Titanium contacts to MoS₂ with interfacial oxide: Interface chemistry and thermal transport

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The deposition of a thin oxide layer at metal/semiconductor interfaces has been previously reported as a means of reducing contact resistance in two-dimensional (2D) electronics. Using x-ray photoelectron spectroscopy with in situ Ti deposition, we fabricate Au/Ti/TiOₓ/MoS₂ samples as well as Au/Ti/MoS₂ and Au/TiOₓ/MoS₂ for comparison. Elemental titanium reacts strongly with MoS₂ whereas no interface reactions are observed in the two types of samples containing TiOₓ/MoS₂ interfaces. Using time-domain thermoreflectance for measurements of thermal boundary conductance, we find that samples contacted with Ti and a thin TiOₓ layer at the interface (~1.5 nm) exhibit the same behavior as samples contacted solely with pure Ti. The Au/TiOₓ/MoS₂ samples exhibit ~20% lower thermal boundary conductance, despite having the same MoS₂ interface chemistry as the samples with thin oxide at the Ti/MoS₂ interface. We identify the mechanism for this phenomenon, attributing it to the different interfaces with the top Au contact. Our work demonstrates that the use of thin interfacial oxide layers to reduce electrical contact resistance does not compromise heat flow in 2D electronic devices. We note that the thicknesses of the Ti and TiOₓ layers must be considered for optimal thermal transport.

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I. INTRODUCTION

Contact resistance presents a major obstacle to the success of two-dimensional (2D) electronics [1,2]. One approach to the reduction of electrical contact resistance is the deposition of thin oxide interlayers at the interface between the semiconductor and the metal [3–9]. Park et al. [3,4] have shown a reduction in electrical contact resistance and an improvement in device stability in MoS₂ field effect transistors with 2 nm TiOₓ films deposited by atomic layer deposition (ALD) at the interface between the MoS₂ and the Ti contact. The observed improvements were attributed to Fermi-level depinning and interface dipole effects. Kim et al. [5], who observed a decrease in Fermi-level pinning with 1 nm interfacial TiOₓ, suggested that the presence of an interfacial oxide reduces the density of metal-induced gap states by blocking the penetration of the electron wave function from the metal. Similarly, Kaushik et al. [6] concluded from density functional theory that the Schottky barrier height is reduced due to charge-transfer doping from the TiOₓ layer to MoS₂. They have experimentally shown a 24-fold reduction in contact resistance and tenfold improvement in on-current and field-effect mobility.

While the use of an interfacial oxide has been found to be highly beneficial to electronic properties in the aforementioned studies, thermal characterization of this interface is relatively lacking. An understanding of thermal transport is crucial as thermal resistances at the contact interface can inhibit heat removal from 2D electronic devices, compromising their performance and reliability [10]. The thermal conductance at the MoS₂/SiO₂ substrate interface present in most 2D devices is typically low, ~14 MW m⁻² K⁻¹ [11]. Therefore caution must be taken when introducing additional interfaces to the device that could potentially increase the total resistance of the system. Our previous work has shown that transport across contact interfaces is highly sensitive to the oxide composition of Ti for graphene as well as bulk substrates [12,13]. McDonnell et al. [14] have demonstrated that Ti/MoS₂ and TiOₓ/MoS₂ interfaces exhibit vastly different chemical compositions and suggested potential detrimental effects on thermal transport due to the higher thermal resistance of TiOₓ compared to metallic Ti. They noted that work by Duda et al. [15] concludes that the removal of native oxide along with the deposition of a Ti adhesion layer has been found to be critical to lowering thermal resistances at metal-semiconductor interfaces. Similarly, Hopkins et al. [16] have shown a substantial decrease in thermal boundary conductance due to the presence of native oxides at metal-semiconductor interfaces. Density functional theory calculations conclude that phonon-phonon coupling and phonon transmission across the metal/MoS₂ interface is strongly dependent on the degree of orbital hybridization at the contact, and that stronger chemical and electronic interactions at the contact result in higher thermal boundary conductance [17,18]. This would imply that the inclusion of oxide instead of metal at the MoS₂ interface could potentially result in diminished thermal transport, warranting an investigation of the thermal boundary conductance across Ti contacts to MoS₂ with interfacial oxides, and the potential dependence of thermal boundary conductance on interface chemistry.

