INTRODUCTION
Phonon scattering at the interface between two materials results in a thermal resistance, $R$ [1]. An ability to accurately predict the thermal resistance of semiconductor interfaces is important in devices where phonon interface scattering is a significant contributor to the overall thermal resistance (e.g., computer chips with high component density). This ability will also lead to improvements in the design of semiconductor superlattices with low thermal conductivity, desirable in thermoelectric energy conversion applications [2].

The two most common theoretical models for predicting the thermal resistance of interfaces are the acoustic mismatch and diffuse mismatch models [1]. While these models have been successful in predicting the thermal resistance of isolated interfaces at temperatures less than $\sim 30$ K [1], they can be an order of magnitude in error at room temperature and above. Neither of these models account for how the atomic-level detail of the interface or the interaction between neighboring interfaces affect the thermal resistance. Furthermore, these models are usually applied under the assumption of linear phonon dispersion (i.e., the Debye approximation) [3–6], which is inaccurate at typical application temperatures, where phonons with wavelengths on the same scale as the interatomic spacing are excited [7]. Here, we use lattice dynamics (LD) calculations, which account for the atomic-level detail of the interface and provide a realistic description of the phonon dispersion, to examine the effect of interface separation distance on the thermal resistance of Si/Ge interfaces.

MODEL
To model the resistance of closely-spaced Si/Ge interfaces, we consider the two computational cells shown in Fig. 1(a). In one cell a thin Ge film with thickness $L_S$ is sandwiched between two semi-infinite leads of Si (the Si/Ge/Si structure). We also consider the opposite situation in which a thin Si film is placed between two semi-infinite leads of Ge (the Ge/Si/Ge structure). For a reference point, we also calculate the thermal resistance of an isolated Si/Ge interface using the computational cell shown in Fig. 1(b), which contains a semi-infinite lead of Si in contact with a semi-infinite lead of Ge. For all three types of computational cell, we refer to the region connecting the left and right semi-infinite leads as the junction. The junction contains all the atoms within the thin film (if applicable) and two atomic layers of each lead species. The computational cells are periodic in the directions parallel to the interface [the $x$- and $y$- directions, see Fig. 1].

The atomic interactions are modeled using the Stillinger-Weber (SW) interatomic potential, which has been parameterized for both Si-Si and Ge-Ge interactions [8, 9]. For the Si-Ge interactions, we use the mixing rules described by Laradji et al. [10]. We model perfect interfaces containing no defects (e.g., species mixing or misfit dislocations). The interfaces are symmetrically strained by setting the lattice constant in the $x$- and $y$- directions to the average of the bulk SW Si and Ge zero-temperature lattice constants. In the lead regions, the layer spacings in the direction perpendicular to the interfaces (the $z$ direction) are chosen to give zero-stress in that direction. Prior to performing the LD calculations, we allow the atoms in the junction to relax to their

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equilibrium positions by quenching the system in a molecular dynamics (MD) simulation to zero temperature.

**METHODOLOGY**

The thermal resistance of the junction region, which contains either one or two Si/Ge interfaces, is defined as [1]

$$ R = \frac{T_L - T_R}{q}, \tag{1} $$

where $q$ is the heat flux across the junction, and $T_L$ and $T_R$ are the temperatures in the left and right leads at the lead/junction boundary (see Fig. 1). At the phonon mode-level, $q$ can be written as [1, 11]

$$ q = \frac{1}{(2\pi)^3} \int_L \sum_{\nu} \bar{h}\omega(\mathbf{k},\nu)|v_z(\mathbf{k},\nu)|\alpha_{L-R}(\mathbf{k},\nu)f_L(\mathbf{k},\nu)Hd\mathbf{k}, \tag{2} $$

$$ -\frac{1}{(2\pi)^3} \int_R \sum_{\nu} \bar{h}\omega(\mathbf{k},\nu)|v_z(\mathbf{k},\nu)|\alpha_{R-L}(\mathbf{k},\nu)f_R(\mathbf{k},\nu)Hd\mathbf{k}, $$

