

January 2015

UNUSUAL THERMAL TRANSPORT IN GRAPHENE / BORON NITRIDE SINGLE INTERFACE & SUPERLATTICE TUNED BY INTERFACIAL ROUGHNESS

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By Vignesh Gouthaman

Entitled

UNUSUAL THERMAL TRANSPORT IN GRAPHENE / BORON NITRIDE SINGLE INTERFACE & SUPERLATTICE
TUNED BY INTERFACIAL ROUGHNESS

For the degree of Master of Science in Mechanical Engineering

Is approved by the final examining committee:

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Date

UNUSUAL THERMAL TRANSPORT IN GRAPHENE / BORON NITRIDE
SINGLE INTERFACE & SUPERLATTICE TUNED BY INTERFACIAL
ROUGHNESS

A Thesis

Submitted to the Faculty

of

Purdue University

by

Vignesh Gouthaman

In Partial Fulfillment of the

Requirements for the Degree

of

Master of Science in Mechanical Engineering

August 2015

Purdue University

West Lafayette, Indiana

ACKNOWLEDGEMENTS

First and foremost I would like to express my most sincere gratitude to Prof. Xiulin Ruan for taking me under his wing. Prof. Ruan has provided valuable insights and continued unwavering guidance throughout my Master's research. His immense knowledge in relevant topics, motivation and leadership has helped me complete my research successfully. I am very glad to have Prof. Ruan as my advisor through the period of my Masters.

I would like to thank my advisory committee members Prof. Bumsoo Han and Prof. Liang Pan for their patience and support through my research. I would like to give a special thanks to Tianli Feng who has worked with me and guided me on this project from the beginning. Tianli has been a pillar of support being ever ready to help me out if and when I had any questions, trivial or complicated. He has been an excellent mentor and I am thankful I got to work alongside him. I believe he will make a really good leader one day. I would also like to thank Eshaan Mathew, Yan Wang and Zuyuan Wang for sharing insights and providing their valuable help along the way.

Finally, I would like to thank my parents, my brother and my sister-in-law for supporting me through my education at Purdue University.

TABLE OF CONTENTS

	Page
LIST OF FIGURES.....	v
NOMENCLATURE	vii
ABSTRACT.....	ix
CHAPTER 1. INTRODUCTION.....	1
1.1 Motivation.....	1
1.2 Review of Thermoelectric Materials	2
1.3 Review of Thermal Management.....	5
1.4 Phonon Transport.....	8
1.4.1 What is a Phonon?	8
1.4.2 Acoustic Phonons (Coherent Phonons)	10
1.4.3 Optical Phonons (Incoherent Phonons)	10
1.4.4 Superlattice and Its Importance	11
1.5 Objective and Scope of Thesis.....	12
CHAPTER 2. METHODOLOGY	13
2.1 Overview.....	13
2.2 Molecular Dynamics	14
2.2.1 Green-Kubo Method	16
2.3 Simulation Setup.....	18
2.3.1 Molecular Structure	18
2.3.2 Boundary Conditions	21
2.3.3 Tersoff Potential.....	22
2.4 Initial Results and Periodic Nature of the Structure	24
2.4.1 Revised MATLAB Code to Generate Molecular Structure.....	26
2.4.2 Importance of Periodicity	27
2.5 Using Green Kubo Method to Predict Thermal Conductivity.....	28
CHAPTER 3. RESULTS AND DISCUSSION.....	31
3.1 Introduction.....	31
3.2 Effect of Non-Periodicity of Superlattice	32
3.3 Effects of Periodic Length on Thermal Conductivity Prediction of Graphene-Boron Nitride.	33
3.4 Relation of L0/W0 or h/w of Teeth for Near Single Interface Systems (Few Interfaces)	36
3.5 Effect of Interfacial Roughness on Thermal Conductivity of System with Respect to the Length of the Teeth and Periodic Length.....	38

	Page
CHAPTER 4. CONCLUSION AND FUTURE WORK.....	43
4.1 Conclusion	43
4.2 Future Work.....	44
LIST OF REFERENCES.....	45

LIST OF FIGURES

Figure	Page
Figure 1-1: Temperature gradient causing charge carriers to flow. This imbalance of charge creates a potential difference which can be measured[32].....	2
Figure 1-2: ZT of many typical thermoelectric materials as a function of year [33]....	3
Figure 1-3: Processor power density over time [34].....	5
Figure 1-4: Transistors per Die over time [34].....	6
Figure 1-5: Snapshot of a typical Si/Ge superlattice nanowire used as model system in the MD simulations. The total length of the wire (L), cross-sectional width (D), and periodic length ($L_p = L_{Si} + L_{Ge}$) are indicated. Color code: yellow: Si, blue: Ge. [35].....	11
Figure 2-1: Flowchart showing the steps of calculations involved in molecular dynamics simulation.....	15
Figure 2-2: System with rough interface visualizing the different terms used.....	19
Figure 2-3: (a) Visualization of entire system using VMD, (b) a close-up look at the carbon atoms, the interface and the boron nitride atoms. (C – Cyan, B – Magenta, N – Blue).....	21
Figure 2-4: Initial results: Studying variation in Thermal Conductivity in smooth interface and rough interface systems with varying periodic lengths keeping system length, width and teeth length and width constant. Red circle points to the unexpectedly low k values.....	24
Figure 2-5: Visualization of the molecular structure produced for the case with $PL = 10\text{\AA}$. Due to the periodic length being very small the structure doesn't seem periodic at all. (C – Cyan, B – Magenta, N – Blue).....	25
Figure 2-6: Revised visualization of the molecular structure produced for the case with $PL = 10\text{\AA}$ using the revised MATLAB code. The lattice structure is now perfectly periodic in nature. (C – Cyan, B – Magenta, N – Blue).....	26
Figure 2-7: HCACF plotted against time steps.....	28
Figure 2-8: Integrated values of the Heat Current Auto-Correlation Function plotted against Time steps. As explained, the plot seems to plateau at about 25000 time steps and later diverge.....	29
Figure 3-1: Initial results: Studying variation in Thermal Conductivity in smooth interface and rough interface systems with varying periodic lengths keeping system length, width and teeth length and width constant. Red circle points to the unexpectedly low k values.....	32
Figure 3-2: Plot of various cases with different periodic length with varying width of teeth (separation between teeth). The different thermal conductivity values are plotted relative to the value of the smooth condition in their respective cases.....	34

Figure	Page
Figure 3-3: Relation thermal conductivity w.r.t h/w or L0/W0 in a case symbolic of single interface system.....	37
Figure 3-4: Effect of teeth on thermal conductivity of a Single Interface. Figure by Zuyuan Wang.....	38
Figure 3-5 Effect of interfacial roughness on thermal conductivity of system with respect to the length of the teeth and periodic length.....	39
Figure 3-6: Size Effect showing that the thermal conductivity of a system will keep increasing for the smooth interface system and plateau off for the system with the rough interface.....	40

NOMENCLATURE

Symbol	Units	Definition
a	m	Cell length
C	J/m ³ K	Volumetric Heat Capacity
f	s ⁻¹	Frequency of heat flux
G	W/m ³ K	Electron to phonon energy transfer per unit volume or electron cooling rate
h	W/m ² K	Interfacial conductance
h _{ep}	W/m ² K	Electron-phonon conductance
h _{pp}	W/m ² K	Phonon-phonon conductance
J	W/m ²	Heat Flux
k	W/mK	Thermal Conductivity
k _B	1.38064E-23 m ² kg/s ² k	Boltzmann Constant
K _e	W/mK	Electron thermal conductivity
k _p	W/mK	Phonon thermal conductivity
\bar{k}	m ⁻¹	Wave vector
L	m	Length of the system
L _p	m	Penetration depth
m	amu	Atomic mass
MF, ω	Hz	Modulation frequency
n _b		Number of basis atoms
\dot{q}	W/m ³	Energy Generation term
t	s	Time
T	K	Temperature
T _e	K	Temperature of electron
T _p	K	Temperature of phonon
V _d		Volume fraction
X	m	Position, Distance
Greek		
α	m ² /s	Thermal Diffusivity

\square	eV	Interaction Potential
ϵ	eV	Potential well depth
λ	m	Mean Free Path
τ	s	Relaxation Time
σ	m	Zero potential energy pairwise separation
v	m/s	Carrier Velocity
ω	Rad/s	Phonon Angular frequency

ABSTRACT

Gouthaman, Vignesh. M.S.M.E., Purdue University, August 2015. Unusual Thermal Transport in Graphene / Boron Nitride Single Interface & Superlattice Tuned by Interfacial Roughness. Major Professor: Xiulin Ruan, School of Mechanical Engineering.

Graphene combined with Boron Nitride is a superlattice that has a lot of potential in terms of tenability. There has been a lot of work that has gone into finding ways to tune the properties of this superlattice to improve its figure of merit. Interfacial roughness if strategically induced is thought to have the potential to increase the thermal conductivity without sacrificing any of the qualities of the superlattice. We perform equilibrium molecular dynamics via Green Kubo method on Graphene/Boron Nitride and study its thermal conductivity under the influence of various parameters that shape the superlattice and its properties. Green Kubo method involves generating the lattice structure and using a pair potential along with boundary conditions to implement equilibrium molecular dynamics. The simulation give us a heat current auto-correlation function (HCACF) which can be used to find the thermal conductivity of the system.

Some important aspects that were found were the importance of ensuring a perfectly periodic lattice structure to make predictions of thermal conductivity as the phonons are extremely sensitive to any irregularities at the interface between two materials.

The thermal conductivity of Graphene Boron Nitride superlattice is found to be dependent on the periodic length of the superlattice. It is found that at 5nm a critical

periodic length is reached where a large amount of medium energy phonons scatter causing the thermal conductivity to drop quickly and then continue rising after that. In terms of single interface there is a relation between the ratio of height and width of the teeth that are induced in the interface to simulate roughness and the thermal conductivity of the material. At a ratio of about 0.25 a maximum thermal conductivity is reached for the Graphene-Boron Nitride superlattice. To enhance the thermal conductivity using interfacial roughness you would need to induce teeth that are 2.5\AA in length in the interface which make it roughly the size of a unit cell hence not causing any disruptions to the phonons and at the same time increasing the thermal transport across the superlattice.

