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Thermal transmission at Si/Ge interface: *ab initio* lattice dynamics calculation

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Abstract. We perform lattice dynamics calculations (LD) on silicon/germanium interfaces using *ab initio* interatomic force constants to predict the interfacial phonon transmission as a function of both phonon frequency and the transmission angle. We carry out a spectral and angular analysis to quantify the contribution of each phonon mode in a given scattering direction. The effect of the interaction range was studied at this interface by taking account of more or less atom layers across the interface. Moreover, we were able to predict the thermal boundary conductance (TBC) as a function of the transmission angle and temperature as well. Our results show that, the thermal energy transmission is highly anisotropic while thermal energy reflection is almost isotropic. In addition, we found that it seems there is a global critical angle of transmission beyond which almost no thermal energy is transmitted. This can be used to device high pass phonon filter via changing the orientation of the interface.

1. Introduction

Since the discovery of thermal resistance at the interface between two media by the pioneering experimental work of Kapitza on superfluid helium/solid interfaces [1], many theoretical attempts have been to understand interfacial heat transport. Among the most popular models, the acoustic mismatch model (AMM) [2] and diffuse mismatch model (DMM) [3] have been proposed. The former model AMM consider the phonons as plane waves experiencing specular transmission at the interface so the transmission is a function of the ratio between the impedances of the two media, while in the latter model DMM, all phonons diffusely scatter at interfaces, and the probability of transmission is determined by a mismatch between the densities of states. Both models fail to predict the thermal conductance measured experimentally [4], but they are still widely used because of their simplicity. In the quest for more accurate models to predict thermal boundary conductance (TBC), several methods have been proposed during the last decade, including molecular dynamics [5, 6], Green function [8] and lattice dynamics [7, 10]. Despite its popularity and wide use, molecular dynamics simulations often rely on the consideration of empirical potentials, which do not describe accurately bulk phonon dispersion. Lattice dynamics calculations have been traditionally devised to give a precise account of bulk phonon dispersion. This level of accuracy has, however, not been reached for describing interfacial heat flow. Let us mention lattice dynamics calculations for one-dimension [9], two-dimension and three-dimension [7] solids. The pioneering work of Young and Maris provided a reasonable agreement with thermorefectance measurements of the Kapitza conductance for interfaces between metals



and dielectrics as long as their Debye temperatures differ by less than a factor of 5 [11]. In this article, we perform lattice dynamics calculations using *ab initio* interatomic force constants in order to quantify phonon transmission at silicon/germanium interface. We show that these calculations provide a full description of the interfacial transmission including the frequencies and directions of both transmitted and reflected phonons and enable us to predict the thermal boundary conductance (TBC) at the interface as a function of the transmission angle.

2. Theoretical Model

In this section, we present the main equations used in lattice dynamics calculations (LD) for a perfect interface between two diamond-like structure solids in three-dimensions. Thereby, we can characterize the properties of incident and excited phonons required to calculate the phonon energy transmission at the interface. The interaction in each medium is supposed to be determined by interatomic force constants $\Phi(\mathbf{r})$ derived from *ab initio* calculations [12]. In the bulk, the equation of motion for an atom j of mass m_j displaced by $\mathbf{u}(\mathbf{r}_j)$ can be read as:

$$m_j \ddot{\mathbf{u}}(\mathbf{r}_j) = - \sum_j \Phi(\mathbf{r}_{jj}) \mathbf{u}(\mathbf{r}_j) \quad (1)$$

where the sum is over all atoms including atom j itself (these are called self-terms) and Φ is the interatomic force constant matrix limited here to the harmonic terms. Eq. 1 admits a general solution of the form :

$$\mathbf{u}(\mathbf{r}_j, t) = \mathbf{A}(\mathbf{k}, \nu) \exp [i(\mathbf{k} \cdot \mathbf{r}_j - \omega t)] \quad (2)$$

This solution represents a wave of mode p propagating in the \mathbf{r} direction with the amplitude $\mathbf{A} = A\mathbf{e}$. Therefore, Eq. 1 can be rewritten as:

$$\mathbf{D}(\mathbf{k})\mathbf{e}(\mathbf{k}, \nu) = \omega^2(\mathbf{k}, p)\mathbf{e}(\mathbf{k}, \nu) \quad (3)$$

\mathbf{D} is a 6×6 dimension matrix called the dynamical matrix and \mathbf{e} is the polarisation vector indicating the direction of the corresponding atomic displacement vector. The interface is represented in Fig. 1, where we divide the system into three regions: the left lead where the incident phonons come from, the central region corresponding to the location of the interface and the right lead where the transmitted phonons come out, denoted by L, C and R, respectively. The interface is oriented to be perpendicular to the z -axis corresponding to the [001] crystalline direction.

