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ABSTRACT

Because of its ultra-wide bandgap, high breakdown electric field, and large-area affordable substrates grown from the melt, $\beta$-Ga$_2$O$_3$ has attracted great attention recently for potential applications of power electronics. However, its thermal conductivity is significantly lower than those of other wide bandgap semiconductors, such as AlN, SiC, GaN, and diamond. To ensure reliable operation with minimal self-heating at high power, proper thermal management is even more essential for Ga$_2$O$_3$ devices. Similar to the past approaches aiming to alleviate self-heating in GaN high electron mobility transistors, a possible solution has been to integrate thin Ga$_2$O$_3$ membranes with diamond to fabricate Ga$_2$O$_3$-on-diamond lateral metal-semiconductor field-effect transistor or metal-oxide-semiconductor field-effect transistor devices by taking advantage of the ultra-high thermal conductivity of diamond. Even though the thermal boundary conductance (TBC) between wide bandgap semiconductor devices and a diamond substrate is of primary importance for heat dissipation in these devices, fundamental understanding of the Ga$_2$O$_3$-diamond thermal interface is still missing. In this work, we study the thermal transport across the interfaces of Ga$_2$O$_3$ exfoliated onto a single crystal diamond. The van der Waals bonded Ga$_2$O$_3$-diamond TBC is measured to be 17−17±2.0 MW/m$^2$ K, which is comparable to the TBC of several physical-vapor-deposited metals on diamond. A Landauer approach is used to help understand phonon transport across a perfect Ga$_2$O$_3$-diamond interface, which in turn sheds light on the possible TBC one could achieve with an optimized interface. A reduced thermal conductivity of the Ga$_2$O$_3$ nano-membrane is also observed due to additional phonon-membrane boundary scattering. The impact of the Ga$_2$O$_3$-substrate TBC and substrate thermal conductivity on the thermal performance of a power device is modeled and discussed. Without loss of generality, this study is not only important for Ga$_2$O$_3$ power electronics applications which would not be realistic without a thermal management solution but also for the fundamental thermal science of heat transport across van der Waals bonded interfaces.

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As an emerging ultra-wide bandgap semiconductor material, $\beta$-Ga$_2$O$_3$ has shown favorable properties for use in power electronics applications, such as an ultra-wide bandgap (4.8 eV) and high critical electric field (8 MV/cm), which predict a Baliga figure of merit that is 3214 times that of Si. However, the thermal conductivity of bulk $\beta$-Ga$_2$O$_3$ (10-30 W/m K, depending on crystal orientation) is at least one order of magnitude lower than those of other wide bandgap semiconductors, for instance, GaN (230 W/m K), 4H–SiC (490 W/m K), and diamond (>2000 W/m K). To utilize Ga$_2$O$_3$ in high frequency and high power switching applications, proper thermal management is essential to avoid device degradation due to poor thermal reliability. This will require the use of high thermal conductivity pathways to pull the heat out of the Ga$_2$O$_3$ devices efficiently through interfacial contacts with low thermal boundary resistance. With its ultra-high thermal conductivity, diamond, which has been extensively studied to dissipate localized self-heating from electronics such as AlGaN/GaN high electron mobility transistors (HEMTs), is a possible solution for Ga$_2$O$_3$ devices as well.

Recently, mechanically exfoliated Ga$_2$O$_3$ nano-membranes have been utilized to fabricate high-current transistors. A record high drain current has been achieved in an exfoliated Ga$_2$O$_3$ field-effect transistor with diamond substrates. This work demonstrates
good device performance but has not quantified the heat transport across the Ga$_2$O$_3$-diamond interface as the Ga$_2$O$_3$ nano-membranes were adhered to diamond via van der Waals forces. The thermal boundary conductance (TBC) of mechanically joined materials could be as low as 0.1 MW/m$^2$ K, while the interfacial thermal conductance of transfer-printed metal films is in the range of 10-40 MW/m$^2$ K.\textsuperscript{15-19} Thermal transport across van der Waals interfaces is limited by the real contact area and low phonon transmission due to weak adhesion energy even if there exists the possibility to achieve a high TBC.\textsuperscript{20-22} Thermal transport across these interfaces remains an open issue due to the limited amount of experimental data available in the literature. Therefore, it is of great significance to study the thermal conductance across Ga$_2$O$_3$-diamond interfaces for both real-world power electronics applications and fundamental thermal science of heat transport across van der Waals interfaces.