CHAPTER 1. INTRODUCTION

1.1 Motivation

If there was one thing that one would say marked the emergence of the 21st century for mankind, it would be computing power. To put it into perspective, the computing power that National Aeronautics and Space Administration (NASA) had at their disposal to put a man on the moon is less than the computing power currently in all our cars. The reason that computing power has reached such high levels is due to the fact that more transistors are being fit into a tiny chip. This brings us to one of the main hurdles faced today, which is Thermal Management. There is strong focus on research which deals with nanoscale energy transport at lengths comparable to the phonon mean free paths [1][2]. Graphene has been a hot topic in the thermoelectric research circles in the recent past and with good reason. Graphene is probably the first true example of a two-dimensional material, and hence has extremely high thermal conductivity[3]. This is precisely why it is such an exciting material to research.

Research has shown that suspending graphene above a substrate leads to substantially improving the quality of the device, but this kind of geometry poses many challenges in terms of functionality[4][5]. In the pursuit of identifying dielectrics that would allow substrate-supported geometry while holding on to the quality of that of a

suspended sample, we come across Boron Nitride[6]. Boron Nitride is especially intriguing because it has a lattice constant similar to Graphene, and it has large optical phonon modes and a large electrical bandgap[6].

Now since graphene by itself has a very high thermal conductivity, there are many ways that are suggested to control the thermal conductivity of Graphene. One of the ways to suppress thermal conduction effectively is by introducing rough boundaries and weakly-coupled interfaces between Graphene and Boron Nitride in the solid[3].

1.2 Review of Thermoelectric Materials

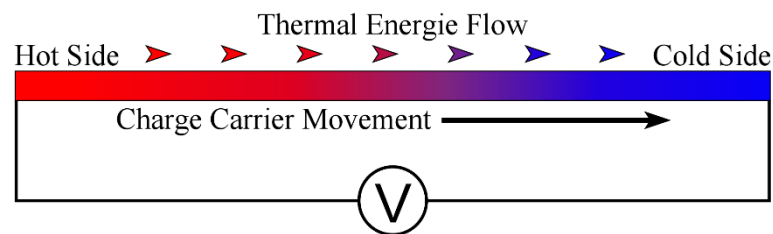


Figure 1-1: Temperature gradient causing charge carriers to flow. This imbalance of charge creates a potential difference which can be measured[32].

The thermoelectric effect involves the fundamental exchange of thermal energy to electrical energy and vice versa. There are two primary effects part of the broader thermoelectric effect. An electric voltage is generated when a temperature gradient is applied across the thermoelectric device, this effect is known as Seebeck Effect. Conversely, a temperature gradient is created when an electric voltage is applied across the device which is known as Peltier Effect.

As shown in figure 1-1, when a conductive material is subjected to a thermal gradient, charge carriers migrate along the gradient from the hot side to the cold side; this is Seebeck

effect. Electrons transfer heat by diffusing heat by the process of colliding with other electrons and by carrying the internal kinetic energy during transport. The process of carrying the internal kinetic energy during transport is known as Peltier effect. As one can see the Seebeck effect and Peltier Effect are the opposite of one another. The applications of the thermoelectric effect range from thermoelectric generators, which essentially function like heat engines. They have use in power plants converting waste heat back to energy. These also find applications in recovering waste heat from the exhaust of automobiles to increase fuel efficiency.

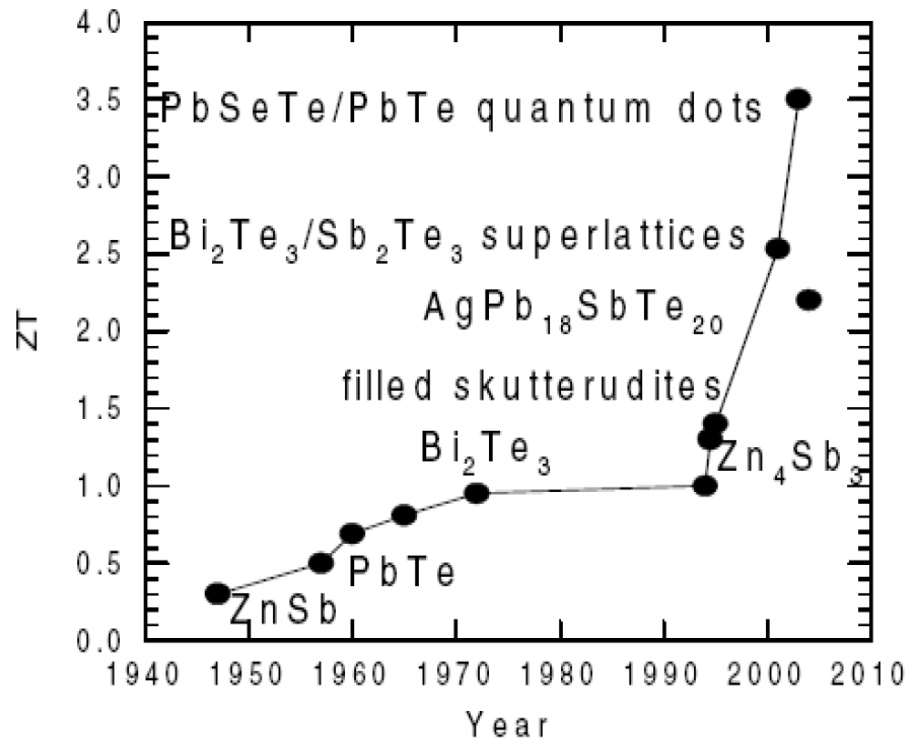


Figure 1-2: ZT of many typical thermoelectric materials as a function of year [33].

A dimensionless number called the figure of merit (ZT) is used to measure the effectiveness of a thermoelectric material.

$$ZT = \frac{\sigma S^2 T}{\kappa_e + \kappa_l} \quad (1.1)$$

In Equation (1.1) above ZT is the figure of merit, σ stands for the electrical conductivity, S stands for the seebeck coefficient, T for temperature in K and κ for the thermal conductivity due to electrons and phonons respectively. The higher the ZT value the more efficient the thermoelectric material. By taking into consideration the maximum refrigeration capacity that can be achieved in a thermocouple that is placed between the plates with two different temperatures (T_1 and T_2), ZT can be derived.

The ratio of the output electric power and the input energy needed to generate the temperature differential is called the thermoelectric efficiency η . The maximum value of efficiency that can be achieved is,

$$\eta_{max} = \frac{\Delta T}{T_h} \left(1 - \frac{1 + \frac{T_c}{T_h}}{\sqrt{1 + ZT} + \frac{T_c}{T_h}} \right) \quad (1.2)$$

Thermoelectric has been talked about for close to 200 years when Thomas Seebeck discovered it in 1821 but ZT remained very low (less than 1) for the most time, until not long ago when they have jumped to the 2-4 range with the introduction of nanostructures. Only now the thermoelectric materials can compete with their mechanical counterparts when it comes to efficiency.

The effect of nanostructures are only beginning to show their own estimated potential. A lot of work needs to be carried out to further increase the efficiency of thermoelectric materials.

1.3 Review of Thermal Management

As technology rapidly progresses on all frontiers; be it power electronics, batteries, personal electronics, computers or all forms of smart technology etc., the main issue that comes up time and time again is the need to extract heat from a small compact region in the body. Here the large scale cooling methods cannot be applied just because of the size constraint being dealt with. Due to exponential growth in power density in electronic chips as shown in figure 1-3, a critical heat dissipation technical problem arises. If this accumulation of heat is not tackled can have a lot of dire consequences, such as affect performance of the appliance, cause failure of the system, reduce lifespan of the item, be a fire hazard etc.

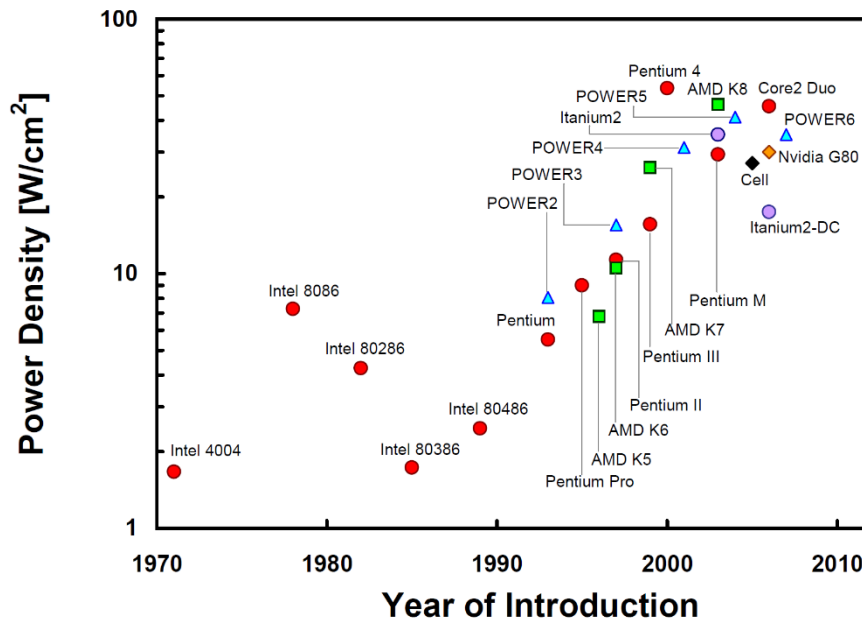


Figure 1-3: Processor power density over time [34].

To address this problem of dissipating heat from the heat-generating electronic, the industry has thus far used cooling by air, cooling by liquid, and phase-change cooling etc. These methods usually involve fins, fans or heat sinks; basically methods where additional

components have to attach to the electronic components. If these tactics are employed then the efficiency of cooling apart from depending on the cooling mechanism itself, they also depend on the thermal contact between the mechanism and heat source. Usually to mitigate the problem of improper contact, a thermal interfacial material (TIM) is applied to help the heat transfer from the heat source to the cooling mechanism. A widely used thermal interfacial material is the thermal grease made out of “silicone oil filled with metal oxides”[7]. The thermal conductivity of the silicone oil is 0.7 W/mK, which is much better as compared to air having 0.026 W/mK at room temperature.