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FIG. 1. (a) TDTR data and best fit for the Au/MoS2 structure. Thermal boundary conductance as a function of interfacial layer thickness for the MoS2 substrates (b) with and (c) without an oxide interlayer. Samples included are Au/Ti (black squares), Au/TiOx (red circles), and Au/Ti/TiOx (blue triangles) in addition to a reference sample of Au/MoS2 (dashed line). The arrows indicate the Ti metal thickness for each Ti/TiOx sample where data are plotted as a function of oxide thickness.

II. EXPERIMENTAL METHODS

We report a process for electron-beam deposition of an interfacial Ti oxide layer in ultrahigh vacuum (UHV) using a partial pressure of O2. The process allows for in situ chemical characterization of the interface with x-ray photoelectron spectroscopy (XPS). We compare the effects of metal (Ti), oxide (TiOx), and metal/oxide heterostructure (Ti/TiOx) films, at a range of thicknesses, deposited on bulk geological MoS2 crystals that are typically used for device fabrication. We use time-domain thermoreflectance (TDTR), an optical pump probe technique, for the measurement of thermal boundary conductance across these interfaces [19–21]. By measuring bulk geological crystals we are able to bypass thermal resistances from substrate/MoS2 interfaces and solely characterize the contact interfaces associated with the MoS2 surface.

Prior to loading to UHV, bulk MoS2 geological crystals (purchased from SPI [22]) were exfoliated with Scotch tape to clean the surface by removing the top layer [14]. Preliminary XPS data were collected in our Scienta Omicron UHV system [23]. All XPS data were acquired at a pass energy of 50 eV, using an Al Kα source with a photon energy of 1486.7 eV. The Mantis QUAD-EVC 4 pocket evaporator was used to deposit Ti onto the sample in situ. The titanium was evaporated at a rate of approximately 1 Å/min. For oxide deposition, a pressure of $5 \times 10^{-6}$ mbar of ultrahigh-purity O2 was maintained in the chamber during deposition. XPS data were acquired after each Ti and TiOx deposition. See the Supplemental Material [24] (Sec. S5) for the calculation procedure for the thickness of the deposited layers using the attenuation of the Mo 3d core-level intensity. The samples were then capped with 1–2 nm Au in situ to prevent oxidation in air upon removal from UHV. An additional ∼70 nm of Au was deposited in an ex situ e-beam evaporator for TDTR measurements.

TDTR is an optical pump probe technique that is widely used to characterize interfacial conductance at a variety of metal contacts. An 80 MHz repetition rate laser centered at 800 nm is split into high-power pump and low-power probe paths. The pump is amplitude modulated using an electro-optic modulator, and frequency doubled to 400 nm before being focused on the sample surface. The probe is mechanically delayed in time, and monitors the thermoreflectance at the sample surface due to temperature perturbations induced by the pump. We specifically modulate the pump at 10.28 MHz to ensure one-dimensionality in our analysis and minimize sensitivity to potential in-plane transport in the MoS2. Indeed, MoS2 in its few-layer and bulk forms has been shown experimentally to have an anisotropic thermal conductivity [25–28]. Modulating at this frequency also improves our sensitivity to the interfacial conductance at these contacts. We estimate the temperature rise of the MoS2 to be on the order of ∼30 K due to the average absorbed power from the pump and probe beams during TDTR experiments, which we calculate based on in- and cross-plane thermal conductivities of MoS2 from the literature [21,25,26] and the numerical solution to the multilayer cylindrically symmetric heat equation used to analyze our TDTR data. Example TDTR data and best fit are shown in Fig. 1(a) for the Au/MoS2 specimen, where we extract a conductance of $20.8 \pm 3.0$ W m$^{-2}$ K$^{-1}$. The error in our reported values reflect the standard deviation from several measurements on each specimen, as well the uncertainty associated with an 8% deviation in the thickness of the Au capping layer. More information regarding TDTR and its analyses can be found in the literature [19,21]. See the Supplemental Material [24] (Sec. S1) for a description of our two-color implementation of TDTR as well as a sensitivity analysis of relevant parameters in the Au/MoS2 system.

