons will affect the local temperature, such that the measurable temperature is no longer the same as the emitted temperature $T_e$. Also, because of the different transmission coefficients of different phonon modes, the reflected phonons are not in equilibrium either. Clearly, the Landauer approach misses this nonequilibrium physics that experiment captures. To remedy this, the impact of transmitted and reflected phonons on the local temperature should be considered.

As shown in FIG. 4(a), the modal phonon emitted temperature on each side of the interface are $T_{\lambda,e1}$ and $T_{\lambda,e2}$, respectively. The modal equivalent equilibrium temperature $T_\lambda$ of phonon mode $\lambda$ on the two sides, as shown in FIG. 4(a), are

$$T_{\lambda,1} = T_{\lambda,e1} - \frac{1}{2}(T_{\lambda,e1} - T_{\lambda,e2})\tau_{1\to2}(\omega), \quad (7)$$

$$T_{\lambda,2} = T_{\lambda,e2} + \frac{1}{2}(T_{\lambda,e1} - T_{\lambda,e2})\tau_{2\to1}(\omega), \quad (8)$$

To calculate the TBC with modal equivalent equilibrium temperature, we first make an assumption that all phonon modes have the same emitted temperatures $T_{e1}$ and $T_{e2}$ on the two sides, respectively. This assumption means that there is no phonon scattering
FIG. 3. The comparison of TBC across Al/Si interface between different Landauer approaches and Experiment.

from the reservoir to the interface, and all the phonon modes preserve the temperature from the isothermal reservoir. The modal equivalent equilibrium temperature $T_\lambda$ of two representative modes $\lambda_1$ and $\lambda_2$ are shown in FIG. 4(b). Considering all modes, the lattice equivalent equilibrium temperatures $T_1$ and $T_2$, which are the local temperature on each side of the interface, are given by:

$$T_1 = \frac{\sum_p \int_0^{+\infty} T_{\lambda_1}(\omega) v_{g1}(\omega) f(T_{e1}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_1(\omega) v_{g1}(\omega) f(T_{e1}) d\omega},$$

$$T_2 = \frac{\sum_p \int_0^{+\infty} T_{\lambda_2}(\omega) v_{g2}(\omega) f(T_{e2}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_2(\omega) v_{g2}(\omega) f(T_{e2}) d\omega}.$$
conservation of energy. The local equivalent equilibrium temperature jump $\Delta T$ then becomes

$$\Delta T = T_1 - T_2 = \frac{\sum_p \int_0^{+\infty} T_{\lambda,1} \bar{h}\omega D_1(\omega) v_{g1}(\omega) f(T_{e1}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_1(\omega) v_{g1}(\omega) f(T_{e1}) d\omega} - \frac{\sum_p \int_0^{+\infty} T_{\lambda,2} \bar{h}\omega D_2(\omega) v_{g2}(\omega) f(T_{e2}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_2(\omega) v_{g2}(\omega) f(T_{e2}) d\omega}.$$

(11)

Now the TBC across the interface can be calculated as:

$$G_{\text{dressed}} = \frac{\sum_p \int_0^{+\infty} \frac{1}{8\pi} k(\omega)^2 \tau(\omega) \bar{h}\omega [f(T_{e1}) - f(T_{e2})] d\omega}{\sum_p \int_0^{+\infty} \frac{1}{8\pi} k(\omega)^2 \tau(\omega) \bar{h}\omega [f(T_{e1}) - f(T_{e2})] d\omega}$$

$$= \frac{\sum_p \int_0^{+\infty} T_{\lambda,1} \bar{h}\omega D_1(\omega) f(T_{e1}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_1(\omega) f(T_{e1}) d\omega} - \frac{\sum_p \int_0^{+\infty} T_{\lambda,2} \bar{h}\omega D_2(\omega) f(T_{e2}) d\omega}{\sum_p \int_0^{+\infty} \bar{h}\omega D_2(\omega) f(T_{e2}) d\omega}.$$

(12)

and the results are shown in FIG. 3 as $G_{\text{dressed}}$ (dressed means the modal $G_{\lambda}$ is dressed by the overall temperature jump $T_1 - T_2$ rather than their respective $\Delta T_{\lambda}$, hence the total $G$ is not a direct summation of $G_{\lambda}$).

The dressed conductance $G_{\text{dressed}}$ assumes that the emitted temperature $T_{\lambda,e}$ of all the modes are the same. However, our recent modal NEMD calculations at the interface [30]...
imply that modal emitted temperatures are different for different phonon modes at the interface. In fact, in typical experimental measurements the thermostats are placed far enough from the interface, so different phonon modes arrive at the interface at different emitted temperatures although they leave the thermostat with the same temperature. Hence, as an alternative to the dressed conductance $G_{\text{dressed}}$, we define another conductance limit with a different assumption that the modal equivalent equilibrium temperature $T_\lambda$ for all the modes are all the same:

$$T_{\lambda,1} = T_1, T_{\lambda,2} = T_2, \Delta T_\lambda = T_1 - T_2 = \Delta T, \quad (13)$$