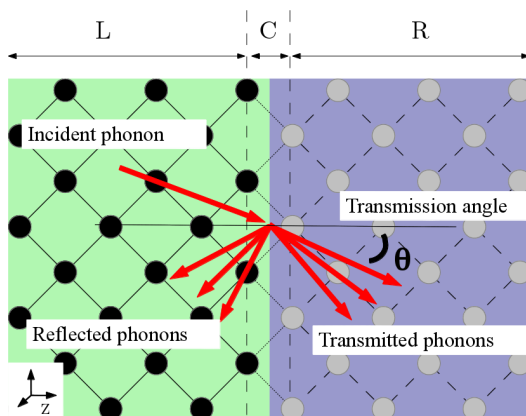


Figure 1. Schematic of the perfect interface between Si/Ge. Coming from the left lead, the incident phonon strikes the interface in the central region and is decomposed into transmitted phonons in the right lead and reflected phonons in the left lead.

After decomposing the dynamical matrix into three or more region-dependent dynamical sub-matrices [10], we are able to determine the excited modes. At the interface, we assume

elastic scattering, in other words, the incident phonon can only excite phonons having the same frequency

$$\omega(\mathbf{k}^L) = \omega(\mathbf{k}^R) = \omega(\mathbf{k}) \quad (4)$$

Also, at the interface the components of the wave vector parallel to the interface are conserved [13]

$$k_x^L = k_x^R = k_x \quad \text{and} \quad k_y^L = k_y^R = k_y \quad (5)$$

With these two requirements, we can find the excited modes by solving a generalized linear eigensystem

$$\begin{pmatrix} -\mathbf{D}^{L'} & M\omega^2\mathbf{I} - \mathbf{D}_S^C & -\mathbf{D}^{R'} & -\mathbf{D}^{R''} \\ \mathbf{I} & 0 & 0 & 0 \\ 0 & \mathbf{I} & 0 & 0 \\ 0 & 0 & \mathbf{I} & 0 \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{D}^{L''} & 0 & 0 & 0 \\ 0 & \mathbf{I} & 0 & 0 \\ 0 & 0 & \mathbf{I} & 0 \\ 0 & 0 & 0 & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{e}' \\ \mathbf{e}'' \\ \mathbf{e}''' \\ \mathbf{e}'''' \end{pmatrix} = \Gamma \begin{pmatrix} \mathbf{e}' \\ \mathbf{e}'' \\ \mathbf{e}''' \\ \mathbf{e}'''' \end{pmatrix} \quad (6)$$

where $\Gamma \equiv \exp(ik_z a/2)$, $\mathbf{e}' = \Gamma\mathbf{e}$, $\mathbf{e}'' = \Gamma^2\mathbf{e}$ and $\mathbf{e}''' = \Gamma^3\mathbf{e}$. The subscript S indicates that the corresponding matrix contains all self-terms. This will give us all possible z -components of the reflected and transmitted wave vectors, but we select only those which have a physical meaning as described by Zhao and Freund [10]. Note also that the order in Γ depends on the number of interacting neighbours that we consider, higher orders correspond to larger interaction range. For some incident wavevectors, the generalized matrix in Eq. 6 may be singular, we solve then this equation by a direct method. We eliminate the cases where $\Gamma = 0$ and $\Gamma = \infty$ which give unphysical values of Γ .

