

**A Molecular Dynamics Study of the Thermal Boundary Conductance of
Stacked Two-Dimensional Materials**

by

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The work done in this thesis has in collaboration with the groups of Dr. Salehi-Khojin and Dr. Aksamija, resulted in a publication (1) and I want to express my gratitude for the opportunity to work together with them.

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LIST OF ABBREVIATIONS

MD	Molecular Dynamics
NEMD	Non-Equilibrium Molecular Dynamics
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
NVT	Constant number (N), volume (V), and temperature (T)
NVE	Constant number (N), volume (V), and Energy (T)
TBC	Thermal Boundary Conductance
2D	Two-Dimensional
Ti	Titanium
MoS ₂	Molybdenum disulphide
SiO ₂	Silicon dioxide
UIC	University of Illinois at Chicago

SUMMARY

With the components driving information technology becoming ever smaller and reaching their limits in size, there has been a shift in focus to develop devices where 2D materials, such as graphene and MoS₂, act as the main functional component, due to their often superior electrical properties to current materials used. Replacing the conductors in transistors for example, where relatively high voltages are applied at high frequencies, with 2D materials, is a very attractive approach for reaching smaller scale, better performing, electronic devices. However, the resistive heating in such devices is a challenge for the same reason, thus careful consideration must be taken in developing and designing it to ensure that heat can dissipate efficiently from the source, which is mostly in the through-plane direction. Efforts have been made to experimentally measure the thermal boundary conductance (TBC) of the interface of MoS₂ with SiO₂, but so far there is no consensus on the value. (2; 3; 4)

When measuring the TBC of a 2D material in experiments, it is not measured directly, but rather inferred from the difference in conductivity between a device with the 2D material inserted, and one without. While the surfaces of the materials by the interface can be observed using microscopy techniques during the production of the device, the surface interactions at an atomic level during a cross-planar heat flow are not easily measured, and this is where molecular dynamics (MD) simulations play an important role: with atomic resolution and with the capability of enforcing heat-flows, the interfaces of the 2D material can be investigated in needed detail to complement the experimental measurements and enrich the analysis. (5)

SUMMARY (Continued)

In this thesis, the first Chapter introduces the reader to the context and the goals of the work. Chapter 2 goes into more detail of explaining thermal conductivity and TBC and what simulation methods were used. Chapter 3 explains how the simulations were set up in detail. In Chapter 4 the results are presented and discussed. Finally, in Chapter 5, concluding remarks are made in the context of experimental results.

CHAPTER 1

INTRODUCTION

1.1 2D materials and Microelectronic Devices

When it comes to 2D materials, such as graphene and transition metal dichalcogenides like MoS₂ used in this study, they have amassed a large amount of interest the past decade due to their exciting properties, such as high electric conductivity, optical and mechanical properties. (6; 7; 8; 9; 10; 11) One of the potential new applications is to replace silicon in traditional semiconductors devices, such as transistors. In a transistor, the 2D material would be embedded between layers of different materials, with resistive heating being prominent during operation. Because of the heat being generated in such small regions, it is important to have efficient heat removal to avoid device failure from overheating. (12) The majority of the heat is dissipated out of the plane of the 2D material and the rate at which heat can be removed is limited by the thermal boundary conductance (TBC) associated with the interfaces below and above the plane.

Knowing what the TBC contributes to the total conductance and how it is affected by the surrounding materials is key to arriving at fully functional, nanoscale electronics based on 2D materials. But despite a lot of effort in recent years, there is an order of magnitude difference between reported values. (2; 3; 4; 13) The TBC can be found from measuring the discontinuity

in the temperature, ΔT , across the interface at a given the heat flux, J , per cross-sectional area A :

$$\frac{J}{A} = \sigma_K \Delta T \quad (1.1)$$

where σ_K is the TBC. Directly measuring ΔT , however, is impractical experimentally, and is typically inferred by measuring the difference in overall thermal conductivity of a test device with and without the 2D material. (1)

1.2 Objectives

The inability to directly measure the TBC of a device is a typical scenario where molecular dynamics (MD) simulations can provide valuable insight on an atomic scale to complement experiments. MD simulations have been used to measure thermal conductivity and TBC successfully for more than a decade (5; 14), and are well suited to investigate the TBC of the 2D material in a test device.