Thermal pads also are a way to increase thermal conductance from the heat source to the cooling mechanism. These are sturdy at room temperature which get soft at temperatures that the electronics operate at. Having discussed all these mechanisms used

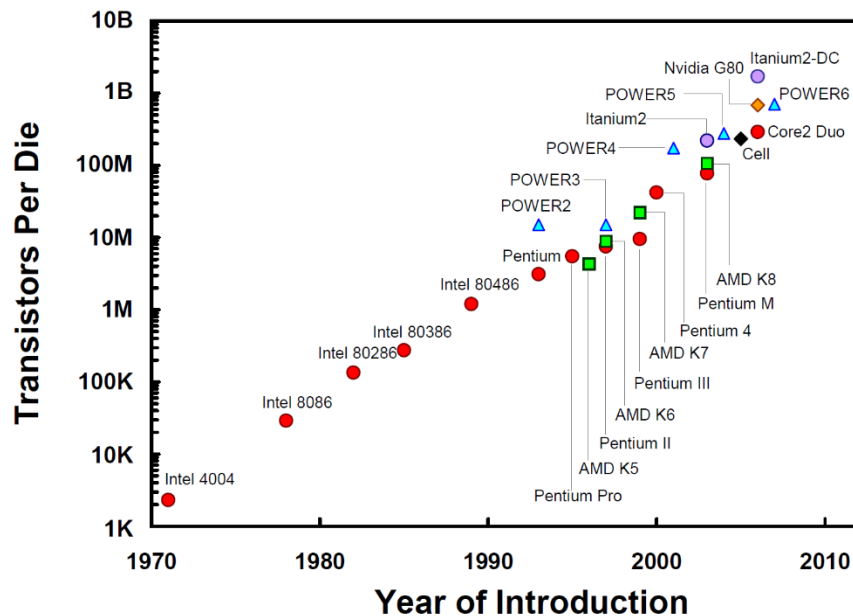


Figure 1-4: Transistors per Die over time [34].

by the industry, these thermal interfacial materials do not dispose heat rapidly enough to

keep the next generation of electronic components cool. To resolve this issue research has been done on carbon nano-tubes in various forms such as aligned CNT arrays and polymer with Carbon Nano Tube, graphene fillers[8][9][10]. Out of this recent research, graphene based thermal interfacial materials have turned out to be extremely immensely promising for the high thermal conductivity and its flexibility letting it conform to other surfaces. [7]

All of the above techniques that have been discussed deal with external features being attached to the target heat source which will eventually have the issue of thermal interfacial resistance. This will reduce their effectiveness in removing the heat from the hot spots. With the power density in today's chips reaching such astronomical levels, there are spots in the chips which reach a power density greater than 100 W/cm^2 which calls for effective cooling techniques directly to the local hotspots. Here it is very interesting to explore the opportunity to use graphene and mesh them with the chips as part of the plane, hence acting as a planar heat dissipater. Graphene would potentially have all the right properties which are being extremely thin hence dissipating heat very effectively and having a high thermal conductivity hence not affecting the performance of the electronic chips.

Now, when the question comes up as in what substrate will be used to integrate the graphene with, SiO_2 substrates would be a standard choice. Graphene devices on SiO_2 are very disordered and show intrinsic properties much lower than graphene itself. Graphene could be suspended above the substrate which leads to considerable improvement in the quality of the device but raises questions about the limitations about the functionality and sturdiness of such a device[6]. There is a need to identify dielectrics that will allow a substrate supported molecular structure and at the same time get to the same quality achieved by the suspended geometry. Boron Nitride comes up as an appealing substrate.

This is due to the fact that Boron Nitride has a lattice constant very similar to graphene, and on top of that it has large optical phonon modes and a large electrical bandgap. Graphene devices on Boron Nitride substrate have carrier inhomogeneities that are much better than devices on SiO₂. The dielectric properties of Boron Nitride compare positively to those of SiO₂ ($\epsilon \approx 3-4$ and $V_{\text{breakdown}} \approx 0.7 \text{ V nm}^{-1}$) with no loss of functionality[11]. Hence, Graphene in combination with Boron Nitride form an excellent combination.

1.4 Phonon Transport

In the sections above we have reviewed thermoelectric effect, thermoelectric materials and basics of thermal management. Heat is mainly carried by phonons and electrons in a solid. Resistance to thermal transport is caused by any inelastic collisions that are faced by these heat carriers. In case of a near perfect bulk semiconductor or insulator, energy is mainly transmitted by the phonons and the conduction is mainly due to phonon-phonon scattering. The reason we will only be focusing on discussing thermal transport by phonons in this document is because: their electronic contribution to the k value is usually many orders smaller for graphene based systems as compared to from lattice contribution. Hence when dealing with a graphene system, dealing with just the phonon transport should be more than enough to get a good understanding of the thermal transport going on within the system.

1.4.1 What is a Phonon?

In semiconductors and insulators, heat is carried primarily by vibrations in the crystal lattice known as phonons. A phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in solids or liquids. Although it is the

quantity of energy that gets transmitted from one end to another, it is designated as a quasi-particle. In the simplest example, let take a one-dimensional chain of atoms connected by springs. We can take the equilibrium separation as d , mass to be m and note down each atom's displacement from its equilibrium position as u_s where s is a character denoting the integer index of the plane. Using Hook's law, we can write down the restoring force as,

$$F_s = -C(u_s - u_{s+1}) - C(u_s - u_{s-1}) \quad (1.3)$$

Which we can write as follows, using the equation of motion for displacements of atoms in the s -plane,

$$m \frac{d^2 u_s}{dt^2} = -C(2u_s - u_{s+1} - u_{s-1}) \quad (1.4)$$

When periodic boundary conditions are applied, we get,

$$u_s(t) = A e^{iksd - i\omega t} \quad (1.5)$$

Where A is the amplitude. The vector k , is related to the vibration frequency as follows,

$$\omega(k) = 2 \sqrt{\frac{C}{m}} \left| \sin\left(\frac{kd}{2}\right) \right| \quad (1.6)$$

The above example shows when we take a solid with only 1 type of atom. When dealing with a solid with more than one atom basis, we usually start with the standard structure with 2 atoms in a single unit cell and phonons propagating in the direction such that successive planes of atoms are all of one type[12]. Solids with more than one atom in its unit cell, exhibit two types of phonons: acoustic phonons and optical phonons.

1.4.2 Acoustic Phonons (Coherent Phonons)

Acoustic Phonons are coherent movements of atoms of the lattice out of their equilibrium positions. If distortion of atoms is in the direction of propagation then, some atoms get closer to each other and some farther away from each other. If the wavelength of a coherent phonon reaches infinity, it corresponds to a simple displacement of the crystal and it doesn't take any energy. Acoustic phonons have a linear relationship between frequency and phonon wavevector for long wavelengths.

1.4.3 Optical Phonons (Incoherent Phonons)

Optical Phonons are incoherent phonons which are out-of-phase movements of the atoms in the lattice, so usually indicated by adjacent atoms moving in opposite directions. They are called optical because in ionic crystals, like sodium chloride, they are excited by infrared radiation.

To indicate acoustic and optical phonons let's take atoms with mass m_1 and mass m_2 that experience displacements from equilibrium u_s and v_s respectively, then writing out the equations of motions gives us[12],

$$m_1 \frac{d^2 u_s}{dt^2} = -C (2u_s - v_s - v_{s-1}) \quad (1.7)$$

$$m_2 \frac{d^2 v_s}{dt^2} = -C (2v_s - u_{s+1} - u_s) \quad (1.8)$$

Sine wave for each atom type will be written as follows,

$$u_s(t) = A e^{iksd - i\omega t} \quad (1.9)$$

$$v_s(t) = B e^{iksd - i\omega t} \quad (1.10)$$

When Equation (1.9) and Equation (1.10) are substituted in Equation (1.8), we get,

$$m_1 m_2 \omega^4 - 2C(m_1 + m_2) \omega^2 + 2C^2(1 - \cos(kd)) = 0 \quad (1.11)$$

Finally, the solution comes down to at ($k=0$)

$$\omega^2(k = 0) = \begin{bmatrix} 2C \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \left(1 - \frac{k^2 d^2}{4} \right) & \text{optic} \\ 0 + \frac{C}{2(m_1 + m_2)} k^2 d^2 & \text{acoustic} \end{bmatrix} \quad (1.12)$$

1.4.4 Superlattice and Its Importance

A superlattice is a periodic structure of layers of two (or more) semiconductor materials. Typically, the thickness of one layer ranges from 1 to 10nm. The superlattice we are aiming to work with during the course of this thesis is of Graphene and Boron Nitride.

The importance of superlattice stems from the fact that if a superlattice is made of two semiconductor materials with different bandgaps, each quantum well meshes together new filtering criteria for charges to flow through the structure. Advances have been made

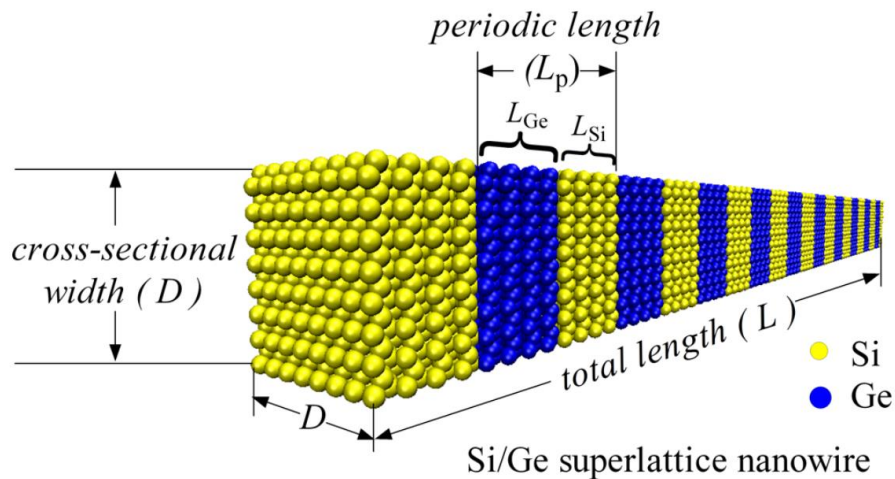


Figure 1-5: Snapshot of a typical Si/Ge superlattice nanowire used as model system in the MD simulations. The total length of the wire (L), cross-sectional width (D), and periodic length ($L_p = L_{Si} + L_{Ge}$) are indicated. Color code: yellow: Si, blue: Ge. [35]

to make ultra-fine semiconductors or which are presently called quantum structures all due to the understanding about superlattices after the proposal in 1970 by Esaki and Tsu[13].