III. RESULTS AND DISCUSSIONS

Thermal boundary conductance, $h_K$, is plotted for structures with and without TiOx in Figs. 1(b) and 1(c),...
Before the deposition of Ti metal (black curve), MoS$_2$ spectra before and after the deposition of 4.1 nm Ti metal in this study. Figure 2(a) shows the core-level XPS spectra of (a) 4.1 nm Ti on MoS$_2$ and (b) 4.6 nm TiO$_x$ on MoS$_2$. We note that the three Au/Ti/MoS$_2$ samples with pure Ti metal overlayers and TiO$_x$ respectively. In the limit of zero TiO$_x$ thickness, corresponding to samples with pure Ti metal overlayers (Au/Ti/MoS$_2$), the average $h_K$ value was approximately 21.5 ± 5.6 MW m$^2$ K$^{-1}$. This value is roughly equivalent to the $h_K$ value of the Au/MoS$_2$ reference sample (20.8 ± 3.0 MW m$^2$ K$^{-1}$). The results are also consistent with previous measured values of metal/MoS$_2$ interfaces [25,29]. We note that the three Au/Ti/MoS$_2$ samples had Ti thicknesses ranging from 2.9 to 5.2 nm and Ti metal thickness had no effect on $h_K$ for these samples, suggesting that the intrinsic resistance of the Ti does not contribute to the overall resistance of the system. Similarly, the figure shows that TiO$_x$/MoS$_2$ samples with TiO$_x$ thicknesses from 1.7 to 4.6 nm all exhibit roughly the same value of 16.0 ± 2.8 MW m$^2$ K$^{-1}$. The lack of thickness dependence of $h_K$ in the Ti/MoS$_2$ and TiO$_x$/MoS$_2$ samples indicates that thermal transport is dominated by interfacial resistances and not by the intrinsic thermal resistance of metal or oxide layers.

Chemical characterization of the Ti/MoS$_2$ and TiO$_x$/MoS$_2$ interfaces is shown in Fig. 2. We implement XPS so as to observe any chemical changes in the underlying MoS$_2$ when in contact with Ti or TiO$_x$. See the Supplemental Material [24] (Sec. S3) for the core-level spectra of all specimens examined in this study. Figure 2(a) shows the core-level XPS spectra before and after the deposition of 4.1 nm Ti metal in UHV. Before the deposition of Ti metal (black curve), MoS$_2$ is characterized by the Mo 3$d_{3/2}$ state at ∼228.9 eV with a spin-orbit splitting value of 3.1 eV, and the S 2$p_{3/2}$ state at ∼161.8 eV with a spin-orbit splitting of 1.2 eV. Following the deposition of Ti, the spectra exhibit new chemical states including Mo metal (Mo$_0$) at 227.5 eV in the Mo 3$d$ spectrum and Ti-S states in the S 2$p$ spectrum. This result is consistent with previous reports of the deposition of Ti in UHV [14].

Figure 2(b) shows XPS spectra corresponding to a sample with 4.6 nm of TiO$_x$. The spectra indicate that the Mo-S bonds are preserved and no chemical reaction occurs between Ti and the substrate. As previously reported by McDonnell et al. [14], the presence of a partial pressure of oxygen during the deposition of Ti on MoS$_2$ inhibits the reaction between them as Ti reacts with oxygen impinging on the surface of the substrate during deposition. The Mo 3$d$ and S 2$p$ core levels exhibit a 0.64 eV shift to higher binding energy, corresponding to a change in the position of the Fermi level. This indicates that the presence of an oxide overlayer causes n-type doping in the sample. This result is similar to that of Kaukshik et al. [6] who reported a 0.5 eV core-level shift for 2 nm of ALD TiO$_2$ on MoS$_2$. We note that the oxide which forms under the deposition conditions in our UHV chamber comprises two chemical states. The TiO$_2$ state has its 2$p_{3/2}$ component at 459.2 eV with a spin-orbit splitting of 5.7 eV and comprises ∼80% of the oxide layer deposited. The second chemical state, which appears at 457.65 eV with a spin-orbit splitting of 5.5 eV corresponds to Ti$_2$O$_3$ [30,31]. See the Supplemental Material [24] (Sec. S4) for the spectral deconvolution of the oxide layer.