In the work presented in this thesis, the objectives are **1.** to directly model the heat transfer normal to the surface of MoS_2 while stacked between Ti and SiO_2 and calculate the TBC of the interfaces using MD simulations and **2.** to compare the TBC of the stacked system to systems with Ti- MoS_2 and MoS_2 - SiO_2 only to assess the effect of stacking.

CHAPTER 2

HEAT CONDUCTION AND MOLECULAR DYNAMICS SIMULATIONS

2.1 Heat Flow and Thermal Conductivity

Thermal conductivity is the measure of the capacity of a material to transport heat and relates heat flux, \mathbf{G} to a temperature gradient, ∇T via Fourier's Law:

$$\mathbf{G} = -K\nabla T \quad (2.1)$$

that is, the heat flux through a surface is proportional to the negative temperature gradient across the surface, where the thermal conductivity, K , is the constant of proportionality. The fact that heat is transported in the system means that it is not in thermal equilibrium since $\nabla T \neq 0$.

When calculating the bulk thermal conductivity K , one assumes that the material within which the heat is transported is homogenous and continuous. Here, continuous assumes an unbroken crystal structure in the case of crystalline materials. When there is a grain boundary in a crystal or when the surfaces of two materials that are held together by Van der Waals forces are considered, the thermal conductivity abruptly changes over a very short distance. This impacts the transport of heat through lattice vibrations, or phonons, which is the largest contributor to the total dissipated heat, across the interface. Because of this imperfect contact of the two sides of the interface, there is a finite *thermal boundary conductance* (TBC) or Kapitza

conductance σ_{κ} , associated with it and therefore also a discontinuity in the temperature, ΔT . The heat flow per area supported by the interface is given by the product of the conductance with the temperature discontinuity (15)

$$\frac{J}{A} = \sigma_{\kappa} \Delta T_{\text{dis}} \quad (2.2)$$

Thus, with knowledge of the cross-sectional area A , the heat flow J and the discontinuity in temperature ΔT_{dis} at the interface, one can calculate the TBC for that interface.

2.2 Molecular Dynamics Simulations

Molecular dynamics simulations is a tool where the motion of particles in a classical system are described at the atomic scale by Newton's equations of motion. A numerical integration method is used to propagate an N-particle system in time by evaluating the forces between pairs of particles at discrete time steps with a separation in time on the order of femtoseconds (10^{-15} s). The small time-step is necessary to capture the high frequency in the vibrations of molecular bonds which are up to the order of 10^{14} Hz. Although there is a multitude of numerical integration methods that one would naively use, not all of them are suited for use in MD simulations. A good time-integration method need to fulfill things such as conservation of energy and momentum, time-reversibility and conservation of phase-space volume. (16; 17) Among the most used methods are the Verlet (18), Leap Frog (19) and the Verlet-Velocity (20) methods, which all fulfill the mentioned requirements.

The forces are evaluated from a so called "force field" describing the interaction potential between all types of particles in the system. It is a sum of different types of potentials where each potential function usually describe different types of interactions, such as coulombic interactions for charged particles or Van der Waals interactions for non-polar, uncharged particles.

2.3 Non-Equilibrium MD and Heat Flow

The use of MD simulations to monitor non-equilibrium transport processes, is almost as old as the development of MD simulations themselves (21; 22; 23), dating back to the 1950's. With the power to manipulate a system in almost any way possible, MD simulations are particularly suited to induce heat flows artificially in equilibrium systems.

One of the advantages in using non-equilibrium molecular dynamics (NEMD) to calculate the thermal conductivity and the TBC is that in a system with an interface, the discontinuity in the temperature, ΔT_{dis} , can be used to calculate the TBC using Equation 2.2, while the temperature gradients in the bulk materials away from the interface can be used to obtain the thermal conductivity, K , through Equation 2.1 or Equation 2.4 below.