In this work, we have mechanically exfoliated a (100) oriented Ga$_2$O$_3$ nano-membrane from an electric field gradient (EFG)-grown commercial (~201) Ga$_2$O$_3$ substrate (Novel Crystal Technology, Japan) with medium-tack dicing saw tape and transferred it on a single crystal (100) CVD diamond substrate (Element Six). Time-domain thermoreflectance (TDTR) was used to measure the Ga$_2$O$_3$-diamond TBC and Ga$_2$O$_3$ thermal conductivity. TDTR is a well-established technique for thermal measurements of both bulk and nanostructured materials. The detailed experimental setup can be found in the literature.\textsuperscript{23} During TDTR measurements, a modulated laser beam (pump) heats the sample surface periodically, while a delayed probe beam detects the temperature of the sample surface via thermoreflectance. The surface temperature variation is related to the thermal properties of the sample. By fitting the TDTR data with an analytical heat transfer solution of the sample, the unknown thermal properties are extracted.\textsuperscript{24,25} Moreover, by combining the picosecond acoustic technique and the membrane thickness measured by an Atomic Force Microscope (AFM), the phonon group velocity across the membrane thickness direction is obtained. Moreover, we use a Landauer approach to calculate phonon transport across Ga$_2$O$_3$-diamond interfaces. Additionally, the effects of Ga$_2$O$_3$-substrate TBC and substrate thermal conductivity on thermal performance of a power electronics device are modelled by an analytical solution.

Figure 1(a) shows a part of the sample scanned by AFM. A blanket layer of Al (~80 nm) was deposited to serve as the TDTR transducer. As the size of the Ga$_2$O$_3$ nano-membrane was approximately 11 µm × 70 µm, a CCD camera integrated in the TDTR system was used to help locate the sample. To obtain the thermal conductivity of the diamond substrate, TDTR was performed on the area which was not covered by the Ga$_2$O$_3$ nano-membrane. The thermal conductivity of the single crystal diamond substrate was determined to be 2169 ± 130 W/m K, which is very close to other values reported in the literature.\textsuperscript{26} This value was used in the data analysis and parameter fittings from the TDTR measurements on the Ga$_2$O$_3$ bonded to diamond. The Al-diamond TBC is also determined in the measurements to be 34 MW/m$^2$ K. Figure 1(b) shows the picosecond acoustic echoes obtained during TDTR measurements. The observed echoes correspond to strain waves that are reflected at interfaces.\textsuperscript{27} Figure 1(c) shows the strain wave traveling distance for each echo. For echo 1, a small valley shows up before a peak, indicating the loose bonding of van der Waals forces at the interface. In this scenario, we pick the middle point of the valley and peak as the echo point ($t_1 = 25$ ps).\textsuperscript{29} The sound speed of Al is 6420 m/s,\textsuperscript{27} so the Al thickness was determined to be 80 nm ($d_1 = v_{Al} \times t_1/2$). For echo 2 (154 ps = 25 ps + 129 ps), it relates to the Ga$_2$O$_3$-diamond interface. The traveling time in Ga$_2$O$_3$ is 129 ps. The thickness of the Ga$_2$O$_3$ layer was determined as 427 ± 3 nm by an AFM. Then the longitudinal phonon group velocity of Ga$_2$O$_3$ in the direction perpendicular to the (100) plane is determined as 6620 m/s, which matched very well with the density functional theory (DFT)-calculated value.

![Image](FIG. 1. (a) AFM image of the center of the Ga$_2$O$_3$ sample. (b) Picosecond acoustic echoes obtained in the TDTR measurements. (c) Echoes which relate to strain wave bouncing back at interfaces.)
The surface roughness of the two surfaces affects the real contact area and, correspondingly, the thermal conductance across this interface. To measure the surface roughness, AFM was used to scan the diamond substrate surface and the top surface of the Ga$_2$O$_3$ membrane. The bottom surface of the Ga$_2$O$_3$ membrane should be similar to or smoother than the top surface. The surface images are shown in Figs. 2(a) and 2(b). The root mean squared (RMS) roughness of diamond and Ga$_2$O$_3$ surfaces is 3.39 ± 0.91 nm and 3.23 ± 0.93 nm, respectively. The sensitivity of our TDTR measurements was determined by considering a fractional change in the thermoreflectance signal due to a fractional change in the independent parameters. Figure 2(c) shows the TDTR sensitivity of the TBC of the Ga$_2$O$_3$-diamond interface, the thermal conductivity of the Ga$_2$O$_3$ membrane, and the TBC of the Al-Ga$_2$O$_3$ interface with a modulation frequency of 2.2 MHz and a 20× objective (pump radius 4.9 μm and probe radius 3.0 μm). The sensitivity of the TBC of the Ga$_2$O$_3$-diamond interface is very large, resulting in accurate measurements of this parameter. Figure 2(d) shows good agreement between the experimental data (red circles) and the fitted curve (blue curve).