Figure 1-5 gives a good illustration of what a superlattice looks like. This is a computer simulated model of a Si/Ge superlattice showing its periodic nature.

1.5 Objective and Scope of Thesis

Through the introduction, the importance of research on graphene based thermoelectric superlattices has been established. Boron Nitride has been shown to have very interesting properties when made into a superlattice with Graphene. If roughness were to be induced in the interface between graphene and boron nitride, it enhanced the contact area between the two materials but also disrupting smooth passage of phonons. The primary motivation behind this research project is, to understand the effect caused by induced roughness between Graphene and Boron Nitride, in single interface and in a superlattice; on thermal transport in the solid. The way roughness has been simulated is by having teeth along the interface. By varying the frequency of teeth and its size the interface can be simulated to be either rougher or less rough. This project will attempt to understand the effect of parameters such as periodic length, teeth length, and width between each tooth on the thermal conductivity of the superlattice. The objective is to understand the competing effects played by the coherent and incoherent phonons travelling through the superlattice.

CHAPTER 2. METHODOLOGY

2.1 Overview

The motivation, introduction and objectives behind this thesis having been discussed in the previous chapter, this chapter will delve into the methods that were employed to achieve the objectives. The thermal transport within the Graphene-Boron Nitride system has been studied using Molecular Dynamics simulations. This chapter provides basic insight about what molecular dynamics is and its importance. There are multiple methods of thermal conductivity prediction and the one used through this research is called Green-Kubo method which is an Equilibrium Molecular Dynamics method. It is important to understand the physics behind the Green-Kubo method. The procedures followed in terms of simulation setup, generating the molecular structure and determining the boundary conditions have been discussed thoroughly.

Some of the steps taken to modify the molecular structure in the simulation system after initial results were analyzed have been discussed along with the importance of perfectly periodic representation of the superlattice. Finally, to wrap up this chapter, the procedure used to predict the thermal conductivity using the Green-Kubo method has been explained. Understanding of the system and the procedures used play a critical part in analyzing the results and making relevant conclusions.

2.2 Molecular Dynamics

Computer simulations are carried out in the hope of understanding the properties of assemblies of molecules with respect to their structure and how they interact with each other in the microscopic scale. These complement the conventional experimental analysis, usually helping us to find out things that cannot be found out in other ways. The two main categories of simulation technique are molecular dynamics (MD) and Monte Carlo (MC); additionally there are a whole lot of hybrid techniques that combine features from the two techniques[14]. The advantage that MD has over Monte Carlo simulations is that it gives a route to dynamical properties of the system like time-dependent responses to perturbations, rheological properties and spectra. Computer simulations act as a bridge between microscopic length and time scales; and the macroscopic world.

In a Molecular Dynamics simulation, the position and momentum space trajectories of a system of classical particles are predicted using Newton's laws of motion[15]. The only inputs required are an atomic structure and an appropriate inter-atomic potential. Using the positions and momenta, it is possible to investigate the thermal transport at an atomic level. Molecular Dynamics simulations have peaked the interest of scientists in the past ten years due to its ability to study thermal transport going on in solids addressing the need to study thermal management in semi-conductors devices.

The flowchart below gives a simplified explanation of the steps involved in the calculations for conducting molecular dynamics.

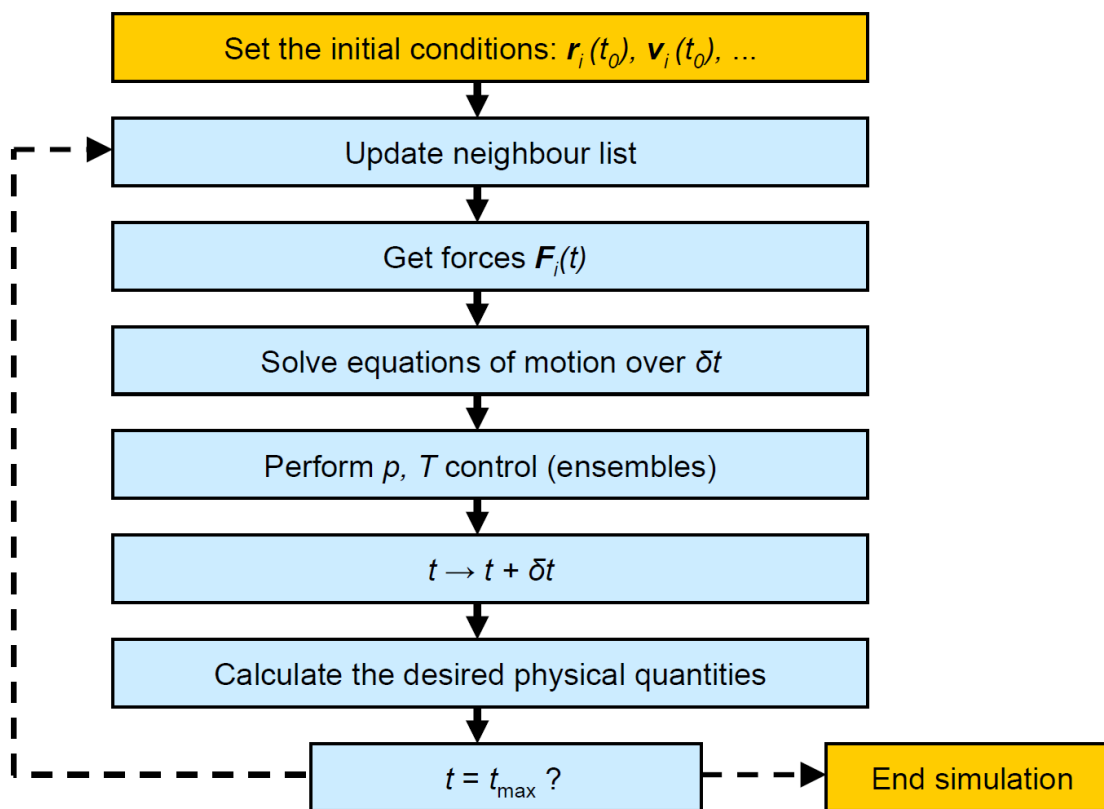


Figure 2-1: Flowchart showing the steps of calculations involved in molecular dynamics simulation.

Once the initial conditions are set, which is usually a random initial velocity given to the a few atoms, then using the forces between adjacent atoms, the position and velocity of the adjacent atoms are updated. Depending on the molecular dynamics simulation type the temperature or pressure is controlled. The time step is increased and the process is repeated until the total time of the simulation has completed.

The forces are derived from the pair potential used which in this case is Tersoff potential between Carbon atoms and Boron Nitride atoms.

$$F = -\nabla V(r) \quad (2.1)$$

$$F_i = \sum_{j \neq i} F_{ij} \quad (2.2)$$

Equations of motion are solved with a finite difference algorithm,

$$\vec{r}_i(t + \delta t) = \vec{r}_i(t) + \vec{v}_i(t)\delta t + \frac{1}{2}\vec{a}_i(t)\delta t^2 \quad (2.3)$$

Although there are many advantages to MD simulations, they do have some shortcomings. Firstly, since all the calculations are based on classical Newtonian physics, quantum effects are not taken into account. Due to this, phonons are considered as classical particles as opposed to being considered as Bosons. At very low temperatures this issue causes inconsistencies in the results [16].

Availability of classical potentials comes in as the second shortcoming. Developing classical potentials can be tedious and ensuring its accuracy can be tough. Hence, classical potentials for inorganic materials are usually difficult to find. This shortcoming can be accounted for “by using ab initio or tight-binding MD which can bypass the need for classical potentials” [7]. As mentioned earlier in this thesis, Tersoff potential has been used for Carbon and Boron Nitride atoms which was provided to me by my colleagues in the research group.

2.2.1 Green-Kubo Method

Two main techniques have been developed to predict the thermal conductivity of a dielectric material using Molecular Dynamics (MD) simulations. The first technique is a direct application of the Fourier Law which is a steady state, non-equilibrium approach

called the Direct Method or Non-Equilibrium Molecular Dynamics (NEMD) method. The second technique is called the Green-Kubo method which is an equilibrium molecular dynamics method.

Although in theory the two techniques would produce the same results, the advantage of Green-Kubo is that it would need a much smaller size of system as compared to the NEMD method. As mentioned earlier, in this document we will concentrate on using the Green-Kubo method.

Thermal conductivity using Green-Kubo method is determined based on the time it takes for the heat current fluctuations in the solid to dissipate. Several research groups have successfully used the Green-Kubo approach to predict the thermal conductivity of multitude of materials like silicon, graphene, Bi₂Te₃ and argon among many others [17][18][19][20]. Considering Green-Kubo's linear response formulation [21], the equation for the lattice thermal conductivity for an anisotropic system is as follows [22]:

$$\kappa_{l,\alpha} = \frac{1}{k_B V T^2} \int_0^\infty \langle S_\alpha(t) \cdot S_\alpha(0) \rangle dt, \alpha = x, y, z \quad (2.4)$$

In the above Equation (2.4), V is the volume of the simulation domain, $\langle S_\alpha(t) \cdot S_\alpha(0) \rangle$ is the heat current auto-correlation (HCACF) in a certain direction where $\langle \dots \rangle$ refers to the ensemble average, T refers to the temperature and t referring to time-step. In MD, the time dependent heat current vector is extracted from the time dependent position and energy of each atom:

$$\mathbf{S} = \frac{d}{dt} \sum_j \mathbf{r}_j E_j = \frac{d}{dt} \sum_j \mathbf{r}_j (E_{k,j} + E_{p,j}), \quad (2.5)$$

In Equation (2.5) \mathbf{r}_j refers to the position of the atom j , $E_{p,j}$ and $E_{k,j}$ referring to the potential and kinetic energy of the atom j . To obtain the thermal conductivity value, the HCACF should be integrated over time.

