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Thermal boundary conductance across metal-gallium nitride interfaces from 80 to 450 K

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Thermal boundary conductance is of critical importance to gallium nitride (GaN)-based device performance. While the GaN-substrate interface has been well studied, insufficient attention has been paid to the metal contacts in the device. In this work, we measure the thermal boundary conductance across interfaces of Au, Al, and Au-Ti contact layers and GaN. We show that in these basic systems, metal-GaN interfaces can impose a thermal resistance similar to that of GaN-substrate interfaces. We also show that these thermal resistances decrease with increasing operating temperature and can be greatly affected by inclusion of a thin adhesion layers. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4902233]

Thermal management has assumed a critical role in the design and development of electronic devices, power generation modules, and waste energy harvesting techniques. For example, power dissipation limits the performance of electronic systems starting from individual microprocessors and scaling up to data centers.[1] In silicon-based microprocessors, operation beyond a few GHz is a challenge due to on-chip power densities exceeding $100\,\mathrm{W\,cm^{-2}}$, far greater than typical cooling capabilities. Even greater power densities have been observed in gallium nitride-based (GaN) radio frequency and amplifier devices.[2,3] Increase in power density leads to massive hot-spots in GaN active regions, which directly lead to underperformance and eventually failure of the these devices. This thermal bottleneck creates a major issue for furthering of GaN-based technologies such as high-electron-mobility transistors (HEMTs) for high frequency devices, light emitting diodes (LEDs) for energy-efficient illumination, RADAR technologies and high performance space satellites.

It is clear that as device dimensions continue to decrease into the micron and sub-micron size range—on the order of typical thermal mean free paths—thermal transport becomes increasingly difficult to mitigate and engineer. In this size regime, the thermal transport is dominated by the thermal boundary conductance (h_K) across interfaces. The control of h_K across GaN contacts has proven to be difficult[4,5] as electric field concentration within the device lead to large hot-spots, while dislocations and other interfacial imperfections[6] further aggravate temperature rises close to the GaN interfaces. Relatively large cross-plane thermal resistances in GaN-based device channels are extremely detrimental to device operation, and have been associated with up to a 40% increase in channel temperature.[5] It is well known, and there is a clear trend in industrial data, that increase in device temperature leads to an exponential decrease in mean time to failure of GaN devices.[8,9] Recent surveys indicate GaN electronic device market is expected to reach billions of dollars by the end of this decade.[10] Without addressing the thermal issues in GaN-based devices, the operational potential of GaN-devices and materials may not be reached, causing severe and detrimental outcomes to the massive investments and economic markets established for these technologies.

Previous studies on thermal boundary conductance across GaN-based interfaces have focused mainly on the GaN/substrate interfaces.[4–6] However, in a typical GaN device, high electric fields can result in significant hot-spots localized near the drain side of the gate contact, emphasizing that the thermal boundary transport at GaN-metal interfaces must also be understood.[7] To address these issues, we can begin by understanding the thermal characteristics of the interfaces between GaN and simple metal electrodes. By using time domain thermoreflectance (TDTR),[11–13] we measure the thermal boundary conductance between thin films of aluminum, gold, and gold with a titanium adhesion layer on $3\,\mu$m thick layers of GaN on sapphire substrates. These measurements are conducted over industry-relevant temperatures, ranging from 80 to 450 K. We show not only a clear dependence on metallic contact and operating temperature but also emphasize that the boundary resistance across these metal-GaN interfaces can be as high or higher than GaN-substrate interface resistances.

The samples were fabricated via metal evaporation onto GaN substrates. Nominally 80 nm of aluminum, gold, and gold films with a titanium adhesion layer were evaporated

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onto [0001] oriented GaN films on sapphire substrates using electron-beam evaporation at 6×10^{-6} Torr using planetary rotation to ensure uniform layer deposition. The GaN films were purchased commercially from University Wafer, Inc. The thickness of the GaN films was 3.2 μm, as measured via ellipsometry. We verify the orientation of the GaN films with electron diffraction using a JEOL 2010F transmission electron microscope (TEM) at 200 keV in wide illumination TEM mode. Prior to metallic deposition, the GaN films are treated with a series of alcohol cleans (methanol, acetone, and isopropyl alcohol). In addition, a subset of the samples was cleaned with an O_2 plasma clean for 30 min. The thicknesses of the metallic layers were confirmed using picosecond acoustics[14,15] and profilometry for Al or profilometry for the Au and Au/Ti films.