The TBC of the Ga$_2$O$_3$-diamond interface was measured to be 17 ± 1.7/±2.0 MW/m$^2$ K and is compared with the TBC of several other diamond interfaces and transferred interfaces in Table I. The error bars (low bar = 1.7 MW/m$^2$ K and up bar = 2.0 MW/m$^2$ K) of TDTR measurements is estimated by a Monte Carlo method. The Ga$_2$O$_3$-diamond TBC is in the TBC range of the transferred metal films on silicon, SiO$_2$, and sapphire substrates (van der Waals force bonded) and is comparable to the TBC of several physical-vapor-deposited metals on diamond (covalent force bonded). The Ga$_2$O$_3$-diamond TBC is mainly affected by three factors: the weak van der Waals force between Ga$_2$O$_3$ and diamond (covalent bonding is much stronger), the small contact area at the interface, and the large phonon density of state (DOS) mismatch between Ga$_2$O$_3$ and diamond. For the Ga$_2$O$_3$-diamond interface, the two materials are bonded by the van der Waals force. Interfacial bonding affects thermal conductance significantly. For instance, the TBC of covalent bonded interfaces is much larger than that of the van der Waals force bonded interfaces because phonon transmission is very low due to the weak adhesion energy of van der Waals interfaces and the large phonon DOS mismatch between Ga$_2$O$_3$ and diamond. The van der Waals force at the Ga$_2$O$_3$-diamond interface should be weaker than those of other polar material interfaces. This further decreases the TBC. In terms of the real contact area at the interface, there are no good methods to measure it. Some calculations indicate that the fractional areal coverage of transferred metal films on silicon or sapphire substrates could reach 25% because of plastic deformation and capillary forces. The transferred metal thin films (Au) are very soft, so the contact area between the metals and substrates could be very large under pressure during the transfer process. However, for the Ga$_2$O$_3$-diamond interface, diamond is known as one of the hardest materials and Ga$_2$O$_3$ is much harder than Au. We can see very small pillars forming surface roughness of both the Ga$_2$O$_3$ and diamond surfaces according to the AFM images. We speculate that these pillars may enlarge the contact area at the interface and enhance thermal transport. Surface-roughness insensitive TBC was observed in van der Waals interfaces before. Our measured Ga$_2$O$_3$-diamond TBC is comparable to the TBC of diamond. For the Ga$_2$O$_3$-diamond interface, the thermal conductivity of Ga$_2$O$_3$, and the TBC of the Al-Ga$_2$O$_3$ interface with a modulation frequency of 2.2 MHz and a 20× objective. (d) TDTR data fitting with a modulation frequency of 2.2× MHz and a 20× objective.
Ga$_2$O$_3$ interfaces for both fundamental science and real-world applications.

Here, we define “diamond interface” as any interface with one side of which is diamond. Diamond has ultra-high thermal conductivity due to the light carbon atom and strong covalent bond among carbon atom, which leads to an ultra-high Debye frequency and cutoff frequency. As a result, the phonon DOS match of diamond and other materials is very poor and the TBC of diamond interfaces is very low. When integrating diamond with other materials to take advantage of its high thermal conductivity, the low TBC of diamond interfaces is usually the bottleneck. This highlights the motivation to study thermal transport across diamond interfaces for both fundamental science and real-world applications.

To understand the phonon transport across the perfect Ga$_2$O$_3$-diamond interface, a Landauer approach with transmission function from the diffuse mismatch model (DMM) is applied to calculate the TBC at the Ga$_2$O$_3$-diamond interface. The general form of the Landauer formula is

$$G = \frac{1}{2} \int D_1(\omega) \frac{d\rho_E}{d\omega} h \nu \frac{\tau_{12}(\theta)}{\sin \theta} d\theta d\omega,$$

where $D$ is the phonon DOS, $\rho_E$ is the Bose-Einstein distribution function, $h$ is the reduced Planck constant, $\omega$ is the phonon angular frequency, $v$ is the phonon group velocity of material 1 (Ga$_2$O$_3$), $\tau_{12}$ is the transmission coefficient from material 1 to 2 (here, it is from Ga$_2$O$_3$ to diamond), $\theta$ is the angle of incidence, and the sum is over all incident phonon modes. The expression of the transmission function from DMM is

$$\tau_{12}(\omega) = \frac{\sum_p M_2(\omega)}{\sum_p M_1(\omega) + \sum_p M_2(\omega)},$$

where $M_p$ is the transmission coefficient from material $p$ to 2 (here, $p = 1$ or 2).

