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ABSTRACT

Silicon Carbide (SiC) is a typical material for third-generation semiconductors. The thermal boundary resistance (TBR) of the 4H-SiC/SiO_2 interface was investigated by both experimental measurements and theoretical calculations. The structure of 4H-SiC/SiO_2 was characterized by using transmission electron microscopy and X-ray diffraction. The TBR was found to be 8.11×10^{-8} m^2K/W at 298 K by the 3ω method. Furthermore, the diffuse mismatch model was employed to predict the TBR of different interfaces, which is in good agreement with measurements. Heat transport behavior based on the phonon scattering perspective was also discussed to understand the variations of TBR across different interfaces. Besides, the intrinsic thermal conductivity of SiO_2 thin films (200–1500 nm in thickness) on 4H-SiC substrates was measured by the 3ω procedure, to be 1.42 W/m K at 298 K. It is believed the presented results could provide useful insights into the thermal management and heat dissipation for SiC devices.

In recent years, the microelectronics industry has made great achievements in promoting the electronic performance of semiconductors. However, due to the increasing power density, heat dispassion has become one of the most important challenges to the performance and reliability of the devices. When the characteristic size shrinks to the order of the mean free path of energy carriers, thermal transport is dominated by the thermal conductance at the interfaces between adjacent materials, rather than the intrinsic thermal properties of materials.[1] Thus, it is an urgent issue to investigate the thermal boundary resistance (TBR) in electronic devices.

Silicon carbide (SiC) is widely recognized as one of the most promising semiconductor materials for new generations of power devices due to the unique advantages in terms of power conversion efficiency, thermal conductivity, and robust mechanical properties.[2] Moreover, SiC is the only known wide-bandgap semiconductor with a native SiO_2 perpetrated in the same way as silicon, which makes it suitable for metal-oxide-semiconductor devices.[3] However, the performance of SiC devices can also be limited by poor heat dissipation owing to the existence of TBR.[4] Particularly, the interface between silicon carbide and silicon dioxide (SiC/SiO_2) is the most common interface for current SiC-based microelectronics devices. Therefore, the TBR of the SiC/SiO_2 interface is critical in thermal analysis and thermal management in SiC devices.

Recently, the TBR across different interfaces, such as Si/SiO_2[5] and Al/Si,[6] has been investigated using MD simulation. However, in MD simulation, constructing a detailed interface model between two different materials that have high density of interface states[7] is a challenging and sophisticated work. Compared to the complexity and time consumption of MD simulations, the acoustic mismatch model (AMM) or diffuse mismatch model (DMM)[8] can avoid the complex interface modeling, yet achieve reasonable prediction on TBR. Thus, the AMM and DMM are easier to employ and then predict the TBR qualitatively and efficiently.

However, the thermal behavior of the SiC/SiO_2 interface is the lack of investigation. Numerous studies have shown that there is a

high density of interfacial traps between SiC and its native oxide,[9–11] which leads to a lower electron mobility. It is still unknown how much the roughness would block phonon transport across the SiC/SiO_2 interface. English *et al.* found that compositional disorder at an interface could strongly reduce thermal interface conductance at high temperature (50% of melting temperature).[12] Liang *et al.* revealed that the thermal accommodation coefficient (TAC) at the smooth and perfect interface is significantly lower than that at a disordered interface.[13] These related results indicate that the interfacial thermal conduction strongly depends on defect density at the interface. Therefore, it is indispensable to determine the TBR across the SiC/SiO_2 interface.

In this work, the TBR of the 4H-SiC/SiO_2 interface is investigated by both the experimental 3ω method and the theoretical diffuse mismatch model. First, the TBR of the Si/SiO_2 interface is investigated to verify the effectiveness of the customized 3ω experimental platform. Then, the thermal conductivities of SiO_2 films with various thicknesses on 4H-SiC substrates are measured. Experimental characterization and theoretical analysis are employed to determine the TBR across the 4H-SiC/SiO_2 interface.