TEM analysis also confirmed that the interface between the various metal films and the GaN substrates are compositionally distinct, with a distinct boundary between the two layers. We expect the presence of a thin (a few monolayers) β-Ga_2O_3 at the GaN surface consistent with findings on similar material systems in the literature.[16–18] Therefore, it is important to note that the thermal boundary conductance that we report is indicative of the efficacy of heat flow from the metal film, across the native oxide and associated interfaces and into the GaN. We revisit these interfacial structures in the discussion of our results.

We measure thermal boundary conductance of various metal-GaN thin film interfaces with TDTR,[11–13] a method which utilizes a train of ultra-fast laser pulses to thermally stimulate the metal contact layer, and time delayed probe pulses to measure the change in thermoreflectance due to the decay of the deposited thermal energy. Specifically, we use sub-picosecond pulses emanating from a Ti:Sapphire laser system with an 80 MHz repetition rate. We modulate the thermal excitation (pump) pulses at 8.8 MHz and use a lock-in amplifier to monitor the thermoreflectivity changes at this frequency with a time-delayed probe pulse for up to 5 ns after the initial heating event. By using pump and probe radii of 25 and 6 μm, respectively, we are able to assume that the thermal decay is nearly one dimensional in the through-plane direction of the sample.[11] The non-room-temperature measurements were performed through a transparent window in a cryostat chilled with liquid nitrogen and temperature controlled with a resistive heater.

The analysis of this data, described in detail elsewhere,[11–13] involves least squares fitting to a model which relates changes in thermoreflectivity of the sample to the thermal conductivity, heat capacity, and thermal boundary conductances in each component of the system. We assume literature values for the thermal conductivity and heat capacity of the Al (Ref. 19), Au (Ref. 20), and GaN (Ref. 21) layers. We analyze sensitivity of our model to these thermophysical characteristics of the system the sensitivity of the ratio of the in-phase to out-of-phase components of the lock-in amplifier to the different parameters in our thermal model.[22,23] High sensitivity to a parameter is reflected by large relative magnitude over the analyzed measurement (or pump-probe delay) time. Figure 1 shows the sensitivity of the thermal conductivity of the metal coating and GaN layer and thermal boundary conductance of the metal-GaN and GaN-Sapphire interfaces at representative temperatures. This sensitivity analysis encompasses the major variable parameters within the sampled penetration depth (on the order of 4 μm at room temperature for these experiments). It is apparent that our measurement is most sensitive to the thermal boundary conductance of the metal-GaN interface over the temperature range of interest in this study.

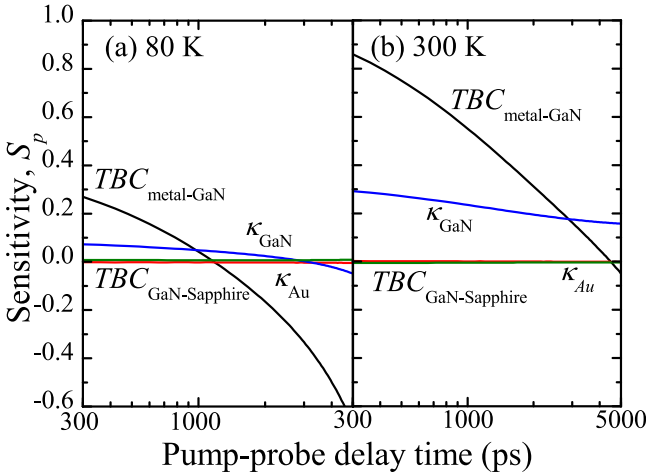

FIG. 1. Sensitivity, S, as a function of time of our TDTR measurements and analysis to various thermophysical parameters, p, in our samples. We plot the thermal sensitivities to the thermal boundary conductances across the metal-GaN and GaN-sapphire interfaces, the thermal conductivity of the GaN and the thermal conductivity of the metal film at (a) 80 K and (b) 300 K. Large relative magnitude of the sensitivity to the thermal boundary conductance indicates that this method is most sensitive to this parameter in our measurements and analyses.