To completely describe the transmission at the interface, we need a set of $6 \times N$ equations, where N is the number of the interacting atomic layers taken into account. The complex displacement vector, $\mathbf{u}(\mathbf{r}_{ij})$ of the i th atom in the j th primitive unit cell in the left lead can be expressed as a superposition of the incident mode and the excited modes in the left lead :

$$\mathbf{u}(\mathbf{r}_{ij}) = \mathbf{A}_i(\mathbf{r}_i, \mathbf{k}, \nu) \exp[i\mathbf{k} \cdot \mathbf{r}_j] + \sum_{\mathbf{k}_r, \nu}^{n_r} \mathbf{A}_r(\mathbf{r}_i, \mathbf{k}_r, \nu) \exp[i\mathbf{k}_r \cdot \mathbf{r}_j] \quad (7)$$

where \mathbf{A}_r is the amplitude of the reflected waves and n_r the number of allowed modes. Similarly, the displacement vector in the outgoing medium (right lead) is

$$\mathbf{u}(\mathbf{r}_{ij}) = \sum_{\mathbf{k}_t, \nu}^{n_t} \mathbf{A}_t(\mathbf{r}_i, \mathbf{k}_t, \nu) \exp[i\mathbf{k}_t \cdot \mathbf{r}_j] \quad (8)$$

The equation of motion of the l th atom layer at interface can be written in the general form:

$$\sum_{\mathbf{k}_{i,r,t}} \left[\left(\omega^2\mathbf{I} - \mathbf{D}_s^L - \mathbf{D}_s^{R,\dagger} - \mathbf{D}_s^{C,l} - \mathbf{D}_s^{int,\bar{l}} \right) \mathbf{A}_{i,r} - \mathbf{D}_{int}^{R,\bar{l}} \mathbf{A}_t \right] = 0 \quad (9)$$

$$\sum_{\mathbf{k}_{i,r,t}} \left[-\mathbf{D}_{int}^{L,\bar{l}} \mathbf{A}_{i,r} + \left(\omega^2\mathbf{I} - \mathbf{D}_s^R - \mathbf{D}_s^{L,\dagger} - \mathbf{D}_s^{C,l} - \mathbf{D}_s^{int,\bar{l}} \right) \mathbf{A}_t \right] = 0 \quad (10)$$

where the sum is over all wave vectors. The first equation Eq. 9 describes the motion of an atom in the incoming medium (left lead). The interactions with the atoms in the left lead are represented by the left dynamical matrix \mathbf{D}_s^L which includes the self-terms. The interactions with the atoms in the right lead across the interface are represented by the right dynamical

matrix with interfacial force constant $\mathbf{D}_{int}^{R\bar{l}}$, from which some terms corresponding to up to the l th neighbour layer were subtracted and added to the right matrix dynamic of the other medium in bulk $\mathbf{D}_s^{R,\dagger}$. The subscript s is always used to indicate that the matrix includes the self-terms, while int indicates that the force constants are calculated across the interface, and \bar{l} (\dagger) refers to up to which layer the corresponding terms are subtracted (resp. added). The matrix $\mathbf{D}_s^{int,\bar{l}}$ contains only the self-terms at interface, from this matrix also some terms of up to l th neighbour were subtracted. Similarly, the second equation Eq. 10 describes the motion of an atom in the outgoing medium (right lead) and the notations remain the same. By solving the previous set of equations, we obtain the amplitude of each excited modes *i.e* reflected A_r and transmitted A_t phonons and then the energy phonon transmission coefficient defined as the fraction of phonon energy transmitted across the interface, can be obtained :

$$\mathcal{T} = \frac{\rho_t}{\rho_i} \sum_1^{n_t} \frac{v_{g,t}^z \cdot |A_t|^2}{v_{g,i}^z \cdot |A_i|^2} \quad (11)$$

where $v_{g,t}^z$ are the group velocities of the transmitted phonons in the direction perpendicular to the interface and n_t is the number of transmitted modes.

3. Results and Discussion

We present now the results obtained by performing the LD calculations on Si/Ge interface as described in the previous section. The interatomic interaction was limited to the 8th neighbours, which corresponds to the 4th unit cell (diamond-like crystals have two atoms per unit cell). Fig. 2 shows the transmission and reflection of all the phonon modes in polar coordinates, and for different interaction ranges that goes from the first unit cell (L1) up to the 4th unit cell (L4). The angular axis is taken as the y -axis. Overall, the transmission coefficient displays a maximum value about 1/2 in the normal transmission direction corresponding to $\theta = 0^\circ$ and it decreases when we go to the grazing direction, $\theta = 90^\circ$. From these curves, we can see that the phonon transmission is anisotropic with relative low values lying in the interval of transmission angle between $\theta = 50^\circ$ and $\theta = 90^\circ$. This transmission angle $\theta = 50^\circ$ beyond which the transmission is small can be seen as a global critical angle. Thermal phonon reflection seems to be almost isotropic with maximum value about 0.7 in the direction of 90° of transmission angle. The transmission coefficient is found to be almost insensitive to the interaction range, but the reflection coefficient displays a little increase when the interaction goes up to the 4th unit cell.