The NEMD setup used in the simulations follow the algorithm described by T. Ikeshoji and B. Hafskjold in 1994. (5) The algorithm relies on establishing a temperature gradient in the system between a heat source and a heat sink and measuring the heat energy Q transferred between them per unit time. The simulation setup have the source and sink regions kept at different constant temperatures while the outside region is simulated at constant energy and the whole system is simulated at constant volume. The source and sink are coupled to heat baths at separate temperatures T_h and T_c , respectively. By monitoring the added heat at the

source or the removed heat from the sink over time, since they are equal under steady state condition, the heat flow, $J = \frac{\Delta Q}{\Delta t}$, can be obtained. The bulk thermal conductivity, K , is then calculated as the heat flow per area per temperature difference, multiplied by the length over which the temperature difference is measured. Putting all the above knowledge together, we have the following equations to rely on when calculating the thermal conductance K and the TBC (σ_K)

$$J = \frac{\Delta Q}{\Delta t} \quad (2.3)$$

$$K = \frac{J}{A \Delta T_{\text{bulk}}} L \quad (2.4)$$

$$\sigma_K = \frac{J}{A \Delta T_{\text{dis}}} \quad (2.5)$$

Here, ΔQ is sampled over the simulation time Δt , while A is the cross sectional area of the material in the plane normal to the heat flow J . ΔT_{bulk} is the temperature difference over length L in the bulk material and ΔT_{dis} is the discontinuity in the temperature across the interface. In the case of a material without any grain boundaries or surfaces, ΔT_{bulk} is just the difference in temperature between the source and the sink: $\Delta T_{\text{bulk}} = T_h - T_c$.

CHAPTER 3

METHODS

(Figure 1 and Section 3.2 are adapted from the Supplementary Information of my publication (1) with the following citation:

Poya Yasaei, Cameron J. Foss, Klas Karis, Amirhossein Behranginia, Ahmed I. El-Ghandour, Arman Fathizadeh, Javier Olivares, Arnab K. Majee, Craig D. Foster, Fatemeh Khalili-Araghi, Zlatan Aksamija, and Amin Salehi-Khojin, "Interfacial Thermal Transport in Monolayer MoS₂- and Graphene-Based Devices", *Adv. Mater. Interfaces* 2017, 1700334.

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3.1 Simulation Details

Four sets of simulations were conducted using different combinations of materials: Ti-MoS₂, MoS₂-SiO₂, Ti-MoS₂-SiO₂ and Ti-SiO₂. The full system containing Ti, MoS₂ and amorphous SiO₂, and the system with only Ti and SiO₂ called the "control", were run to be compared with experimentally available TBC values extracted by collaborators from Salehi-Khojin's group.

(1) In addition to comparing simulations to experimental systems, two simulations with only Ti-MoS₂ and MoS₂-SiO₂, were conducted to investigate the contribution to the overall TBC from each of the interfaces with MoS₂.

The molecular dynamics (MD) simulations were carried out using the software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) (24) and the thermal conductivi-

ties were calculated from non-equilibrium molecular dynamics (NEMD) simulations. (5; 25) The bulk conductivity (K) of the SiO_2 and Ti substrates as well as the Kapitza conductance (TBC) of MoS_2 -substrate boundaries were calculated from NEMD trajectories, in which a temperature gradient was imposed across a thermally equilibrated system while being kept at constant energy and volume. After reaching a steady state, the heat flow was monitored by measuring the amount of heat required to maintain the temperature gradient and was used to calculate the thermal conductivities from Equation 2.4 and Equation 2.5. The interatomic potentials in SiO_2 , MoS_2 , and Ti were modeled using the Tersoff (26), Stillinger-Weber (27) and Embedded Atom Method (28) forcefields, respectively. The Van der Waals interactions between MoS_2 and each substrate were described by 6-12 Lennard-Jones potentials (29; 30; 31) with parameters for mixed interactions calculated using the Lorentz-Berthelot mixing rules. (32; 33) Simulations were carried out at constant volume using periodic boundary conditions in the x-and y-directions and at a time step of 0.1 fs. For equilibrium simulations in the NVT ensemble, the temperature was kept constant using the Nosé-Thermostat of LAMMPS. (34)