In order to obtain the TBR between the 4H-SiC/SiO_2 interface by the 3ω method, five different thicknesses of the SiO_2 film were deposited by Plasma Enhanced Chemical Vapor Deposition (PECVD) on the Si and 4H-SiC substrate, respectively. Additionally, the feasibility of our customized 3ω measurement platform was validated for the TBR of the Si/SiO_2 interface. The details on sample preparation, measurement process, as well as characterization methods are addressed in the supplementary material. In the following, the measurement of the 4H-SiC/SiO_2 interface was conducted by the customized 3ω measurement platform. The apparent thermal conductivity values of the SiO_2 thin film samples with thicknesses varying from 200 to 1500 nm are between 0.96 and 1.32 W/m K at 298 K. The apparent thermal resistances of the SiO_2 thin films on the 4H-SiC substrate are plotted in Fig. 1.

The intrinsic thermal conductivity of the SiO_2 thin film on the 4H-SiC substrate was found to be 1.42 W/m K, which is slightly greater than that of the SiO_2 film on Si. This can be attributed to the preparation of two films, which are deposited separately in different PECVD equipment. The TBR of the 4H-SiC/SiO_2 interface was calculated to be 8.11×10^{-8} m^2K/W at 298 K, which is about 4 times higher than that of Si/SiO_2. A larger TBR of 4H-SiC/SiO_2 implicates that a high density of imperfections exists at 4H-SiC/SiO_2 interfaces, which restrains phonon heat transport across the interface. The TBR of the 4H-SiC/SiO_2 interface in our work is the same order of magnitude as that of similar heterogeneous interface systems presented in the literature. The previously reported TBR between highly dissimilar materials at room temperature measured by the time-domain thermoreflectance (TDTR) method ranges from 3.33×10^{-8} to 1.25×10^{-7} m^2K/W.[14]

The interface structure is an important factor to heat transport across the heterogeneous interface, which affects the phonon transport and scattering at interfaces. As shown in Fig. 2(a), potential damage in the near-surface region of the 4H-SiC substrate can be observed, and the disordered 4H-SiC layer has a thickness of 3–5 nm. As aforementioned, structural disorder would lead to an increase in the TBR due to the increased number of phonons scattering in the disordered region.[15] Additionally, multivacancy defects induced by threefold coordinated O and C interstitial atoms and lattice mismatch of 4H-SiC and SiO_2 materials[11] were observed at the 4H-SiC/SiO_2 interface close to the side of amorphous SiO_2. These vacancy defects would reduce the effective contact area compared to smooth contacting surfaces, which would predominantly increase the TBR. Meanwhile, the vacancy defects would increase the phonon scattering with defects and reduce phonon transmission at the interface, which would eventually increase the TBR. Generally, the defect density at the Si/SiO_2 interface remains one to two orders of magnitude lower than that typically found at the 4H-SiC/SiO_2 interface,[16] which contributes to a lower value of TBR of the Si/SiO_2 interface.

Nevertheless, MD simulations have shown that TBR of graphene/copper decreases with the increase in roughness,[17] which arises from the high local pressure between graphene and the copper substrate. Several Green's function calculations suggest that interface roughness induced by atomic mixing can increase phonon transmission and interfacial thermal conductance of the Si-Ge interface by providing channels of transmission for nonspecular in-plane momentum.[18,19] Besides, the interfacial roughness could decrease TBR due to the

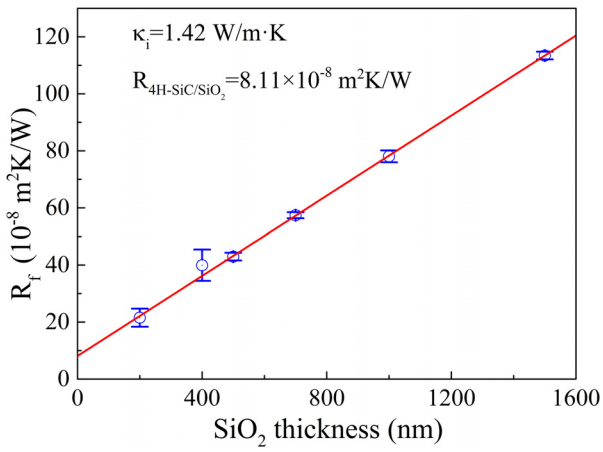

FIG. 1. Apparent thermal resistance (R_f) of SiO_2 thin films on the 4H-SiC substrate with respect to the film thickness. The TBR of the 4H-SiC/SiO_2 interface is obtained from the linear fitting of the measured data (red solid line).