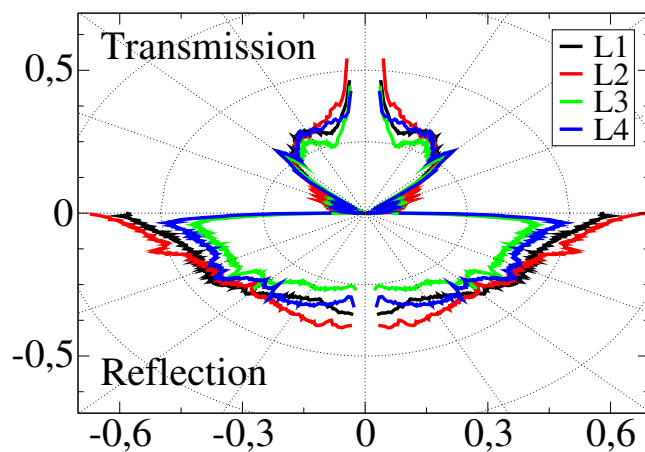


Figure 2. (Color inline) Phonon energy transmission at Si/Ge in polar coordinates for different interaction ranges. L1 refers to the interaction limited to only the nearest unit cell while L4 refers to the interaction up to the 4th unit cell.

We have performed a spectral and angular analysis to quantify the contribution of each phonon mode in a given scattering direction. Fig. 3 depicts this analysis showing that the transmission is highly anisotropic and we found that the probability of transmission is more important in the normal direction up to a transmission angle of $\theta = 50^\circ$. In this orientation, phonons at frequencies higher than 20 rad/ps have a larger probability to be transmitted than phonons having lower frequency. For frequencies lower than 10 (rad/ps), we observe that energy transmission has a limit beyond which the phonon transmission is very low, which confirms the existence of a critical angle at least for these low frequency phonons.

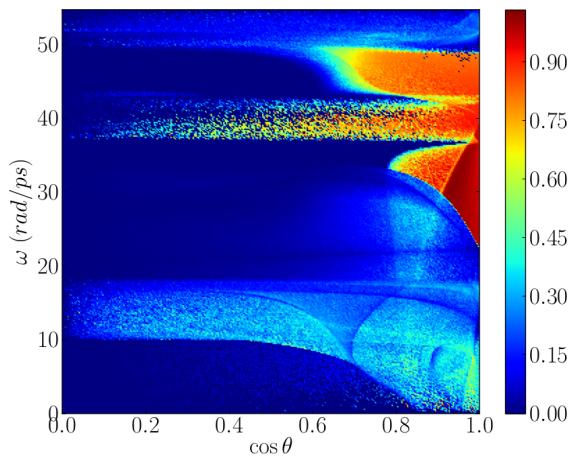


Figure 3. (Color inline) Colormap of the phonon energy transmission at Si/Ge interface as a function of both the angular frequency and the transmission angle. The interaction range was taken up to 2nd unit cell here.

We have also predicted the thermal boundary conductance (TBC) at silicon/germanium interface, which was found to be $G_{\text{Si/Ge}} \simeq 200$ (MW/m²/K) at room temperature when the interaction is limited to the first nearest unit cell (L1). The same value was predicted by Tian *et al* [14] for ideal Si/Ge interface using Green's function. In Fig. 4, we plotted the cumulative TBC as a function of the transmission angle, and we see that a significant contribution to energy transmission across the interface comes to large extent from angular directions close to normal incidence. This is an expected result as the transmission in these directions has been found to be more important. Note also that the TBC exhibits a significant drop in magnitude when the interaction range goes beyond the first unit cell (L1). This behaviour may be surprising and contrary to the intuition, nevertheless, it proves that enhanced interfacial bonding does not imply better phonon transmission. Therefore, we can conclude that to predict accurately the TBC, it is mandatory to consider at least three nearest unit cells, and that popular short range potentials describing diamond like crystals such as the Stillinger-Weber or the Tersoff potentials, will do a poor job in predicting interfacial heat transfer. Unfortunately, a direct comparison with experiments is not possible since we are not aware of an experimental data reporting the TBC of a single Si/Ge interface.