In some materials where the fluctuations are long lived, the autocorrelation function dies out slowly. This means that it requires a very large simulation domain in the direction of the temperature gradient to accurately predict the thermal conductivity and eliminate the size effect. On the other hand in amorphous materials we don't encounter this issue as the thermal fluctuations quickly dampen as the mean free path of the phonons are comparatively small [23].

2.3 Simulation Setup

Prior to conducting the molecular dynamics simulation the setup needs a few key components to be arranged for. These include: the setting up of molecular structure which is in the form of a text file consisting of spatial coordinates of all the atoms in the system; the Tersoff potential file which consists of the potential between atoms of Carbon and Boron Nitride; setting up of boundary conditions and finally the job file that will execute the simulation with the help of the computing cluster.

2.3.1 Molecular Structure

Since, the aim is to study the effect of roughness at the interface between Graphene and Boron Nitride, there would be two broad types of system that would be set up. One system would be with smooth interface (no roughness induced at the interface) and the

other type of system would be with the roughness induced. Now, before we go into how we will create the lattice structure coordinate file, it is important to discuss how the roughness will be simulated at the interface.

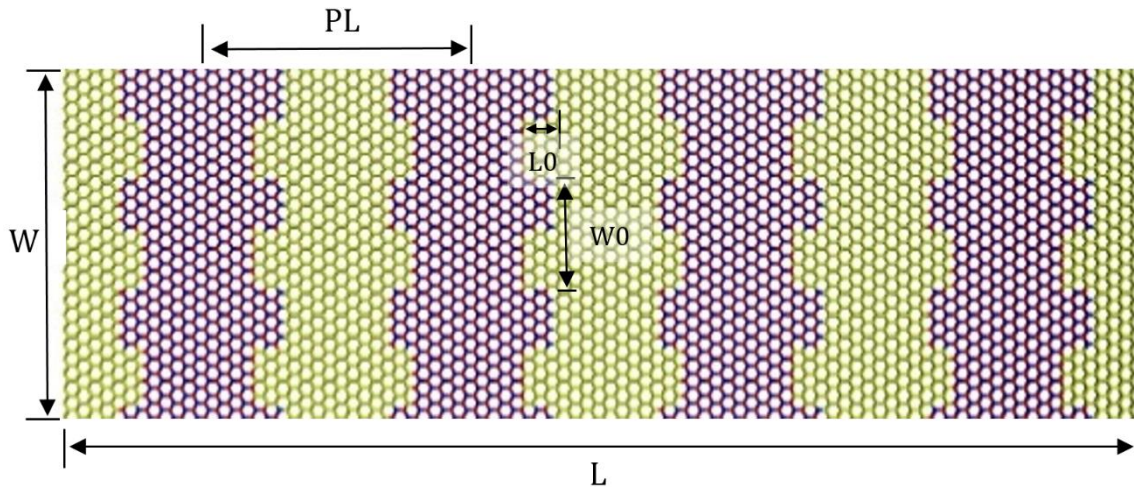


Figure 2-2: System with rough interface visualizing the different terms used.

In the figure 2-2 above, PL stands for Periodic Length of the superlattice, L stands for the length of the system, W stands for the width of the system, L0 stands for the length of the teeth and W0 stands for the separation between successive teeth.

The roughness that is to be simulated at the interface between Graphene and Boron nitride will be in the form of teeth. Now for all the simulations that have been done on rough interfacial systems, it is modeled such that the teeth are equidistant from one another and the width of teeth is half of W0 shown in figure 2-2 above. By controlling the length L0 of the teeth and the width W0 of the teeth at the interface we can simulate the controlled roughness effect at the interface. The larger the value for W0 is smoother the interface, the smaller the value for W0 the rougher the interface. Similarly, the higher the value of L0 the rougher is the interface considered, and closer the value of L0 to zero the smoother it

is considered. For most cases the width W of the system has been arbitrarily set to be half of the length L of the system. The length however has been chosen according to the parameter that is being evaluated or with relative to the periodic length PL of the system.

To generate the molecular structure in the form of a text file having the coordinates for all the atoms, a code in MATLAB was written. This code would act as the blueprint to generate the lattice structure irrespective of the parameters. The code was written in such a way that it would be universal for all the cases studied in this thesis. As mentioned above L_0 refers to the length of the teeth and to produce the lattice structure for smooth interface all that had to be done was set L_0 to be 0 and it should generate a smooth interface superlattice.

The logic that was used to write the code was that, the length of the system would be divided by the periodic length to give number of periods in the x-direction, and similarly the width of the system would be divided by W_0 to give the number of teeth pairs in the y-direction. Number of unit cells were then calculated in the x direction by dividing the length of the system with length of the unit cell and rounding down the number. The length of the unit cell can be calculated by taking the average of the lattice constant of carbon and boron nitride. The length in the x direction is then reset to the value that one gets when multiplying the number of unit cells to the length of the unit cell. This is done so the system is the exact length of an integer multiple of atoms placed side by side. The coordinates are then started from [0 0 0] and written into a text file one by one updating every time one goes onto the next atom.

When the MATLAB file is run, it generates two output files. The first file is a text file with coordinates of each atom in the system and the second is a .xyz file that can be

used to visualize the system using the VMD software. The figure 2-3(a) and (b) show the entire system with the smooth interface and a close up of the atoms.

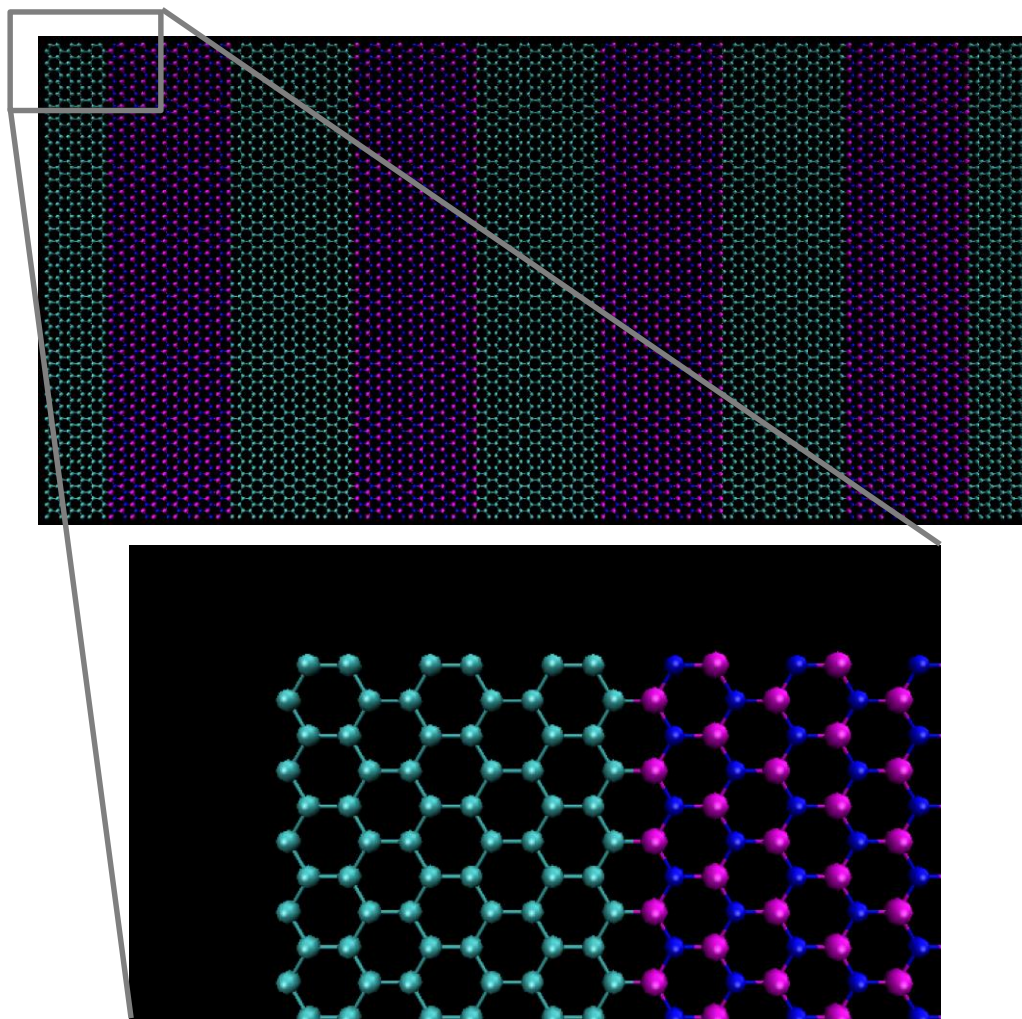


Figure 2-3: (a) Visualization of entire system using VMD, (b) a close-up look at the carbon atoms, the interface and the boron nitride atom (C – Cyan, B – Magenta, N – Blue).

2.3.2 Boundary Conditions

Periodic boundary conditions are applied in x-direction and y-direction which refer to the length and the width of the system which means the system goes on for infinite length

and infinite width. What this means for the atoms on the boundary of the set system is that the particles interact across the boundary, and they can exit one end of the box and re-enter the other end. A periodic dimension can change in size due to constant pressure boundary conditions or box deformation.

The boundary condition in the z-direction (depth) is set as non-periodic and shrink wrapped. This means that the particles do not interact across the boundary and do not move from one side of the box to the other. The position of the face is set so as to encompass the atoms in that dimension (shrink wrapping), no matter how far they move.