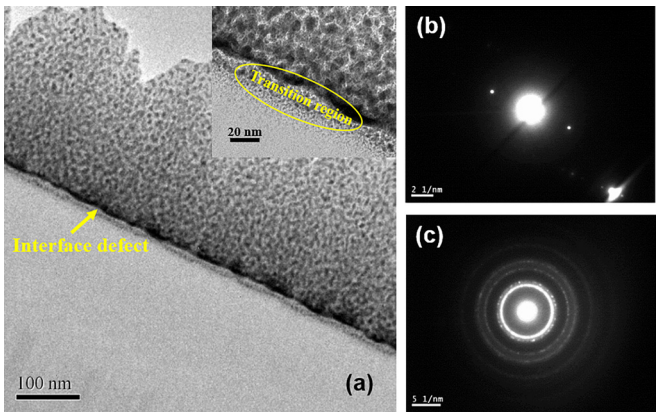

FIG. 2. The cross-sectional TEM image of the 4H-SiC/SiO_2 interface and SAED pattern on both sides of the 4H-SiC/SiO_2 interface. (a) Interface TEM image with 100 nm in scale. The inset represents the magnified region with 20 nm in scale; (b) 4H-SiC SAED pattern; (c) SiO_2 SAED pattern.

increased interface areas and the "phonon bridging" effect,[20] where two materials are assumed to come into contact with each other perfectly. Thus, TBR could decrease against the rough interfaces due to the increase in the contact strength, effective contact area, or new channels of phonon transmission when two dissimilar materials are perfectly contacted, which is not valid in samples of this work.

Meanwhile, selected area electron diffraction (SAED) was employed to determine the state of the materials on both sides of the 4H-SiC/SiO_2 interface. Figures 2(b) and 2(c) show that the 4H-SiC substrate is in a typical crystalline state, while the SiO_2 film is polycrystalline. Generally, the thermal conductivity of the crystalline material is much higher than that with the amorphous state, and the thermal conductivity of the bulk crystal SiO_2 is about 10.4–11.3 W/m K. Therefore, the higher thermal conductivity of the SiO_2 film on the 4H-SiC substrate can be interpreted in terms of the polycrystalline state.

Since the roughness of the experimentally manufactured interface is usually large, the commonly used DMM is applied to analyze the thermal boundary resistance of Si/SiO_2 and 4H-SiC/SiO_2 interfaces. Considering an interface between two materials, namely, A and B, a phonon with frequency ω and mode j that is incident on the interface from A can either scatter back into A or transmit into B. The DMM assumes that scattering at the interface is completely diffusive in nature. The probability of a phonon diffusively scattering across the interface is affected by the density of states and phonon group velocity on each side of the interface. Under the assumption of diffusive scattering, as well as invoking the principle of detailed balance,[8] the transmission coefficient from materials A to B ($\alpha_{A\to B}$) can be calculated as

$$\alpha_{A\to B} = \frac{\sum_j D_{B,j} v_{B,j}}{\sum_j D_{A,j} v_{A,j} + \sum_j D_{B,j} v_{B,j}}, \tag{1}$$

where D is the phonon density of states, v is the phonon group velocity for the phonon mode of interest at frequency ω, and the subscript j refers to the phonon polarization.

According to the Landauer formula, the interface thermal conductance (G) can be predicted by

$$G = \frac{1}{4}\sum \int_0^{\omega_A^v} D_A(\omega) \frac{\partial n(\omega, T)}{\partial T} \hbar\omega v_A \alpha_{A\to B}(\omega) d\omega, \tag{2}$$

where ω^v is the cut-off frequency and $n(\omega,T)$ is the Bose-Einstein distribution function.