and the average temperature of $T_1$ and $T_2$ equals the average of $T_{e,1}$ and $T_{e,2}$. This assumption would require the phonons to generally have different emitted temperatures $T_{\lambda,e}$ (unless a constant transmission coefficient which does not change with frequency or even a unity transmission for all phonon modes which recovers the imaginary interface case). This assumption actually renders all phonons in local thermal equilibrium and give a different TBC, which we call the intrinsic conductance $G_{\text{intrinsic}}$. The $G_{\text{intrinsic}}$ can be calculated as:

$$G_{\text{intrinsic}} = \frac{q}{\Delta T} = \frac{\sum_\lambda q_\lambda}{\sum_\lambda \Delta T_\lambda} = \frac{\sum_\lambda q_\lambda}{\sum_\lambda \Delta T_\lambda} = \frac{\sum_\lambda q_\lambda}{\sum_\lambda T_{\lambda,1} - T_{\lambda,2}} = \sum_\lambda G_\lambda. \quad (14)$$

We call it $G_{\text{intrinsic}}$ because it is a simple summation of the modal conductance $G_\lambda$ due to the fact that all the phonon modes are in local equilibrium near the interface, unlike $G_{\text{dressed}}$. With the intrinsic conductance, if $\tau_{12} = 1$, the zero resistance can be correctly predicted. The results of $G_{\text{intrinsic}}$ across the Al/Si interface is shown in FIG. 3. Both $G_{\text{dressed}}$ and $G_{\text{intrinsic}}$ are significantly larger than that from the original Landauer approach and even the original radiation limit, and can now bound the experimental data at the entire temperature range. These two conductances can only be distinguished using our modal and nonequilibrium approach while not in the gray approach where all phonon modes have the same $T_e$ and $T_1$, $T_2$ at the same time. Our modal nonequilibrium approach brings quantitative agreement with experiment in reach.

Then we apply the non-equilibrium Landauer approach to the ZnO/GaN interface. As mentioned earlier, in the previous thermal boundary conductance study of ZnO/GaN interface [15], it was found that the Landauer approach with transmission from DMM underpredicts the TBC measured from experiments by nearly a factor of two. We suspect that the discrepancy can come from the same issue of not including phonon nonequilibrium.
FIG. 5. The phonon dispersion relations of ZnO and GaN calculated from first principles.

Following the similar method we use for Al/Si interface, the phonon dispersion relations of ZnO and GaN are calculated from first principles as shown in FIG. 5. Then the original and nonequilibrium Landauer approaches, and the radiation limit are applied to the ZnO/GaN interface to calculate TBC with transmission from DMM with modal equivalent equilibrium temperature \( T_\lambda \) correction. As shown clearly in FIG. 6, the experiment results even exceed the original radiation limit, which cannot be explained from the orginal Landauer approach because the radiation limit is considered as the upper limit of TBC. With our nonequilibrium Landauer approach, TBC results from both \( G_{\text{dressed}} \) and \( G_{\text{intrinsic}} \) are much higher than \( G_{\text{original}} \) and can now bound the experimental results. The comparison between our results with the experimental results from Ref. [15] is shown in FIG. 6. Our results once again can well explain the experimental data.

Interestingly, if we compare the \( G_{\text{dressed}} \) and \( G_{\text{intrinsic}} \), it can be found that for the Al/Si interface, \( G_{\text{dressed}} \) is larger, while for the ZnO/GaN interface, \( G_{\text{intrinsic}} \) is larger. In fact, it is related to the relation between modal heat flux and transmission. If the modes carrying large heat flux have high transmission coefficient, \( G_{\text{intrinsic}} \) can be very high because of the
large difference between $\Delta T_e$ and $\Delta T_\lambda$, and as a result $G_{\text{intrinsic}}$ is larger than $G_{\text{dressed}}$. On the other hand, if modes carrying large heat flux and modes with high transmission coefficient are different, $G_{\text{intrinsic}}$ is usually smaller than $G_{\text{dressed}}$. For a perfectly matched interface, DMM will yield transmission coefficient of 0.5 and $G_{\text{dressed}}$ is always twice $G_{\text{original}}$, if the mismatch between two materials across the interface is small, usually $G_{\text{intrinsic}}$ is larger than $G_{\text{dressed}}$.

To summarize, the Landauer approach with transmission from mismatch models is often applied to predict the TBC at the interface. However, it often underestimates the conductance as compared to experimental results. We have modified the original Landauer approach to include the effects of phonon local nonequilibrium, and term it "nonequilibrium Landauer approach". Our approach on Al/Si and ZnO/GaN interfaces shows that the experimental TBC results do not actually exceed the Landauer results or the radiation limit,
and our dressed and intrinsic conductance can both predict higher TBC than the original radiation limit. Our work sheds important insights in interpreting experimental data for thermal interfaces, especially the highly matched interfaces.