2.3.3 Tersoff Potential

Now that the lattice structure and boundary conditions have been explained, the potentials between carbon atoms and boron nitride atoms needed for the molecular dynamics simulations can be calculated using the Tersoff Potentials. The group of potentials developed by Tersoff [24] in 1988, based on the concept of bond order, means that the bond strength of two atoms is not constant, but depends on the local environment. This idea is to use the coordination of an atom as the variable controlling the energy. However, in semiconductors, instead of the focus being on the atoms is on the bonds: that is where the electronic charge is sitting in covalent bonds.

The Tersoff potential is a three-body potential function which specifically includes an angular contribution of the force. The potential; is widely used at preent in various applications for silicon, carbon, germanium etc.

It is written as following:

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (2.6)$$

$$V_{ij} = f_C(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \quad (2.7)$$

Where the potential energy is decomposed into a site energy E_i and a bonding energy V_{ij} , r_{ij} is a distance between the atoms i and j . f_A and f_R are the attractive and repulsive pair potential respectively, and f_C is a smooth cutoff function.

$$f_R(r) = A e^{-\lambda_1 r} \quad (2.8)$$

$$f_A(r) = -B e^{-\lambda_2 r} \quad (2.9)$$

$$f_C(r) = \begin{cases} 1, & r < R - D \\ \frac{1}{2} - \frac{1}{2} \sin\left(\frac{\pi(r-R)}{D}\right), & R - D < r < R + D \\ 0, & r > R + D \end{cases} \quad (2.10)$$

R and D are chosen so as to include the first neighbor shell only for selected structure (for carbon $R = 1.8\text{\AA}$). The f_C function decreases from 1 to 0 in the range $R - D < r < R + D$.

The primary feature of this potential is the presence of the b_{ij} term. What this term means is that the strength of each bond depends on the local environment and is lowered when the number of neighbors is relatively high [25]. Tersoff potential is not a pair potential as b_{ij} is not constant. The basic idea is that a bond ij is weakened by the presence of other bonds such as for ex. ik involving atom i . The amount of weakening is determined by where these other bonds are located. Angular terms are necessary to build a realistic model [26].

2.4 Initial Results and Periodic Nature of the Structure

Although this section is named as initial results, it deals more with an important lesson learnt from an initial set of results which caused a rethink on the process with which the lattice structure was generated. One of the trends that were to be studied and on the agenda was the variation of thermal conductivity with respect to varying periodic length keeping the length and width of the system, teeth length and teeth width constant.

As the results came in something seemed out of place. As shown in figure 2-4 the thermal conductivity values for cases with periodic length from 10Å to 40Å seem

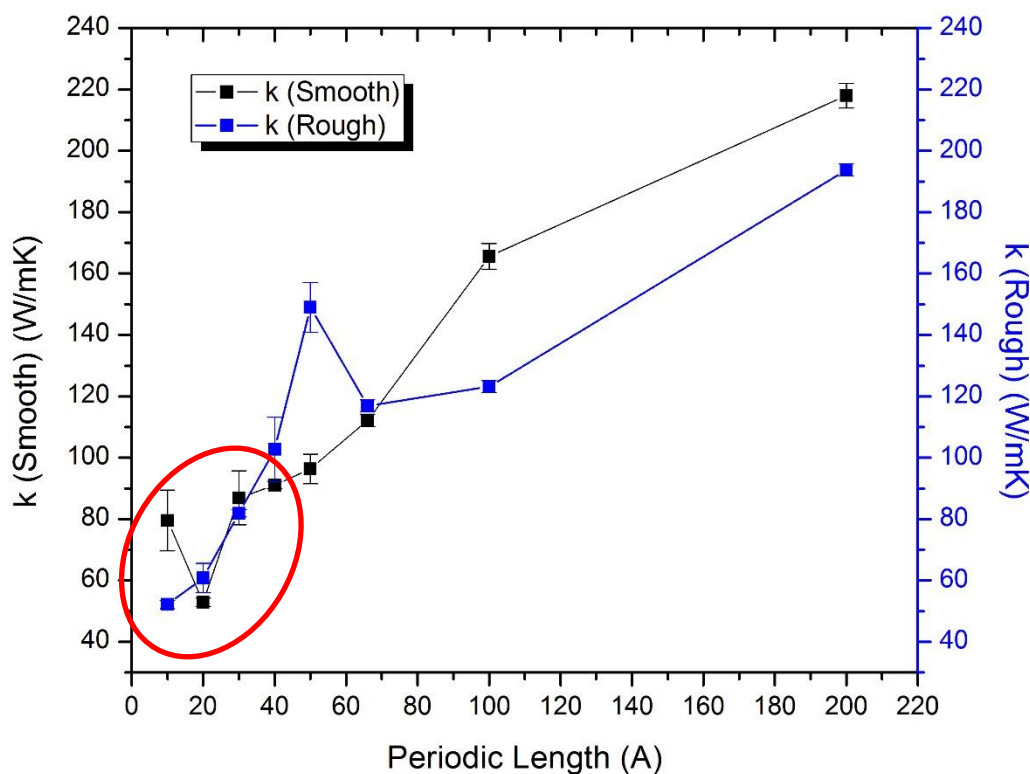


Figure 2-4: Initial results: Studying variation in Thermal Conductivity in smooth interface and rough interface systems with varying periodic lengths keeping system length, width and teeth length and width constant. Red circle points to the unexpectedly low k values.

unexpectedly low i.e below 100 W/mK when the expected values should come in around 150 W/mK. The values for the higher periodic lengths (50Å - 200Å) are around expected values.

To understand the issue, the molecular structure was visualized for the lower periodic lengths. The structure as shown in figure 2-5 showed that due to the periodic lengths being small and only a few multiples higher than the lattice constant of carbon and boron nitride, were causing the atomic placement to be inconsistent from period to period.

This means that the method in which the molecular structure was being generated has to be modified. Although at higher periodic lengths (50Å - 200Å) the structure is perfectly periodic but as the periodic lengths decrease even small variations cause the loss of the periodic nature of the super-lattice and when the PL comes down to 10Å the amount of variation almost completely takes the periodic nature out of the system hence resulting in very low thermal conductivity due to very high levels of phonon scattering at the

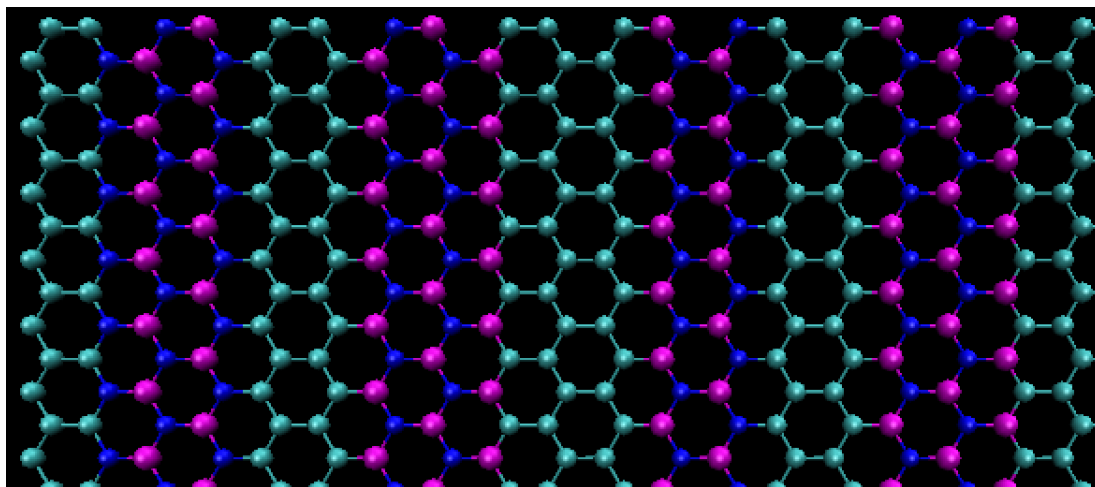


Figure 2-5: Visualization of the molecular structure produced for the case with PL = 10Å. Due to the periodic length being very small the structure doesn't seem periodic at all (C – Cyan, B – Magenta, N – Blue).

interfaces. This level of randomness in the molecules almost compares to interfacial mixing which causes disruptions of superlattice phonons as shown by Huberman *et al* causing the thermal conductivity to drop [27]. Hence, the MATLAB code used to generate the lattice structure was modified.

2.4.1 Revised MATLAB Code to Generate Molecular Structure

The goal was to ensure perfect periodicity of the atoms. For this, the length of the system was divided by the periodic length for that case and round the number to get the number of periods. The new length would be the perfect integral of unit cells. All of these steps are still the same as was done before. What was changed in the revised code was that once the number of unit cells needed for one period was calculated, the period was constructed and then for every period after the first period was perfectly replicated. The first atom in the first period would be the first atom in the second period. Due to this, at very small periodic lengths we ended up with situations such that the graphene band would

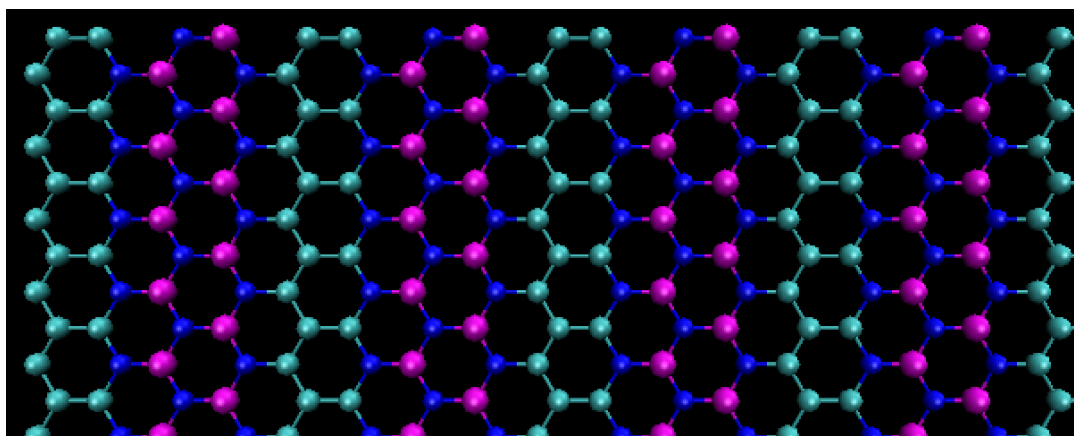


Figure 2-6: Revised visualization of the molecular structure produced for the case with $PL = 10\text{\AA}$ using the revised MATLAB code. The lattice structure is now perfectly periodic in nature (C – Cyan, B – Magenta, N – Blue).

be slightly wider or narrower than the boron nitride band but more importantly the superlattice was perfectly periodic. Figure 2-6 shows the exact same case as in figure 2-5 with $PL = 10\text{\AA}$ but constructed with the revised MATLAB code.