The measured thermal boundary conductances across the various metal-GaN interfaces are plotted in Fig. 2. In general, the thermal boundary conductance follows the typical temperature-dependent trends observed in previous measurements[24] and predicted by the mismatch theories;[25] specifically, the thermal boundary conductance increases with temperature and follows a similar trend as the metal film phononic heat capacity. At room temperature, the lowest

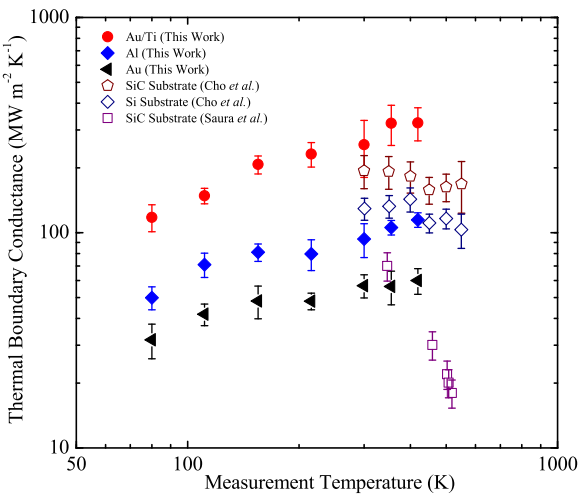

FIG. 2. Thermal boundary conductance as a function of temperature across the metal-GaN interfaces measured in this study (solid symbols) and various GaN-substrate samples from previous literature (GaN-SiC: Cho *et al.*,[34] GaN-Si: Cho *et al.*,[34] GaN-SiC: Sarua *et al.*[4]).

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boundary conductance was found in the Au-GaN system at $56.7 \pm 7.0\,\mathrm{MW\,m^{-2}\,K^{-1}}$ and the highest was Au with an adhesion layer of Ti at $256.6 \pm 76.1\,\mathrm{MW\,m^{-2}\,K^{-1}}$. Thermal boundary conductance at the Al-GaN interface shows improvement over Au only, but not to the extent of the Au-Ti system. It is clear that the enhancement gained from the more chemically intimate adhesion[26,27] with the Au-Ti-GaN system provides the best thermal management solution in GaN devices. Enhanced thermal boundary conductance in the Au-Ti system as compared to the Au system can be largely attributed to an increase in coupling of phonon modes across the interface. This increased coupling is due to both additional adhesion of the Ti layer to the oxide layer on the GaN and an increase in the phonon bandwidth in the Ti. As discussed in previous modeling-based work,[28,29] with enhanced bonding and higher frequency phonon modes in the Ti adhesion layer, phonon modes in the Au film are able to better couple to higher frequency modes in the GaN than would be possible with the less intimate bonding in the absence of the adhesion layer.[30,31] The change in thermal boundary conductance over temperature is consistent with this multi-mode phonon coupling enhancement. Our findings agree well with other modeling and experimental works involving metal-GaN systems.[28,32,33]

In Fig. 2, the initial increase of thermal boundary conductance with increased temperature is ascribed to the population of phonon modes in the metal films increasing up to the Debye temperature of the film. Any further increase with temperature above this point could be indicative of inelastic scattering, or multiple phonons in the metal scattering at the interface and emitting a higher frequency phonon in the substrate.[28,29,40,41] The flattening of the trends in thermal boundary conductance around the Debye temperature of the metal leads us to conclude that the thermal transport across the metal-GaN interface is largely limited by the phonon population in the metal. The enhancement from the adhesion layer is evident in the temperature trends as well. The absence of an adhesion layer results in thermal boundary conductance limited by the gold phonon population, thus a flat trend in the Au-GaN thermal boundary conductance. With the Ti adhesion layer, we see further increase beyond the Au Debye temperature due to the effects of enhanced bonding leading to the discussed multi-mode phonon coupling as well as the increased phonon bandwidth leading to temperature trends flattening out closer to the Debye temperature of titanium.

An important consideration in the discussion of thermal boundary conductance of the metal-GaN interface is the well known β-Ga_2O_3 native oxide layer that can form on the GaN surface when exposed to air.[16–18,42] While only a few monolayers thick,[17] this layer can contribute to the bonding characteristics and the sharpness of the interface at the metal-GaN interface. Aluminum, in particular, has been shown to absorb the oxygen on the GaN surface and form a thin layer of Al_2O_3 at the interface.[16] These thin oxide layers prevent direct interaction between the metal and GaN, and can contribute to the mechanisms described above to further limit the thermal boundary conductance.[23,43]