3.2 Detailed System Setup

The initial structure of Ti and MoS_2 were built from their crystallographic structures. (28; 30) The amorphous structure of SiO_2 was created by heating up a SiO_2 crystal to 7000 K in 0.5 ns of simulation followed by 1 ns of equilibration at 7000 K and cooling down to 300 K in 2 ns. These simulations were performed at a constant volume that matches the size of the Ti and MoS_2 in the x-y plane. The size of the simulation cell for all systems was chosen such that the cell included an integer number of crystallographic building blocks of Ti and MoS_2 .

The resulting systems were 108.15 Å by 106.15 Å in the x-y plane. The thickness in z were 55 Å and 110 Å, for Ti and SiO₂ respectively. The systems were minimized and subsequently equilibrated in the NVT ensemble for a minimum of 20 ps. Equilibration was assumed to be reached when the total system energy plateaued. To calculate the thermal conductivity, a temperature gradient was set up in the equilibrated systems normal to the material interfaces and the system was simulated in the NVE ensemble. The heat flux was monitored until the system reached a steady state which was typically achieved in 100 to 300 ps. Under steady state conditions, by knowing the temperature drop across the interfaces, the thermal boundary conductance was calculated using the accumulated heat added to or removed from the hot and cold regions, respectively, during the length of the simulation using Equation 2.5. All heat flux simulations used for data collection were run for 1 ns or until the statistical error associated with the total heating/cooling was less than 10%. Temperature profiles along the z-axis were acquired by dividing the system into equal sized bins of 10 Å in width and calculating the average temperature from atomic velocities for each bin over the total simulation time. The jump in temperature across the boundary used in the calculation of the boundary conductance was measured as the difference in temperature between the two bins adjacent to each other on each side of the boundary. For the Ti-MoS₂-SiO₂, Ti-MoS₂ and Ti-SiO₂ systems, a slab with a thickness of 10 Å at the upper end of the Ti was set to be the heat source. For the MoS₂-SiO₂ system, the entire MoS₂ sheet was the heat source. In the Ti-MoS₂-SiO₂, MoS₂-SiO₂ and Ti-SiO₂ systems, the heat sink was set as a 10 Å slab at the lower end of the SiO₂. For the Ti-MoS₂ system, the heat sink was set up in the MoS₂ sheet (see Figure 1).