2.4.2 Importance of Periodicity

The importance of having a perfectly periodic lattice structure has been underscored by the need for the above revision in the MATLAB code. The periodicity is the main aspect of a superlattice. There has been research conducted studying the effects of interfacial mixing, which means irregularities at the interface where atoms of one element swap places with atoms of another element. This causes heavy disruptions of superlattice phonons decrease thermal conductance at the interface by a considerable amount [27]. Lacking a perfectly periodic structure does disrupt the phonons but not to the extent that interfacial mixing does as one still has a consistently uniform interface even though the atoms at the interface are not consistent through different periods. It will be evident from the results discussed in the next chapter the influence that perfect periodicity has on the thermal conductivity. The perfectly periodic structure produces considerably higher thermal conductivity values and are consistent with expected values for a Graphene-Boron Nitride superlattice.

2.5 Using Green Kubo Method to Predict Thermal Conductivity

Thermal conductivity for the Graphene-Boron Nitride super-lattice is simulated with the use of equilibrium molecular dynamics (Green-Kubo theory) [21]. The heat current vector for a pair potential can be written as follows:

$$\mathbf{S} = \frac{1}{2} \sum_{i,j} (\mathbf{F}_{ij} \cdot \mathbf{v}_i) \mathbf{r}_{ij,o} \quad (2.11)$$

Where \mathbf{v}_i refers to the atom i velocity and \mathbf{F}_{ij} refers to the force between the two atoms (i & j). As the atoms in a solid vibrate in a local vicinity, the heat current $\mathbf{S}(t)$ can be written in terms of the distance between the two atoms denoted by $\mathbf{r}_{ij,o}$. The thermal conductivity is deduced using the heat current auto-correlation function [28].

$$\kappa_{l,\alpha} = \frac{1}{k_B V T^2} \int_0^\infty \langle S_\alpha(t) \cdot S_\alpha(0) \rangle dt, \quad (2.12)$$

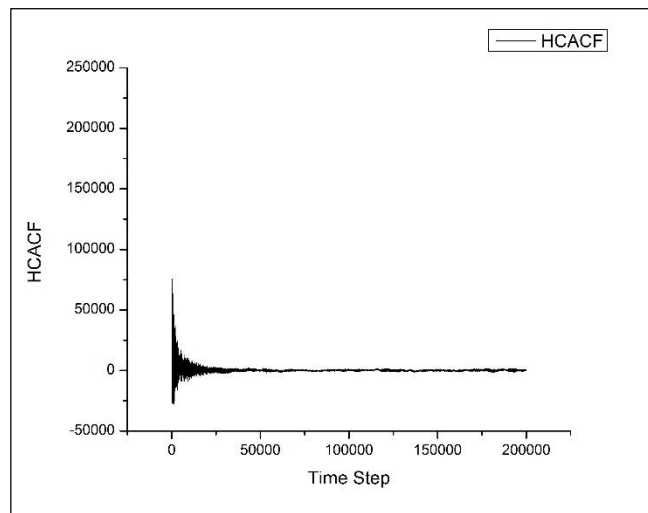


Figure 2-7: HCACF plotted against time steps.

In Equation (2.12), V is the volume of the domain, T being the temperature, k_B is the boltzmann constant and $\langle S_\alpha(t).S_\alpha(0) \rangle$ is the heat current auto-correlation function (HCACF).

The simulation is first run in NPT 5000000 time steps where each time step is 0.5 fs ($5 \times 10^{-16} s$) that means the NPT runs for about 2.5 ns. We then change to NVE for the whole system. The values for HCACF are obtained after processing of data obtained from the last full cycle of time steps as shown in figure 2-8 below. The direct integral of Heat

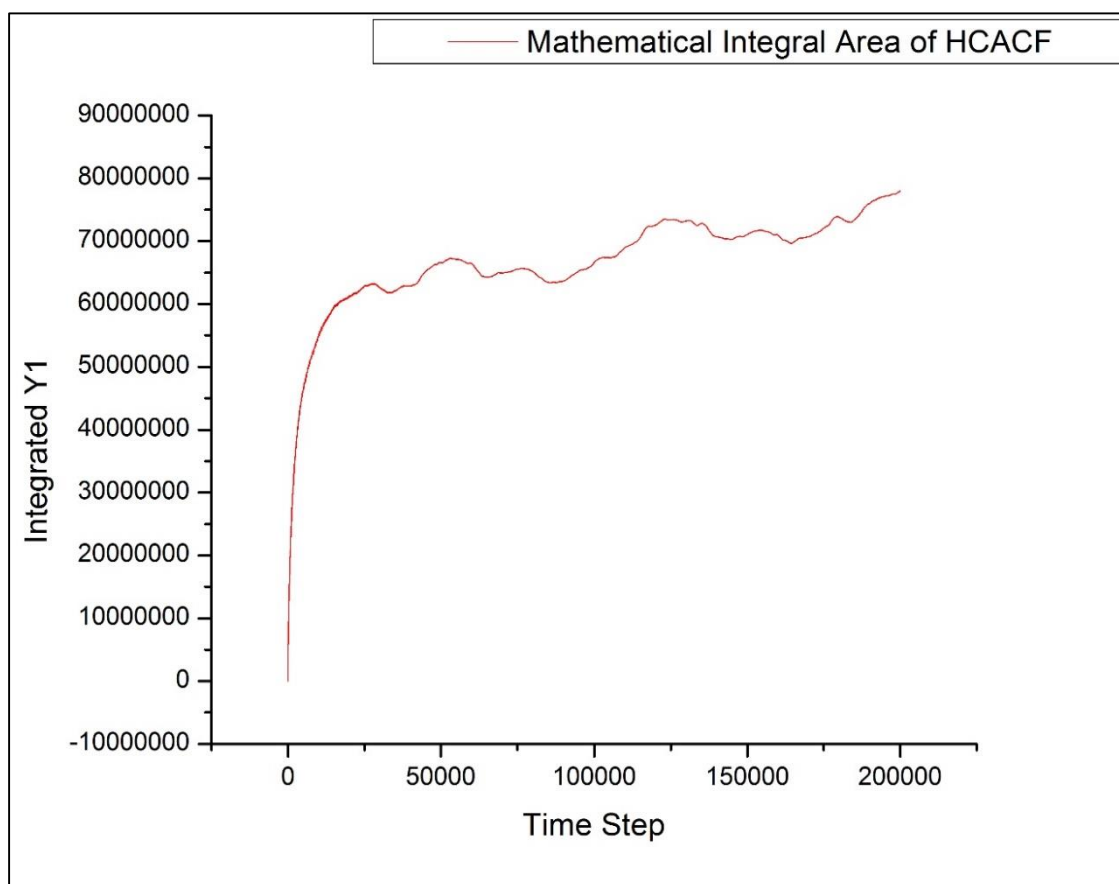


Figure 2-8: Integrated values of the Heat Current Auto-Correlation Function plotted against Time steps. As explained, the plot seems to plateau at about 25000 time steps and later diverge.

Current Auto-Correlation Function plateaus initially then diverges later on. This is a very common feature of Molecular Dynamics simulations [29].

The value at which this integral curve converges is plugged into Equation (2.12) where all the constants are then plugged in such as Boltzman constant k_B , set Temperature T and Volume of the simulation domain. This is how the thermal conductivity is calculated using the Green Kubo Method of Equilibrium Molecular Dynamics.

CHAPTER 3. RESULTS AND DISCUSSION

3.1 Introduction

The aim of this research is to gain understanding of how interfacial roughness impacts the thermal conductivity of Graphene-Boron Nitride superlattice. We will aim to simulate cases to understand the impact of varying periodic length, varying the roughness in the form of teeth size and spacing of the teeth at the interface, and understanding effect of a roughness in a single interface system. At the end of this chapter, apart from discussing the results from this research, results that have been recently researched by the scientific community will be discussed.

As mentioned earlier, the roughness in the interface has been simulated in the form of teeth. The length of the teeth and the width/separation between consecutive teeth can be controlled hence controlling roughness per say. The more the length of the tooth the rougher it is considered and vice versa. Similarly is the teeth are far apart it is considered to be smoother as compared to having teeth extremely close to each other.