4. Conclusion

In summary, we have used LD calculations together with *ab initio* interatomic force constants to quantify phonon transmission at silicon/germanium interface and predict the thermal boundary conductance. These calculations have allowed us to quantify the transmission and reflection coefficients as a function of transmission angle, enlightening the important contribution of the phonons which are transmitted in the normal direction. A spectral and angular analysis of phonon transmission has been done to elaborate a complete view on the contribution of each phonon mode in a given scattering direction. Finally, we have emphasized the necessity to take into account at least three interacting unit cells to properly describe the TBC at Si/Ge interfaces. This work may be extended in different ways. First, it may be employed to predict

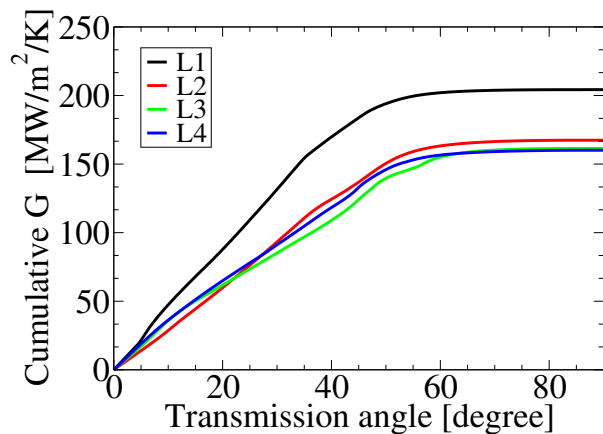


Figure 4. (Color inline) The cumulative TBC at room temperature for Si/Ge interface for different interaction ranges.

phonon scattering at rough interfaces following the lines of [15]. This may shed light on the possibility to enhance heat conduction through periodic patterned interfaces as considered in [16]. Another extension concerns the possibility to build multiscale models of phonon transport across solid multilayers and superlattices. To this end, the phonon transmission coefficient calculated here from first principles calculations may serve as input in a Monte Carlo simulation of the Boltzmann Transport Equation, which generally employs empirical transmission coefficient method to describe phonon scattering at interfaces. This will permit to simulate heat transport in devices having realistic sizes still keeping a microscopic description of interfacial conduction.

5. Acknowledgments

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References

- [1] P.L. Kapitza, *J. Phys. (USSR)*, **4** 181 (1941)
- [2] W.A. Little, *Can. J. Phys.* **37** 334 (1959)
- [3] E.T. Swartz and R.O. Pohl, *Rev. Mod. Phys.* **61** 605 (1989)
- [4] D.G. Cahill, W.K. Ford, K.E. Goodson, G.D. Mahan, A. Majumdar, H.J. Maris, R. Merlin and S.R. Philpot, *J. Appl. Phys.* **93** 793 (2003)
- [5] E.S. Landry and A.J.H. McGaughey, *Phys. Rev. B* **80** 165304 (2009)
- [6] S. Merabnia and K. Termentzidis, *Phys. Rev. B* (2012) **86** 094303
- [7] D.A. Young, and H.J. Maris, *Phys. Rev. B* **40** 3685 (1989)
- [8] W. Zhang, T.S. Fisher and N. Mingo, *AMSE J. Heat Transfer* 129 (2007) 483
- [9] L. Zhang, P. Keblinski, J.S. Wang, and B. Li, *Phys. Rev. B* **83** 064303 (2011)
- [10] H. Zhao and J.B. Freund, *J. Appl. Phys.* **97** 024903 (2005)
- [11] R.J. Stoner and H.J. Maris, *Phys. Rev. B* **48** 16373 (1993)
- [12] M. Aouissi, I. Hamdi, N. Meskini and A. Qteish, *Phys. Rev. B* **74** 054302 (2006)
- [13] S. Pettersson and G.D. Mahan, *Phys. Rev. B* **42** 7386-7390 (1990)
- [14] Z. Tian, K. Esfarjani, and G. Chen, *Phys. Rev. B* **86** 235304 (2012)
- [15] Zhao, H. and Freund, J. B., *J. Appl. Phys.* **105** 013515 (2009)
- [16] S. Merabnia and K. Termentzidis, *Phys. Rev. B* **89** (2014) 054309