Unlike the pure metal and oxide samples, $h_K$ of the Au/Ti/TiO$_x$/MoS$_2$ samples exhibits a decrease with increasing oxide thickness, with no apparent dependence on metallic Ti thickness, as shown in Fig. 1. The two samples with TiO$_x$ thicknesses ≤1.5 nm have $h_K$ values comparable to that of the Au/Ti/MoS$_2$ and Au/MoS$_2$ samples, whereas the Au/Ti(1.7 nm)/TiO$_x$(2.0 nm)/MoS$_2$ is comparable to the Au/TiO$_x$/MoS$_2$ samples with no metal overlayer, within uncertainty. The reduction in $h_K$ for this sample could be due to two possible reasons. The first is the increase in the oxide thickness compared to the heterostructures with TiO$_x$ thickness ≤1.5 nm. However, given that no oxide thickness dependence for $h_K$ of the Au/TiO$_x$/MoS$_2$ samples is observed, the increased oxide thickness is unlikely to be the dominant factor here. The second explanation is that the thickness of the Ti in the heterostructure (1.7 nm) is quite thin. From previous works, it has been shown that a reduction in the interfacial conductance is observed as the thickness of an interfacial adhesion layer becomes very thin (e.g., Cu and Cr) [32]. This reduction in our experiment is explained using similar predictions of accumulated thermal boundary conductance, whereby phonons in Ti with wavelengths less than the total Ti thickness participate in transport across the interface. In this way, the reduction in the population of Ti phonons due to a decrease in total Ti thickness ultimately results in a reduced $h_K$ at the interface. We believe this to be the case when the thickness of the Ti becomes very thin in the heterostructures, making our results consistent with those of Jeong et al. [32].

The XPS spectra of a Ti(2.7 nm)/TiO$_x$(1.5 nm)/MoS$_2$ sample are shown in Fig. 3. The TiO$_x$/MoS$_2$ interface (red curve) is chemically identical to that shown in Fig. 2(b), exhibiting a n-type Fermi-level shift and no other chemical changes following the deposition of Ti metal (blue curve). The only observable changes are broadening of the peaks
and an increase in noise, which occurs due to scattering and attenuation in the TiO$_x$ and Ti overlayers [33]. The lack of interface reactions with the presence of interfacial oxide is one possible explanation for the Fermi-level depinning effect reported by others [3–5]. Fermi-level pinning has been attributed to interfacial reaction products which create new electronic states within the semiconductor band gap [34]. By blocking interface reactions via direct contact with an unreactive oxide layer, MoS$_2$ retains its intrinsic band structure with no new states which could pin the Fermi level.

It is clear from comparison of Figs. 2(b) and 3 that interface chemistry does not explain the differences in behavior of $h_K$, as the TiO$_x$/MoS$_2$ interfaces in both the pure oxide and metal/oxide samples are chemically identical. Therefore, the behavior of $h_K$ is likely dominated by one of the other interfaces present in the device. For the metal/oxide heterostructure, these interfaces include Au/Ti and Ti/TiO$_x$, whereas the oxide sample contains only Au/TiO$_x$. The resistance from the Au/Ti interface is not a contributing factor, since thermal transport across metal/metal interfaces is governed by electrons near the Fermi energy, yielding thermal boundary conductance values that are far higher than those across metal/nonmetal interfaces (i.e., negligible thermal resistances at these metal/metal interfaces) [35–38]. The negligible contribution of this interface is evident in Fig. 1, which shows that Au/Ti/MoS$_2$ exhibits the same $h_K$ as the Au/MoS$_2$ reference sample, and is consistent with previous measurements of thermal boundary conductance at Au/graphene and Au/Ti/graphene interfaces [39].