The thermal conductivity of the Ga$_2$O$_3$ nano-membrane was measured as 8.4 ± 1.0 W/m K, which is lower than the value of bulk Ga$_2$O$_3$ in this direction (about 13 W/m K). Here, TDTR is more sensitive to cross-plane thermal conductivity instead of in-plane ones. The thickness dependent thermal conductivity of Ga$_2$O$_3$ thin films from the literature and this work are summarized in Fig. 3. For a certain crystal orientation, the thermal conductivity of Ga$_2$O$_3$ thin films decreases with film thickness. The phonon mean free path in bulk Ga$_2$O$_3$ ranges from several nm to several µm. Phonons with long mean free paths scatter with film boundaries. The additional film boundary scattering reduces phonon mean free path and reduces thermal conductivity. For instance, the thickness of our Ga$_2$O$_3$ nano-membrane is 427 nm. The phonons with mean free path larger than 427 nm have large possibility to scatter with the film boundaries. The film boundary scattering limits the phonon mean free path in the cross-plane direction and correspondingly reduces cross-plane thermal conductivity. Size effects in nanoscale Ga$_2$O$_3$ electronics would result in further-reduced thermal conductivity, leading to heat dissipation problems in these devices. This highlights the demand of proper thermal management for Ga$_2$O$_3$ electronics.

![FIG. 3. Thickness dependent thermal conductivity of Ga$_2$O$_3$ thin films. The data for the unintentionally doped (UID) and Sn-doped (−201) orientated thin films are from Ref. 37. The blue and red lines are the bulk values in (−201) orientation and perpendicular to (100) orientation.](image-url)
where $M$ is the phonon number of modes. Because the transmission function from DMM does not depend on the angle of incidence, the Landauer formula can be simplified as

$$G = \sum_{\omega} \frac{1}{4} \int D_1(\omega) \frac{d\phi_{o}}{dT} \hbar \omega v_{l1}(\omega) \tau_{l1}(\omega) d\omega.$$

The phonon properties of diamond are obtained from first principles calculation with Vienna *Ab initio* Simulation Package (VASP), and the phonon properties of Ga$_2$O$_3$ are from Materials Project.$^{46-45}$

The calculated phonon transmission coefficients are shown in Fig. 4(a). The low transmission coefficients at low frequency are derived from the acoustic branches. The number of phonon modes of three dimensional material is proportional to the square of wavenumber, which equals to phonon angular frequency over group velocity for acoustic branches at low frequency, as the phonon dispersion relation is almost linear near the gamma point. For the longitudinal acoustic (LA) polarization, the phonon group velocity of diamond perpendicular to the (100) plane is 17 553 m/s, while the phonon group velocity of Ga$_2$O$_3$ perpendicular to the (100) plane is 6809 m/s, which means that the group velocity of diamond is 2.38 times that of Ga$_2$O$_3$, and the number of modes of diamond LA at low frequencies is only 15% of that of Ga$_2$O$_3$. As a result of the large difference between the acoustic group velocities, the phonon transmission coefficient is very low at low frequencies. For most interfaces involving diamond, the transmission is usually low because of the large phonon group velocity and high cutoff frequency of diamond. At high frequencies, the wavenumber of Ga$_2$O$_3$ at a certain frequency is relatively close to that of diamond, and the transmission coefficient increases.

The calculated TBC from the Landauer approach is 312 MW/m$^2$ K, as shown in Fig. 4(b), at the Ga$_2$O$_3$ cutoff frequency. Because of the complex crystalline structure (large unit cell) of Ga$_2$O$_3$, there are a large number of optical phonon modes. As a result, acoustic phonons of Ga$_2$O$_3$ only contribute to about 8% of the total TBC, while optical phonons contribute to about 92%. The calculated TBC is significantly larger than the measured value. The difference between the theoretical TBC and the measured TBC is attributed to the interfacial bonding and real contact area at the interface as discussed above. The van der Waals bonding at the Ga$_2$O$_3$-diamond interface is much weaker than covalent bonds, which reduces TBC significantly.$^{17,20,31,32}$ We also calculated the radiation limit of TBC of the Ga$_2$O$_3$-diamond interface as 426 MW/m$^2$ K.$^{46,47}$ The radiation limit assumes the phonon transmission coefficient as one from one side of the interface to the other side when phonons at a certain frequency from that side have a lower number of modes. Phonon density of states of Ga$_2$O$_3$ and diamond are from their phonon dispersion relations. Both DMM-based Landauer and radiation limit cannot capture inelastic scatterings; however, the calculated results shed light on the possible TBC with a perfect interface, which guide the material growth and device design.