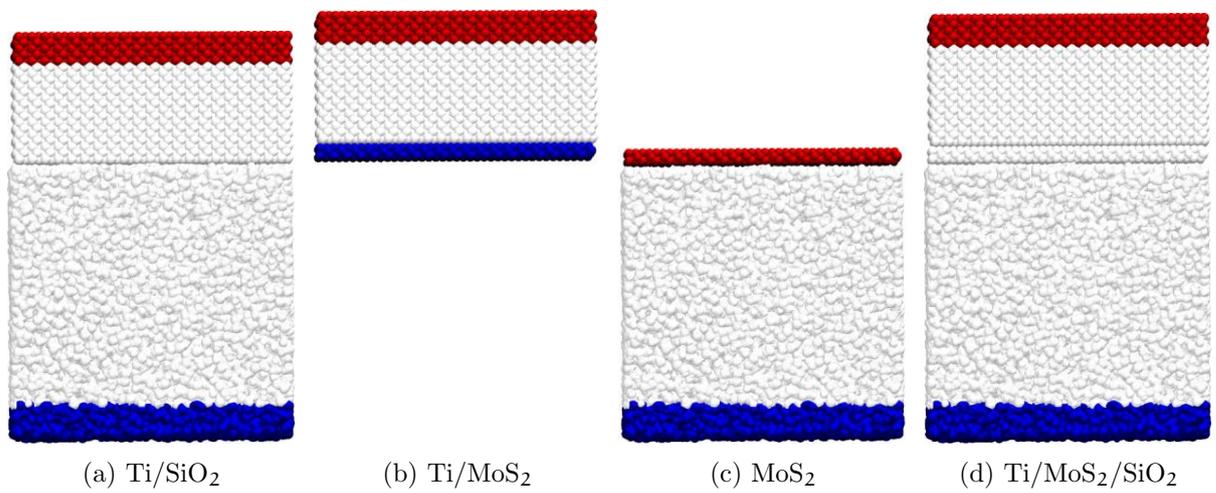


Figure 1: Representation of the heat sources (red) and the heat sinks (blue) for each of the four systems simulated. In Ti and SiO₂, the thermostatted regions are approximately 10 Å thick. In MoS₂ the whole layer acts source/sink.

CHAPTER 4

RESULTS AND DISCUSSION

(Table I and Figure 2 is adapted from my publication (1) with the following citation:

Poya Yasaei, Cameron J. Foss, Klas Karis, Amirhossein Behranginia, Ahmed I. El-Ghandour, Arman Fathizadeh, Javier Olivares, Arnab K. Majee, Craig D. Foster, Fatemeh Khalili-Araghi, Zlatan Aksamija, and Amin Salehi-Khojin, "Interfacial Thermal Transport in Monolayer MoS₂- and Graphene-Based Devices", *Adv. Mater. Interfaces* 2017, 1700334.

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4.1 Results

The obtained temperature profiles for each system are plotted in Figure 2 together with the system it was extracted from. The obtained TBC values for the interfaces of each system are listed in Table I. The bulk thermal conductivities were calculated using the temperature gradient in each material. For the full system, the individual TBC values for Ti/MoS₂ and MoS₂/SiO₂ were calculated using the jump in temperature at the corresponding interface, while the TBC for Ti/SiO₂ *across* MoS₂ was calculated with the jump in temperature between Ti and SiO₂, ignoring the temperature of MoS₂. This resembles how the TBC at the Ti/SiO₂ interface with MoS₂ inserted is inferred in experiments and can thus be used for comparison to experiments.

The bulk thermal conductivity of Ti and SiO₂ were found to be 2.6 and 0.9 W m⁻¹ K⁻¹, respectively. While the finite size of the system is not expected to affect the TBC of the

boundaries, it may affect the bulk conductivity of the substrates calculated from the simulations. The value for SiO_2 compares well to known experimental values of $1.1 - 1.4 \text{ W m}^{-1} \text{ K}^{-1}$. (35) The value for Ti, however, is well below the experimental value of $21.9 \text{ W m}^{-1} \text{ K}^{-1}$. (36) This is explained by the fact that MD simulations do not include the electronic contribution to the thermal conductivity. This contribution is estimated to $19.44 \text{ W m}^{-1} \text{ K}^{-1}$ using Wiedemann-Franz law (37) and using standard values of electrical conductivity and Lorentz number of $2.4 \cdot 10^6 \text{ S m}^{-1}$ and $2.7 \cdot 10^{-8} \text{ W } \Omega \text{ K}^{-2}$. (36; 38) Subtracting the electronic contribution from the experimental value of the total thermal conductivity of Ti gives a phonon contribution of $2.46 \text{ W m}^{-1} \text{ K}^{-1}$ which is close to the result from the MD simulations.