To determine the extent of the contribution of the thermal conductances across the Au/TiO$_x$, Au/Ti, and Ti/TiO$_x$ interfaces to the overall measured $h_K$, we fabricated several reference samples. The samples included Au/Ti (2.3 nm)/Au/O/Au, Au/TiO$_x$ (2.0 nm)/Au/O/Au, and Au/Ti(2.2 nm)/TiO$_x$(4.4 nm)/Au/O/Au. The appearance of O at the interface arises due to residual oxygen present at the Au/Au interface following a UV-O$_3$ treatment, as discussed later. By measuring $h_K$ from each of these stacks we are able to isolate each of the interfaces and determine the interface contributions to the measured $h_K$ from series resistance model. See Supplemental Material [24] (Sec. S2) for further discussion of the specific model implemented. We first deposited 80 nm Au on single-crystal sapphire (Al$_2$O$_3$) with a 5 nm Al adhesion layer in a cleanroom evaporator at high vacuum (HV). Al$_2$O$_3$ was selected as our substrate to maximize sensitivity to potentially large conductances. The conductance at the Au/Al/Al$_2$O$_3$ interface was found to be $49 \pm 5.0$ MW m$^{-2}$ K$^{-1}$. Following this measurement, the surface of the Au was cleaned via UV-O$_3$ exposure as described elsewhere [40] to remove adventitious carbon. The sample was loaded back into UHV. Since the process was found to leave residual oxygen on the Au surface, the sample was capped with $\sim 2$ nm Au in UHV to create a pristine surface before depositing subsequent Ti layers. Three separate samples with Ti (2.3 nm), TiO$_x$ (2 nm), and Ti(2.2 nm)/TiO$_x$(4.4 nm) were created and capped with $\sim 1-2$ nm Au. To account for the contribution of residual oxygen at the interface between the HV and UHV Au, we fabricate a reference sample that is a UV-O$_3$ treated HV Au sample that is then capped with Au in UHV. This sample is measured to determine the contribution of the oxygenated Au interface to the total interfacial conductance in structures containing Ti and TiO$_x$.

Following the UHV deposition processes, the samples were transferred back to the HV electron-beam evaporator, and capped with $\sim 67$ nm of Au following an O$_2$ plasma cleaning procedure. TDTR was performed on the samples, fitting for the conductance across the newly deposited interfacial structure as the underlying Au/Al/Al$_2$O$_3$ interfacial conductance was measured prior to the deposition of the structures. The conductance across the Au/Au interface containing residual oxygen from the UV-O$_3$ process is measured to be $376 \pm 31$ MW m$^{-2}$ K$^{-1}$, and is accounted for in subsequent derivations of Au/Ti and Au/TiO$_x$ conductances. When accounting for this additional resistance, $h_K$ of the Au/Ti interface is found to be $1680 \pm 190$ MW m$^{-2}$ K$^{-1}$. We estimate this to be the lower bound for the conductance at the Au/Ti interface, based on the limitations of TDTR to measure ultrahigh boundary conductances, quasiballistic influences as a result of the thickness of the Ti layer, and extrinsic or chemical effects that prevent the Au/Ti interface from being an otherwise perfect interface. An additional possible explanation will be addressed later. Regardless, the conductance of metal-metal interfaces is quite high—the electron diffuse-mismatch model predicts a conductance of $5970$ MW m$^{-2}$ K$^{-1}$ at the Au/Ti interface at room temperature [35]. Thus, the contribution of the Au/Ti interface in the total interfacial resistance is negligible compared to other resistances present in these systems.

The Au/TiO$_x$ (2 nm)/Au/O/Au conductance is measured to be $44.5 \pm 3.2$ MW m$^{-2}$ K$^{-1}$, resulting in an interfacial conductance at the Au/TiO$_x$ interface to be $101 \pm 11$ MW m$^{-2}$ K$^{-1}$, once the Au/O/Au interface is accounted for. The measured conductance across the Au/Ti(2.2 nm)/TiO$_x$(4.4 nm)/Au interface is $65.2 \pm 4.5$ MW m$^{-2}$ K$^{-1}$, and suggests that the conductance of the Ti/TiO$_x$ interface, with a value of $459 \pm 87$ MW m$^{-2}$ K$^{-1}$, is large compared to that across the Au/TiO$_x$. Our results imply that the conductance of Au/TiO$_x$ interface presents a non-negligible thermal resistance due to the relative weak atomic interactions between Au and TiO$_x$; in fact, in the case of this Au/TiO$_x$/Au/Al/Al$_2$O$_3$ multilayer film system, the Au/TiO$_x$ offers the limiting thermal resistance to heat flow. See the Supplemental Material [24] (Sec. S2) for a complete derivation of the above values.
The thermal conductance across the Au/TiO\textsubscript{x}/MoS\textsubscript{2} interface can be modeled with a series resistance approach:

$$\frac{1}{h_{K,\text{meas}}} = \frac{1}{h_{K,\text{Au/TiO}_x}} + \frac{1}{h_{K,\text{TiO}_x/MoS}_2},$$

where $h_{K,\text{meas}}$ is the measured conductance across the Au/TiO\textsubscript{x}/MoS\textsubscript{2} interface (averaged over all TiO\textsubscript{x} thicknesses), $1/h_{K,\text{Au/TiO}_x}$ is the resistance of the Au/TiO\textsubscript{x} interface, and $1/h_{K,\text{TiO}_x/MoS}_2$ is the resistance of the TiO\textsubscript{x}/MoS\textsubscript{2} interface. Again, we neglect the contribution from the intrinsic resistance of the TiO\textsubscript{x} layer based on the constant boundary conductance observed for the range of TiO\textsubscript{x} thicknesses that are presented in Fig. 1. Taking $h_{K,\text{meas}}$ to be $16.0 \pm 2.8$ MW m\textsuperscript{-2} K\textsuperscript{-1}, and $h_{K,\text{Au/TiO}_x}$ from our measurements on this control interface discussed above, we calculate $h_{K,\text{TiO}_x/MoS}_2$ to be $19.1 \pm 3.8$ MW m\textsuperscript{-2} K\textsuperscript{-1}. The larger comparable conductance at the TiO\textsubscript{x}/MoS\textsubscript{2} interface as compared to $h_{K,\text{meas}}$ suggests that the Au/TiO\textsubscript{x} interfacial conductance is again playing a non-negligible role in the reduction of heat transport across these interfaces, albeit the TiO\textsubscript{x}/MoS\textsubscript{2} represents the dominant thermal resistance in this system. This reduction can be circumvented by implementing a Ti/TiO\textsubscript{x} heterostructure at the interface, provided that the Ti layer is thicker than $\sim 2$ nm as discussed previously, whereby we see an increased boundary conductance compared to just a TiO\textsubscript{x} adhesion layer. In all, this also suggests that the Ti/TiO\textsubscript{x} conductance is negligible compared to that of the Au/TiO\textsubscript{x} and TiO\textsubscript{x}/MoS\textsubscript{2} interface, allowing for a compromise of transport properties from both an electrical and thermal perspective. The values of the various interfaces with Ti and MoS\textsubscript{2} are summarized in Table I.

XPS characterization of the Au/Ti and Au/TiO\textsubscript{x} interfaces shows that chemical bonding occurs at Au/Ti interfaces while no chemical interactions are observed in Au/TiO\textsubscript{x} interfaces. The formation of intermetallic compounds in Au/Ti interfaces deposited in UHV at room temperature has been reported previously [41–43]. Figure 4 shows XPS acquired on Ti and TiO\textsubscript{x} samples deposited in our UHV system before and after the deposition of $\sim 3$ Å of Au. In the Ti 2p spectrum of the Ti metal sample shown in (a), the spectrum exhibits a core-level shift of 0.15 eV as well as broadening due to the presence of Au-Ti bonding at the interface following the deposition of Au. The TiO\textsubscript{x} spectra shown in (b) acquired before and after Au deposition overlap perfectly showing no change in binding energy or line shape. In the Au 4f spectrum in (c), Au deposited on Ti exhibits a prominent asymmetry and a 0.33 eV shift to higher binding energy which is characteristic of intermetallic formation [44], while Au deposited on TiO\textsubscript{x} retains the line shape and binding energy of elemental Au indicating no interaction occurs. The observed bonding at the Au/Ti interface is a potential explanation for the lower measured $h_K$ of the Au/Ti interface in comparison with the value calculated based on the electron diffuse-mismatch model, which does not account for the formation of an intermetallic compound at the interface [35]. It has been shown previously that the thermal boundary conductance can become dominated by the

![Image](https://example.com/image.png)

**FIG. 4.** Ti 2p spectra acquired on (a) Ti and (b) TiO\textsubscript{x} films before and after the deposition of Au, with Au 4f spectra corresponding to these samples shown in (c).