where $L$ and $R$ denote the left and right leads, $\hbar$ is Planck’s constant divided by $2\pi$, $\mathbf{k}$, $\mathbf{v}$, and $\alpha$ are the phonon wavevector, polarization, and frequency, $v_z$ is the z-component of the phonon group velocity, $H$ is equal to one for phonons traveling towards the junction and zero otherwise, and the first (second) integral is over the first Brillouin zone of the left (right) lead. The phonon transmission coefficient, $\alpha_{L-R}$, is defined as the fraction of the incident phonon energy that is transmitted from the left lead to the right lead. The variables $f_L$ and $f_R$ are the distributions of phonons incident on the junction from the left and right leads. If the temperature change within each lead over the distance of one phonon mean free path is small compared to $T_L - T_R$, these distribution functions may be approximated by the equilibrium Bose-Einstein distribution, $f_{BE}(\alpha, T)$, at $T_L$ or $T_R$ [12]. We assume this condition to be true and will comment on the validity of this assumption in the discussion of our results.

When $T_L - T_R$ is much less than the average temperature of the junction, Eq. (2) can be combined with Eq. (1) to obtain [13, 14]

$$ R = \left[ \frac{1}{(2\pi)^3} \int_L \sum_{\nu} \bar{h}\omega|v_z|\alpha_{L-R}Hd\mathbf{k} \right]^{-1}. \tag{3} $$

We use LD calculations under the harmonic approximation to evaluate $R$ from Eq. (3). The integral in Eq. (3) is calculated numerically using Monte-Carlo integration with $25 \times 10^3$ random phonon wavevectors in the first Brillouin zone corresponding to the two-atom diamond unit cell. For each of the six phonon polarizations at each wavevector, $\alpha_{L-R}$ is calculated using the scattering boundary method [14, 15]. The LD calculations are performed for thin films with thicknesses up to 20 atomic layers (~3 nm).

Due to the harmonic approximation, our calculation of $R$ is only valid when (i) there is no phonon-phonon scattering within the junction, and (ii) the phonon interface scattering is elastic (i.e., the incident, reflected, and transmitted phonons have the same frequency). To examine the effects of diffuse phonon-phonon scattering and inelastic scattering, we calculate $R$ in the high temperature-limit and compare the results to separate predictions from classical direct-method MD simulations. The MD simulations naturally incorporate the combined effects of elastic and inelastic phonon scattering and diffusive and ballistic phonon transport. Our MD simulations are also performed using the SW potential and the predictions are made at a temperature of 500 K, where quantum effects are expected to be negligible. Further details related to our MD simulations can be found elsewhere [16].

**RESULTS**

For the isolated Si/Ge interface, we calculate the thermal resistance to be $3.0 \pm 0.1 \times 10^{-9}$ m²-K/W, in good agreement with the value of $2.85 \times 10^{-9}$ m²-K/W calculated by Zhao and Freund using a similar LD-based model and the SW potential [13]. We attribute the small difference between the calculations to lattice mismatch strain, which was not accounted for by Zhao.
and Freund. Our LD-calculated value is also in good agreement with our MD-predicted value of $2.8 \pm 0.2 \times 10^{-9} \text{ m}^2\text{-K/W}$ at a temperature 500 K.

The LD-calculated thermal resistances of the Si/Ge/Si and Ge/Si/Ge structures are shown in Fig. 2. The MD-predicted thermal resistances and the values of the thermal resistance in the diffuse limit, $R_{DL}$, reached when $L_S$ is much greater than the bulk phonon mean free path of the thin film species, are also provided for comparison. The thermal resistance in the diffuse limit is

$$ R_{DL} = 2R_{iso} + \frac{L_S}{k}, \quad (4) $$

where $R_{iso}$ is the thermal resistance of the isolated Si/Ge interface, and $k$ is the bulk thermal conductivity of the thin film species. For our calculation of the diffuse limit, we use MD-predicted values of $R_{iso}$ and $k$ [17].