In the control simulation where MoS_2 is not present, the TBC at the Ti/ SiO_2 interface is $57.7 \text{ MW m}^{-2} \text{ K}^{-1}$. With the MoS_2 inserted in the system, the TBC calculated for Ti to SiO_2 is lowered to $10.9 \text{ MW m}^{-2} \text{ K}^{-1}$. However, comparing single interfaces with each other, the TBC between MoS_2 and Ti calculated in the single interface system is $7.9 \text{ MW m}^{-2} \text{ K}^{-1}$, while for the stacked system the same interface has a TBC of $13.7 \text{ MW m}^{-2} \text{ K}^{-1}$, an increase of about 70 %. A more pronounced increase, with a factor of 3.5, for the TBC is seen at the interface between MoS_2 and SiO_2 , where the single interface system has a value of $15.6 \text{ MW m}^{-2} \text{ K}^{-1}$ and the interface in the stacked system is $54.6 \text{ MW m}^{-2} \text{ K}^{-1}$.

The first thing to note about the results of the TBC is that for the system without MoS_2 , the value for the Ti/ SiO_2 is within the range of experimental values. The value obtained with MoS_2 inserted is not as close being about 50 % of the experimental value, but considering the

one order of magnitude discrepancy in the literature mentioned in the introduction this is still an acceptable result.

Interestingly, the comparison of TBC between the single interface systems with the fully stacked system shows that the interfaces of MoS₂ with Ti and SiO₂, respectively, can not be acquired individually and then used in a stacked system as two independent interfaces, and a full system analysis is needed to arrive at correct TBC values.

The most intriguing result, however, is that the TBC for the MoS₂/SiO₂ interface in the stacked system, 54.6 MW m⁻² K⁻¹, is very close the value found in the Ti/SiO₂ system, 57.7 MW m⁻² K⁻¹. This suggests a that when put on top of MoS₂, the Ti enhances the TBC between MoS₂ and SiO₂ in such a way that the MoS₂ layer acts as a "skin" to the Ti surface and almost keeps the same TBC as the Ti/SiO₂ interface has.