While interfaces in GaN-based devices vary significantly in material constituents and methods of processing, the interfaces chosen in this study aim to provide a reference for fundamental understanding of the GaN-metal interface that is critical to establishing a framework for thermal engineering of the contact component of devices. A comparison of the findings in this work to previous works concentrated on the GaN-substrate interface helps to give context to the metal-GaN interface with respect to thermal management. We see that at relevant operating temperatures (around 400 K) a Au-GaN interface can exhibit thermal conductance as low or lower than that found in a GaN-SiC substrate interface measured by Sarua *et al.*,[4] and comparable to the thermal boundary conductance across GaN-sapphire and GaN-Si interfaces.[4,44] While the use of Al leads to some improvement in thermal boundary conductance as compared to this GaN-substrate interface, the addition of the adhesion layer in the Au-Ti-GaN system enables the significant increase in thermal conductance. This improvement emphasizes the role that material selection and bonding characteristics can have on the thermal gradients at GaN-contact interfaces.

We note that the temperature trends that we observe in the thermal boundary conductance of the metal-GaN interfaces differ from those reported by Sarua *et al.*[4] for a GaN-SiC interface. The interface conductance studied in that work was across a highly defective nucleation layer (necessary for GaN growth on SiC substrates) and the trend with increasing temperature may reflect the decrease in thermal conductivity of the nucleation layer more so than a trend of conductance across the effective GaN-SiC interface.

Our measurements agree relatively well with previous reports in the literature of metal-GaN thermal boundary conductances, the room temperature values of which are summarized in Fig. 3. The thermal boundary conductance of aluminum on GaN was found to be slightly lower by Cho *et al.*,[34] but we attribute this discrepancy to differences in sample configuration and processing. Our findings fall directly in line with our previous molecular dynamics simulations for Al-GaN interfaces, in which we parameterized potentials specifically for the Al-GaN system. Therefore, our reported results in Fig. 3 can serve as a validation of our previous potential development for MD simulations.[35,36] Furthermore, the thermal boundary conductance between Au

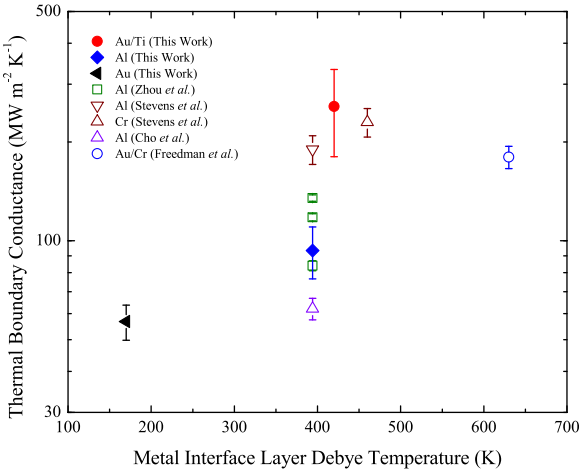

FIG. 3. Comparison of room temperature thermal boundary conductances across various metal-GaN interfaces as a function of interface metal Debye temperature.[34–39]

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and GaN with a Cr adhesion layer measured by Freedman *et al*.[38] agrees well with our Au-Ti-GaN measurements, indicating the similar thermal response of a Cr or Ti adhesion layer for Au contacts on GaN. We have also included the measurements of thermal boundary conductance across Al-GaN and Cr-GaN interfaces by Stevens *et al*.,[37] the discrepancy seen here could be due to the work of Stevens *et al*. pre-Al sputtering procedure to remove the native oxide layer on GaN.[37] We have previously shown that removing the native oxide layer between Al and Si will increase the thermal boundary conductance,[23,43] consistent with our assertion about the discrepancy between our and Al-GaN data of Stevens *et al*.. Understanding the contributions of the various metal systems measured and reported here provide a starting point in the basic thermal science of GaN-metal interactions and enable design of the much more complex contacts needed to operate high power devices.

In summary, we report on the thermal boundary conductance between Au, Al, and Au with a Ti adhesion layer on GaN over temperatures ranging from 80 K to 450 K. We find that the inclusion of a Ti adhesion layer between Au and GaN can increase the efficacy of heat flow across this interface by a factor of five, which we attribute to both an increase in Au adhesion along with a wider bandwidth of phonon modes in the thin Ti layer. The values for thermal boundary conductance found at these basic metal-GaN interfaces are similar to those found in GaN-substrate interfaces in high power device applications. While the majority of heat flow in an active device follows a pathway through the substrate in the most common devices, understanding the fundamentals of GaN-metal thermal transport is crucial for devices heat sinked through their metal contacts as well as comprehensive thermal engineering in typical bottom mounted devices.

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