To understand the impact of the Ga$_2$O$_3$-substrate TBC on the thermal performance of a power device, we use an analytical solution for the temperature rise in multilayer structures with discrete heat sources.$^{48}$ The modeled device consisted of a 500-nm (100) Ga$_2$O$_3$ layer atop a substrate consisting of either high quality diamond, SiC, or Si. The Ga$_2$O$_3$ layer was prescribed an anisotropic thermal conductivity with $k_\parallel = 12$ W/m K and $k_\perp = 21$ W/m K in accordance with published values.$^{49}$ The modeled device structure was a 10 finger device with 50 µm gate-to-gate spacing. The heat sources were each assumed to be $4 \times 150$ µm, and the total domain was 2000 × 2000 µm. A total power density of 10 W/mm was applied to the simulated device. The device structure and simulated heating can be seen in Figs. 5(a) and 5(b), Figure 5(a) shows the schematic diagram of the modeled device demonstrating the cross section and heat source spacing. Figure 5(b) shows the top view of the simulated device (a Ga$_2$O$_3$-diamond TBC of 100 MW/m$^2$ K on a diamond substrate with a thermal conductivity of 2000 W/m K). As expected, the applied power leads to an increase in peak temperature at each Ga$_2$O$_3$ finger. The impact of the Ga$_2$O$_3$-substrate TBC was evaluated by adjusting its value in the model from 10 to 300 MW/m$^2$ K for each substrate material. Figure 5(c) shows the device temperature distribution across the center of the fingers for a simulated Ga$_2$O$_3$ on diamond device with a TBC value of 17, 100, and 300 MW/m$^2$ K. The decrease in TBC would increase the temperature rise significantly, especially when the TBC is not large. As shown in Fig. 5(d), when the Ga$_2$O$_3$-substrate TBC is small, TBC is the dominant factor limiting heat dissipation. When TBC goes beyond 70 MW/m$^2$ K, substrate thermal conductivity is the dominant factor which limits device thermal dissipation. Additionally, as long as the TBC value is not too low, it is crucial to have a high thermal conductivity substrate. For instance, a SiC substrate with a TBC of 300 MW/m$^2$ K shows a maximum temperature of 283 °C, while using a diamond substrate...
substrate with a TBC of 17 MW/m² K (much lower than 300 MW/m² K), as measured in this work, results in a similar maximum temperature rise. This result demonstrates the importance of implementing a high thermal conductivity substrate such as diamond into Ga2O3 power devices. Because of the relatively low thermal conductivity of Ga2O3, even a relatively low TBC value (but equal to or larger than 17 MW/m² K) for a device on diamond will outperform a device on a SiC substrate with an exceptional TBC. This will be useful in guiding device design when integrating Ga2O3 with high thermal conductivity substrates.

In summary, a possible solution to cool Ga2O3 electronics is to integrate thin Ga2O3 membranes with diamond to fabricate Ga2O3-on-diamond devices by taking advantage of the ultra-high thermal conductivity of diamond. A good understanding of the TBC between Ga2O3 and diamond is still lacking. In this work, we measured the TBC of the interfaces of smooth exfoliated Ga2O3 and polished single crystal diamond. The longitudinal phonon group velocity in the direction perpendicular to the (100) plane of Ga2O3 is 6620 m/s, which matched very well with the DFT-calculated value (6809 m/s). Reduced thermal conductivity of the Ga2O3 nano-membrane (8.4 ± 1.0W/m K) was observed and attributed to size effects (phonon-boundary scatterings). The van der Waals Ga2O3-diamond TBC was measured to be 17 ± 1.7/±2.0 MW/m² K, which is in the TBC range of transfer-printed metal films and comparable to the TBC of several physical-vapor-deposited diamond interfaces. This value is relatively quite high by taking the weak bonding strength and small contact area into consideration. The TBC calculated with a Landauer approach and DMM is 312 MW/m² K, which sheds light on the possible TBC we can achieve. The thermal performance of Ga2O3-on-diamond devices was modeled to study the effect of Ga2O3-substrate TBC and substrate thermal conductivity. Our study is important for both applications of power electronics thermal management and fundamental understanding of heat transport across van der Waals interfaces.

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