The thermal resistances of the Si/Ge/Si and Ge/Si/Ge structures calculated from LD initially increase with increasing $L_S$ and then to level off to nearly the same constant value when $L_S \approx 2$ nm. The trend of an increasing thermal resistance with increasing $L_S$ is reasonable because when $L_S < 2$ nm, a large fraction of the atoms in the thin film region are bonded with atoms in the lead regions. The dynamics of the atoms in the thin film are thus similar to the dynamics of atoms in the leads and the thermal resistance is small. As $L_S$ increases, more atoms in the thin film region are bonded to atoms of the same species and have bulk-like dynamics, leading to higher thermal resistance. Because of the independence of the thermal resistance to $L_S$ for $L_S > 2$ nm, we extrapolate the LD calculations at $L_S = 3$ nm up to $L_S = 30$ nm to allow for comparison to the MD predictions.

The MD-predicted thermal resistances of the Ge/Si/Ge structures are in qualitative agreement with the LD calculations, indicating that the phonon transport within the thin Si film is primarily ballistic (ballistic transport is assumed in the LD calculations). Different behavior is observed, however, for the Si/Ge/Si structures. While the MD-predicted thermal resistances of the Si/Ge/Si structures also increases rapidly with increasing $L_S$, the thermal resistance does not level off to a constant value but instead continues to increase towards the diffuse limit. This trend indicates that the phonon transport within the thin Ge film is partially diffuse.

We suggest a qualitative explanation for the observed differences between the Si/Ge/Si and Ge/Si/Ge structures. From our LD calculations, we find that the phonon transmission coefficients are zero in both the Si/Ge/Si and Ge/Si/Ge structures above the maximum phonon frequency in SW Ge of 11 THz. Because this frequency is less than the maximum acoustic phonon frequency in SW Si of 13 THz, the thermal transport within the thin Si film in the Ge/Si/Ge structure is carried entirely by acoustic phonon modes, which have long phonon mean free paths and are likely to travel ballistically across the thin film. In the Si/Ge/Si structure, however, the thermal transport in the thin Ge film is due to a combination of acoustic and optical modes. Due to the lower phonon mean free path of optical modes than acoustic modes, the optical modes in the thin Ge film are more likely to scatter diffusely with other phonons. We note that fully diffusive phonon transport is not expected until $L_S$ is many times greater than the bulk phonon mean free paths, which we estimate from kinetic theory to be 50 nm in both SW Si and Ge at a temperature of 500 K [18].

The LD-calculated thermal resistances of the isolated Si/Ge interface and the Ge/Si/Ge structures are 10-20% greater than the corresponding MD-predicted values. This discrepancy may be due to our use of the equilibrium Bose-Einstein distribution, evaluated at either $T_L$ or $T_K$, to approximate the distribution of phonons incident on the interface. An alternative approximation is to evaluate the Bose-Einstein distribution at the local temperature a distance of one phonon mean free path away from the junction. This approximation has recently been shown by Aubry et al. to lead to improved agreement between thermal resistance predictions obtained by direct-method MD simulations and from Eq. (1) for the Σ3(111) grain boundary in SW Si [19].
SUMMARY AND CURRENT WORK

Lattice dynamics calculations have been used to examine the effect of separation distance on the thermal resistance of closely-spaced Si/Ge interfaces in the high-temperature limit. We predict the thermal resistance of both the Si/Ge/Si and Ge/Si/Ge closely-spaced interface structures to initially increase rapidly with increasing thickness of the thin film before reaching constant values for thicknesses greater than ∼3 nm. The LD-calculated thermal resistances were compared to values predicted from direct method MD simulations, which require no assumptions about the nature of the phonon transport. From these comparisons, we deduced that the phonon transport within the thin Si film in the Ge/Si/Ge structure is primarily ballistic while the transport within the thin Ge layer in the Si/Ge/Si structure is partially diffuse.

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REFERENCES

[18] The phonon mean free path is estimated using the phonon sound speed (taken as the average of the three [100] acoustic phonon group velocities in the $\kappa \to 0$ limit) and the bulk thermal conductivity predicted using MD and the SW potential.

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