Figures 3(a)–3(c) show the phonon dispersions and density of states for Si, 4H-SiC, and SiO_2 crystals calculated with the GULP code,[21] respectively. The phonon group velocities are derived from phonon dispersions. Tersoff potentials are applied for Si[22] and 4H-SiC,[23] while core-shell spring potential is used for SiO_2.[24] The calculation results are in good agreement with other results from first-principles theory.[25–27] As shown in Fig. 3(d), the transmission coefficient of phonons in 4H-SiC to SiO_2 is larger than that of the Si/SiO_2 interface, which is attributed to the higher discrepancy of phonon DOS between 4H-SiC and SiO_2 compared to that between Si and SiO_2. As illustrated in Eq. (1), the higher the discrepancy of phonon DOS, the larger the transmission coefficient would be.

In our DMM predication, the TBR of the Si/SiO_2 interface is 6.88×10^{-9} m^2K/W, while for the 4H-SiC/SiO_2 interface, the value is 2.72×10^{-8} m^2K/W at 298 K. Our results are close to other reported

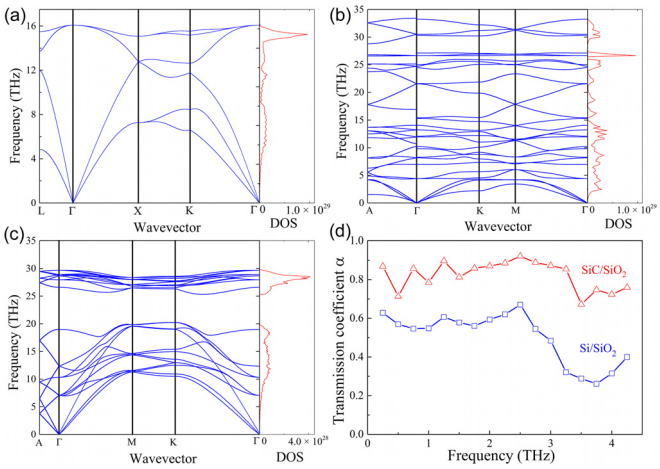

FIG. 3. Phonon dispersions and density of states (DOS) of (a) Si, (b) SiO_2, and (c) 4H-SiC. (d) The transmission coefficient (α) of Si/SiO_2 and 4H-SiC/SiO_2 interfaces.

results for other similar interfaces listed in Table I. Additionally, the experimental results are generally two to three fold of the predicted values, which could be interpreted by considering the limitations and assumptions made in DMM. There are three main mechanisms that DMM could underestimate TBR. First, when calculating the phonon dispersion relation by using lattice dynamics, the material structure is assumed to have a perfect crystallinity. However, the samples of the SiO_2 film in this work are amorphous. There are obvious differences in PDOS between the amorphous structure and the crystallized structure. For instance, due to much more scattering, the peaks in PDOS of amorphous are widened and are not as sharp as that of the crystal structure.[31] The overlapping region of PDOS increases by using the crystal structure, which also increases the phonon transmission probability across the interface, and thus underestimates TBR. Second, DMM assumes perfectly contacted rough scattering interfaces with no imperfections. That is, it cannot assess the effects of defects and disorder, which generally exist at the interface. As shown in Fig. 2, defects and disorder in the near-surface region of the 4H-SiC substrate are observed. These defects and disorders make the contact area smaller than that of smooth contacting surfaces,[32] and also induce more scatterings of phonons.[15] It contributes to a larger TBR of experimental results, and similar results are observed at the Au-Si[33] and Al-Si[15]

TABLE I. The thermal boundary resistances. (Unit: m^2K/W).

Samples	Theoretical prediction	Experimental measurement
Si/SiO_2	6.88×10^{-9} (298 K)	2.13×10^{-8} (298 K)
4H-SiC/SiO_2	2.72×10^{-8} (298 K)	8.11×10^{-8} (298 K)
Si/Al (DMM)	3.70×10^{-9} (300 K)[28]	…
Si/SiO_2 (MD)	4.27×10^{-9} (300 K)[5]	…
Si/graphene (MD)	4.3×10^{-8} (300 K)[29]	…
Si/GaN (micro-Raman)	…	7.5×10^{-8} (420 K)[30]
SiC/GaN (micro-Raman)	…	1.2×10^{-7} (420 K)[30]

interface. Third, DMM inherently assumes diffusive thermal transport across interfaces, which might not be always true. It is shown that DMM could underestimate TBR when there are nondiffusive phonon scatterings at interfaces by using both theoretical calculations and molecular dynamics.[34] Therefore, the assumption of totally diffusive scattering in DMM is potentially inevitable to contribute the discrepancy between the computational value and the experimental value. On the other side, another limitation of DMM may overestimate TBR. That is, DMM does not take account of the inelastic scattering of phonons at interfaces, while inelastic scatterings would provide more channels for phonon transport and reduce TBR.