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[1] E. Pop, S. Sinha, and K. Goodson, *Proceedings of the IEEE* **94**, 1587 (2006).
[2] A. L. Moore and L. Shi, *Materials Today* **17**, 163 (2014).
[3] J. Shi, Y. Dong, T. Fisher, and X. Ruan, *Journal of Applied Physics* **118**, 044302 (2015).
[4] J. Shi, Y. Zhong, T. S. Fisher, and X. Ruan, *ACS Applied Materials & Interfaces* **10**, 15226 (2018).
[5] R. Landauer, *IBM Journal of Research and Development* **1**, 223 (1957).
[6] W. A. Little, *Canadian Journal of Physics* **37**, 334 (1959).
[7] E. T. Swartz and R. O. Pohl, *Reviews of Modern Physics* **61**, 605 (1989).
[8] R. J. Stoner and H. J. Maris, *Physical Review B* **48**, 16373 (1993).
[9] C. Jeong, S. Datta, and M. Lundstrom, *Journal of Applied Physics* **111** (2012), 10.1063/1.4710993.
[10] T. S. Fisher, in *Thermal Energy at the Nanoscale* (WORLD SCIENTIFIC, 2013) pp. 87–111.
[11] P. Reddy, K. Castelino, and A. Majumdar, *Applied Physics Letters* **87**, 211908 (2005).
[12] J. C. Duda, T. E. Beechem, J. L. Smoyer, P. M. Norris, and P. E. Hopkins, *Journal of Applied Physics* **108**, 073515 (2010).
[13] X. Li and R. Yang, *Physical Review B - Condensed Matter and Materials Physics* **86** (2012), 10.1103/PhysRevB.86.054305.
[14] P. M. Norris, N. Q. Le, and C. H. Baker, *Journal of Heat Transfer* **135**, 061604 (2013).
[15] J. T. Gaskins, G. Kotsonis, A. Giri, S. Ju, A. Rohskopf, Y. Wang, T. Bai, E. Sachet, C. T. Shelton, Z. Liu, Z. Cheng, B. Foley, S. Graham, T. Luo, A. Henry, M. S. Goorsky, J. Shiomi, J.-P. Maria, and P. E. Hopkins, *Nano Letters*, acs.nanolett.8b02837 (2018).
[16] Y. Zhou, Z. Fan, G. Qin, J.-Y. Yang, T. Ouyang, and M. Hu, *ACS Omega* **3**, 3278 (2018).
[17] M. L. Huberman and A. W. Overhauser, *Physical Review B* **50**, 2865 (1994).
[18] M. Hu, P. Keblinski, and P. K. Schelling, *Physical Review B* **79**, 104305 (2009).
[19] H. K. Lyeo and D. G. Cahill, *Physical Review B - Condensed Matter and Materials Physics* **73**, 1 (2006).
[20] P. E. Hopkins, *Journal of Applied Physics* **106**, 013528 (2009).

[21] M. Paulsson, T. Frederiksen, and M. Brandbyge, *Physical Review B* **72**, 201101 (2005). arXiv:0505473 [cond-mat].

[22] S. Sadasivam, N. Ye, J. P. Feser, J. Charles, K. Miao, T. Kubis, and T. S. Fisher, *Physical Review B* **95**, 1 (2017). arXiv:1609.03063.

[23] T. Lu, J. Zhou, T. Nakayama, R. Yang, and B. Li, *Physical Review B* **93**, 085433 (2016).

[24] Z. Lu, Y. Wang, and X. Ruan, *Physical Review B* **93**, 064302 (2016).

[25] K.-H. Lin and A. Strachan, *The Journal of Chemical Physics* **143**, 034703 (2015).

[26] P. E. Hopkins, J. L. Kassebaum, and P. M. Norris, *Journal of Applied Physics* **105**, 023710 (2009).

[27] M. Rosochowska, K. Chodnikiewicz, and R. Balendra, *Journal of Materials Processing Technology* **145**, 207 (2004).

[28] S. Simons, *Journal of Physics C: Solid State Physics* **7**, 4048 (1974).

[29] T. Zeng, Gang Chen, *Microscale Thermophysical Engineering* **5**, 71 (2001).

[30] T. Feng, W. Yao, Z. Wang, J. Shi, C. Li, B. Cao, and X. Ruan, *Physical Review B* **95**, 1 (2017). arXiv:1703.10957.

[31] A. J. Minnich, J. A. Johnson, A. J. Schmidt, K. Esfarjani, M. S. Dresselhaus, K. A. Nelson, and G. Chen, *Physical Review Letters* **107** (2011), 10.1103/PhysRevLett.107.095901.

[32] C. Monachon and L. Weber, *Journal of Applied Physics* **113**, 183504 (2013).

[33] R. B. Wilson and D. G. Cahill, *Nature Communications* **5**, 5075 (2014). arXiv:arXiv:1011.1669v3.

[34] R. M. Costescu, M. A. Wall, and D. G. Cahill, *Physical Review B* **67**, 054302 (2003).

[35] S. Shin, M. Kaviany, T. Desai, and R. Bonner, *Physical Review B* **82**, 081302 (2010).

[36] G. Kresse and J. Hafner, *Physical Review B* **47**, 558 (1993).

[37] G. Kresse and J. Furthmüller, *Computational Materials Science* **6**, 15 (1996).