### Table I. Measured and derived values of Ti/TiO\textsubscript{x} structures on MoS\textsubscript{2} and sandwiched between Au.

| Interface                  | Au/Ti\textsuperscript{a} | Au/TiO\textsubscript{x}\textsuperscript{a} | Ti/TiO\textsubscript{x}\textsuperscript{a} | Au/MoS\textsubscript{2} | Au/Ti/MoS\textsubscript{2} | Au/TiO\textsubscript{x}/MoS\textsubscript{2} | Au/Ti/TiO\textsubscript{x}/MoS\textsubscript{2} | TiO\textsubscript{x}/MoS\textsubscript{2}\textsuperscript{b} |
|----------------------------|---------------------------|------------------------------------------|------------------------------------------|---------------------------|------------------------------------------|------------------------------------------|------------------------------------------|------------------------------------------|
| $h_K$(MW m\textsuperscript{-2} K\textsuperscript{-1}) | 1680 ± 190 | 101 ± 11 | 459 ± 87 | 20.8 ± 1.1 | 21.1 ± 5.7 | 16.0 ± 2.8 | 21.5 ± 1.6 | 19.1 ± 3.8 |
| $R_K$(m\textsuperscript{2} K GW\textsuperscript{-1}) | 0.59 ± 0.07 | 9.91 ± 1.07 | 2.18 ± 0.41 | 48.1 ± 2.54 | 47.4 ± 12.8 | 62.5 ± 10.9 | 46.5 ± 3.46 | 52.4 ± 10.4 |

\textsuperscript{a}Denotes values that are derived from measurements.

\textsuperscript{b}Denotes the average of the heterostructures with TiO\textsubscript{x} thicknesses of 1.5 and 2.0 nm, omitting that with 1.7 nm Ti. Other values are averaged from all samples of that type.
thermal conductance of an interfacial compound layer [35]. Furthermore, intermetallic compounds have been found to exhibit low values of thermal conductivity in comparison with their pure metal constituents [45]. Nevertheless, the electron mediated thermal transport at the metallic Au/Ti interface results in a $h_K$ value that is far higher than that corresponding to Au/TiO$_x$.

We note that while the conductance of the Au/Ti/MoS$_2$ interface is similar to that of the Au/Ti/TiO$_x$/MoS$_2$ interface, and offers improved thermal management as compared to using TiO$_x$ alone, the use of Ti inherently modifies the underlying MoS$_2$. In devices contingent on just a monolayer of the dichalcogenide, where the electronic density of states departs significantly from its bulk counterpart [46,47], metrical redistribution. TiO$_2$ in contact with MoS$_2$ has also been previously shown to not heavily alter the density of states in each material, as they still maintain direct band gaps [49]. This, combined with the improved conductance when implementing a Ti/TiO$_x$ heterostructure as an adhesion layer, offers a unique avenue for managing thermal and electronic transport properties in material systems contingent on the integration of MoS$_2$.

### IV. CONCLUSIONS

In summary, we find that Au/TiO$_x$/MoS$_2$ exhibits $\sim$20\% lower thermal boundary conductance than Au/Ti/MoS$_2$. Samples with a thin TiO$_x$ layer ($\sim$1–1.5 nm) at the interface between Ti and MoS$_2$ exhibit the same thermal boundary conductance as those with pure Ti metal. The difference in $h_K$ between the TiO$_x$/MoS$_2$ and Ti/TiO$_x$/MoS$_2$ samples is observed despite the chemically identical TiO$_x$/MoS$_2$ interfaces present in both samples. The differences in $h_K$ arise due to the different interfaces with the top Au contact. Whereas Au/Ti has negligible resistance, that of Au/TiO$_x$ is substantial making this interface the dominant resistor in the system. Our results suggest that thin interfacial oxide layers which can be used to enhance electronic properties have no negative impact on thermal transport in 2D electronic devices. The thickness of the Ti layer in the Ti/TiO$_x$ structure must be considered when implementing this type of contact.

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