Moreover, both the predicted and experimental results demonstrate that the 4H-SiC/SiO_2 interface has a higher thermal resistance than the Si/SiO_2 interface. On one hand, the different phonon DOS between 4H-SiC and Si is attributed to the difference in TBR between heterogeneous interfaces. As in Eq. (1), the interfacial thermal conductance is influenced by phonon DOS, phonon group velocity, and the transmission coefficient. While the phonon density of states and group velocity are the intrinsic properties of the material, the transmission coefficient is determined by both materials across the interface [Eq. (S6) in the supplementary material]. As shown in Fig. 3(d), the highest frequency of the acoustic phonons in SiO_2 is 4.2 THz, which means that phonons in 4H-SiC with a frequency higher than 4.2 THz are restricted to transport through the interface, and thus, only the transmission coefficients of phonons with frequencies below 4.2 THz are calculated. Our calculation results show that the 4H-SiC/SiO_2 interface has a slightly higher phonon transmission efficiency than the Si/SiO_2 interface in general, and the group velocity of 4H-SiC is about 1.5 times of that of Si. However, the phonon DOS of 4H-SiC is about an order of magnitude lower than that of Si when the frequency is below 4.2 THz. The lower phonon DOS of 4H-SiC at low frequency can be attributed to the lighter atomic mass of C compared to Si, which makes the 4H-SiC lattice have more vibration modes at higher frequency.[35] Therefore, lower phonon DOS of 4H-SiC at frequency below 4.2 THz implicates that heat carriers that can pass through the 4H-SiC/SiO_2 interface is less than the Si/SiO_2 interface, causing higher TBR at the 4H-SiC/SiO_2 interface. On the other hand, when a film is deposited on the substrate with higher thermal conductivity, the influence of TBR on the heat transport might be more significant. Kuzmik *et al.* measured the TBR of Si/GaN and SiC/GaN interfaces using the micro-Raman spectroscopy technique.[30] The TBR of the Si/GaN interface is 7.5×10^{-8} m^2K/W, while the TBR of the SiC/GaN interface is 1.2×10^{-7} m^2K/W, which also supports the fact that the SiC substrate with higher thermal conductivity introduces larger TBR of the SiC/GaN interface compared to that of the Si/GaN interface.

In summary, the thermal boundary resistance of both the 4H-SiC/SiO_2 and Si/SiO_2 interfaces was measured by the 3ω method. It was found the TBR between the SiO_2 thin film and the 4H-SiC substrate is 8.11×10^{-8} m^2K/W, which is about 4 times higher than that of the Si/SiO_2 interface. The TBR of these two interfaces is within the same range of the previously reported TBR of similar interfaces at room temperature. Additionally, the TBR of the 4H-SiC/SiO_2 and Si/SiO_2 interfaces is predicted to be 2.72×10^{-8} and 6.88×10^{-9} m^2K/W, respectively, by DMM, which matches well with our experimental results. Furthermore, the discrepancy between the two selected interfaces in this work was ascribed to two potential explanations. One is the higher density of imperfections at 4H-SiC/SiO_2 interfaces, which affects phonon heat transport across the interface significantly. The other is that the DOS of low frequency acoustic phonons in 4H-SiC is lower than that of Si, leading to less heat carriers in 4H-SiC transport through the interface. The presented work on TBR of the 4H-SiC/SiO_2 interface is believed to pave the way for heat dissipation, thermal analysis, and thermal management in high power density devices.

See the supplementary material for the sample preparation, measurement process, characterization methods, heat transport across the Si/SiO_2 interface, apparent thermal conductivity and apparent thermal resistance of the SiO_2 thin films on the Si substrate at 298 K, energy dispersive spectrometer (EDS) characterization for the 4H-SiC/SiO_2 interface, and details of numerical calculations.

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