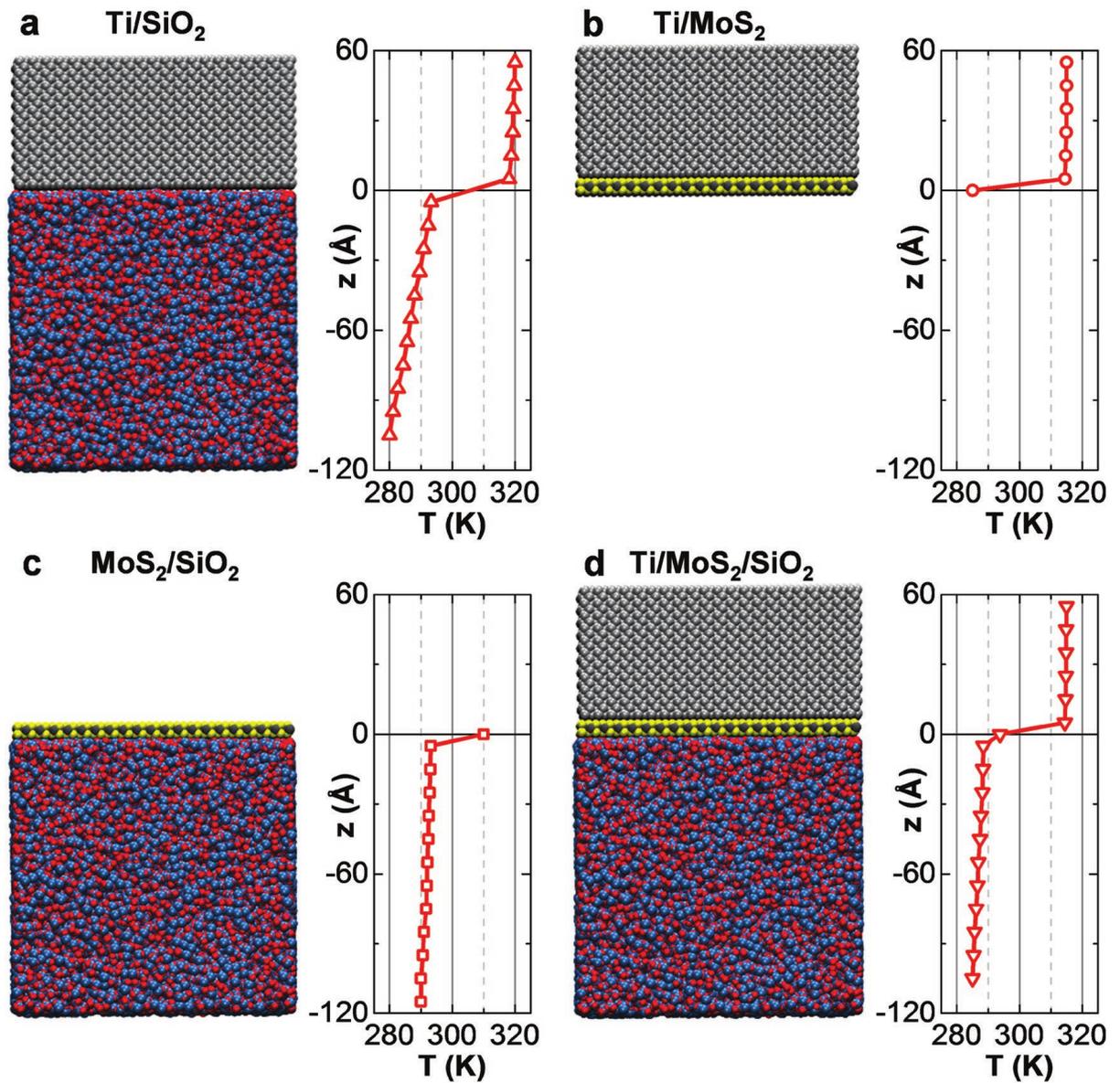


Figure 2: a–d) Snapshots of the four simulation systems consisting of Ti, MoS₂, and SiO₂. For each system, the temperature profile normal to the plane of MoS₂ obtained from the NEMD simulations is shown. The temperature profiles are used to calculate the TBC at each boundary. Figure reprinted from previous publication (1)

TABLE I: CALCULATED THERMAL BOUNDARY CONDUCTANCES

	TBC-MD [MW m ⁻² K ⁻¹]	TBC-Experiment [MW m ⁻² K ⁻¹]
MoS ₂ /SiO ₂	15.6	
Ti/MoS ₂	7.9	
Ti/SiO ₂	57.7	56-74
Ti/MoS ₂ /SiO ₂	10.9	20.3-33.5
MoS ₂ /SiO ₂ (*)	54.6	
Ti/MoS ₂ (*)	13.7	

TBCs from the MD simulations along with the experimental data from Salehi-Khojin's group. (1) The top three rows are from single interface systems and the bottom three rows are values from the stacked system (two interfaces). Individual interface values of the stacked system were calculated using the temperature drops between the two sides of the interface. (*) shows the extracted values from triple-stack simulations. Table reprinted from previous publication (1)

CHAPTER 5

CONCLUSIONS

In conclusion, NEMD simulations have for the first time¹ been conducted to investigate the effect on TBC of a 2D material, MoS₂, when inserted between Ti and SiO₂. The simulations show that the TBC of MoS₂ in a stacked system *can not* be modelled as two separate interfaces in a series, and that the full system with substrate, 2D material and metal layer has to be considered to correctly account for the thermal resistance added to the total thermal resistance of the system. Comparing the single interface systems (Ti-MoS₂ and MoS₂-SiO₂) to the double interface system (Ti-MoS₂-SiO₂), the TBC increases for both the Ti-MoS₂ and the MoS₂-SiO₂ interfaces when MoS₂ is inserted by a factor of 1.7 and 3.5, respectively. This relatively large effect on the TBC of stacked 2D materials is thus an important factor to consider when designing nano-electronic devices and must be taken into consideration at contact metals and gate dielectrics.

Assuming proper force field parameters exist, the simulation methods used in this study can be generalized to any other metal, substrate or 2D-material. Thus, if one wishes to investigate new materials, the author hopes that this thesis and the published material (1), can serve as a good reference and inspiration to future investigations.

¹To the best of the author's knowledge

APPENDICES

Appendix A

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