3.2 Effect of Non-Periodicity of Superlattice

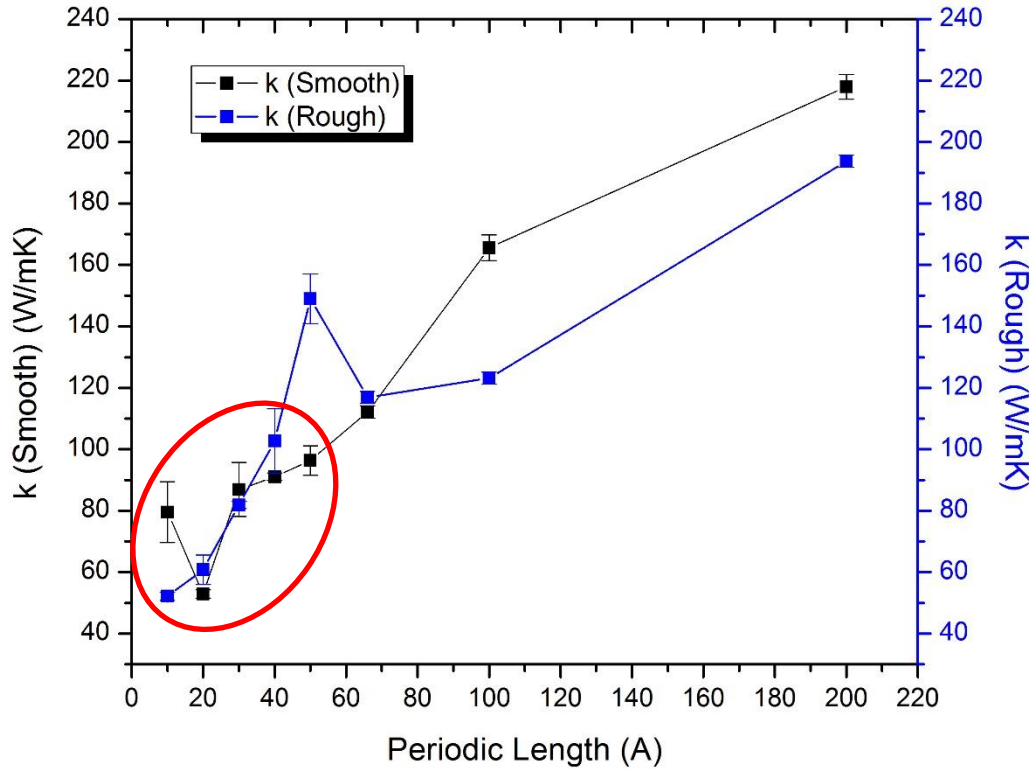


Figure 3-1: Initial results: Studying variation in Thermal Conductivity in smooth interface and rough interface systems with varying periodic lengths keeping system length, width and teeth length and width constant. Red circle points to the unexpectedly low k values.

Although we discussed about these initial results in the previous chapter, it is still useful to discuss what we can learn from those results which were unintended but at the same time very informative. The parameters that were kept constant for this setup were the length of the system which was maintained at $L = 200\text{\AA}$ for all the cases except when $PL = 100\text{\AA}$ and $PL = 200\text{\AA}$ where the system had to be longer. The tooth length was set at $L_0 = 2.5\text{\AA}$ and the width or separation between consecutive teeth $W_0 = 20\text{\AA}$.

The thermal conductivity for the different systems were all expected to lie in the range of 125W/mK to 250W/mK but as we see in figure 2-4 cases with PL less than 50 Å it was not the case. Almost all the cases with low periodic length returned extremely low thermal conductivity values.

Although the reason behind this is understood and rectified for all cases that came afterward, it is interesting to see the effects of disrupting the periodicity of a superlattice by as little as one extra layer of certain atoms or one less layer of certain atoms. In the scientific paper written by Huberman et al, they have discussed the effects of interfacial mixing and they have showed how this mixing is extremely disruptive to medium frequency phonons which dominate the in-plane thermal transport resulting in under prediction of thermal conductivity [27]. The atomic structure created due to small periodic lengths aren't as disruptive as interfacial mixing, but we get the idea about how it affects the thermal conductivity prediction.

The thermal conductivity prediction for PL = 50 Å and higher are consistent with the other cases and expected results.

3.3 Effects of Periodic Length on Thermal Conductivity Prediction of Graphene-Boron Nitride.

In this case study we take four cases, each with its mini cases. The graph that we would be interested to generate will have these four cases in comparison to each other. The first case has periodic length set at PL = 100Å and Teeth length L0 = 10Å, the second case has periodic length PL = 100 Å and Teeth length L0 = 2.5 Å, the third case has periodic length PL = 200Å and Teeth Length L0 = 10 Å and finally the fourth case has periodic

length $PL = 50 \text{ \AA}$ and Teeth length $L0 = 2.5 \text{ \AA}$. The four cases were chosen to get an idea of the trend due to two factors, primarily periodic lengths 50 \AA , 100 \AA and 200 \AA and Teeth Lengths 2.5 \AA and 10 \AA .

The aim of this case was to find out how roughness affects the thermal conductivity of the system. The aim was to check if in any of the cases induced roughness was able to actually increase the thermal conductivity of the system where our datum was the thermal

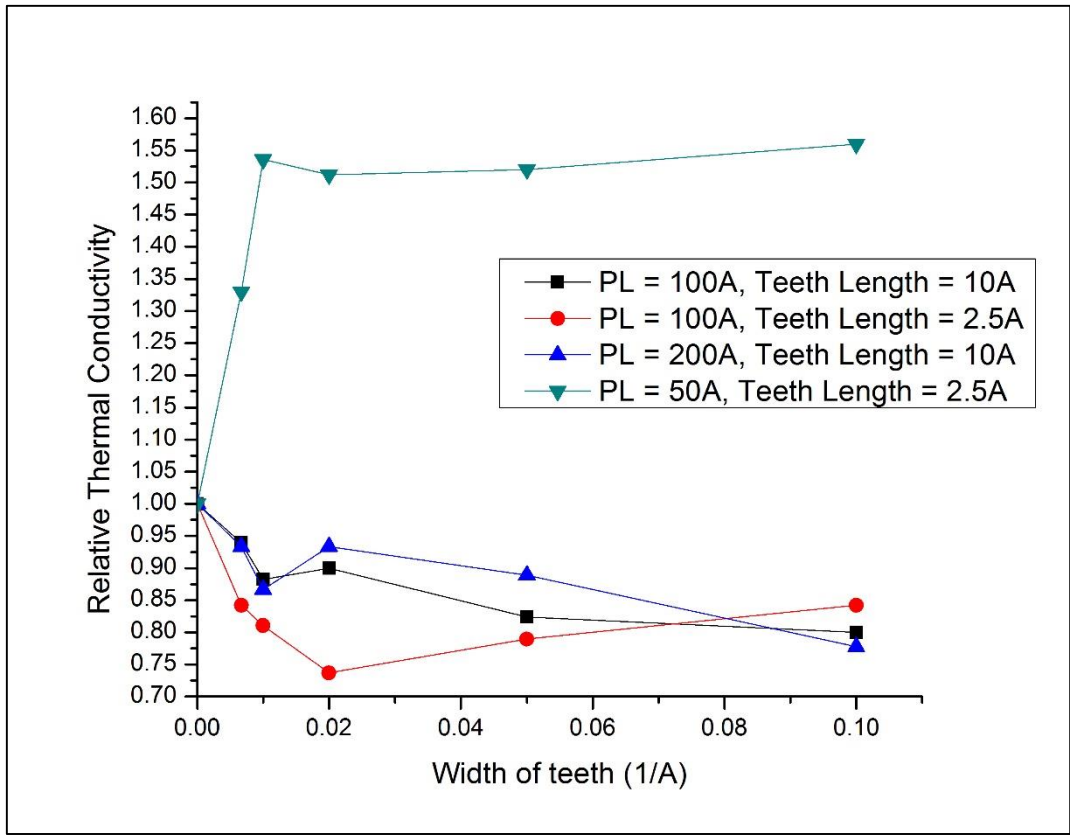


Figure 3-2: Plot of various cases with different periodic length with varying width of teeth (separation between teeth). The different thermal conductivity values are plotted relative to the value of the smooth condition in their respective cases.

conductivity obtained from the smooth case (no teeth). Hence, in the figure 3-2 above, all the thermal conductivity values are relative to the value for the smooth case set in their

respective parameters. This will show us the trend of the thermal conductivity due to induced roughness depending on periodic length.

From the figure 3-2 above we see that for the case with periodic length $PL = 50\text{\AA}$ and teeth length $L_0 = 2.5\text{\AA}$ the thermal conductivity values for the rough cases are actually higher than what it is for the smooth condition without teeth at the interface. This means in this condition the roughness is actually enhancing the thermal transport capacity of this system.

Since the result for the case is distinctly separate from the other cases, the results were verified a few more times to be sure and every way that was simulated confirmed the results shown in figure 3-2. The physics behind this phenomenon is due to coherent and incoherent phonons. Now, coherent phonons are phonons that have a wavelength greater than the periodic length of the superlattice while incoherent phonons have wavelengths less than the periodic length of the superlattices. In common man's terms incoherent phonons 'see' the interface and scatter at the interface. When the periodic length is small the incoherent phonons do scatter at the interface but bulk of the energy is transported by the coherent phonons hence this doesn't affect the thermal conductivity to a great extent. On the other extreme when the periodic length is extremely large, the coherent phonons which need to have a wavelength larger than the periodic length carry little to no energy at all due to its very large wavelength and almost all of the energy is transported by the incoherent phonons. Since the periodic lengths are very large in this case, the incoherent phonon scattering at the interface does not affect the thermal conductivity to a huge extent. Having said this, there lies a region where the periodic length is about the same size as the wavelength of a large number of phonons. As the period of superlattice increases to a

critical value near 5 nm the lattice thermal conductivity drops sharply to a minimum, and beyond that it smoothly increases with the period. Ertekin et al have shown that the minimum in the thermal conductivity arises from a competition between lattice dispersion and anharmonic effects such as interface scattering [30]. They have also shown that this 5nm critical period is irrespective of the length of the system and is dependent on the material properties which also makes sense and is supported by the results that we have gotten.

The above explanation gives the reason as to why the smooth interface has a sudden dip in thermal conductivity but the reason the thermal conductivity is actually increasing for the cases with teeth in the interface are due to a couple of reasons. One could be due to increased surface area at the rough interface. Second could be because of angled bonds at the rough interface between Carbon and either Boron or Nitride. It has been shown that angled bands transmit thermal energy much more effectively than perpendicular atomic bonds.

3.4 Relation of L_0/W_0 or h/w of Teeth for Near Single Interface Systems (Few Interfaces)

During one of the simulation studies of a system with $PL = 200\text{\AA}$ the thermal conductivity values for the smooth case was coming to be lower than the case with teeth length 2.5\AA and 10\AA . This seemed strange because according to size effect: when the length of the system becomes larger the thermal conductivity from the smooth case becomes higher than the k value from the cases with teeth / induced roughness. The length

of the system was 400\AA . Having a periodic length of 200\AA meant that there were only 2 periods in the systems. This meant the interfaces were quite far away from one another.

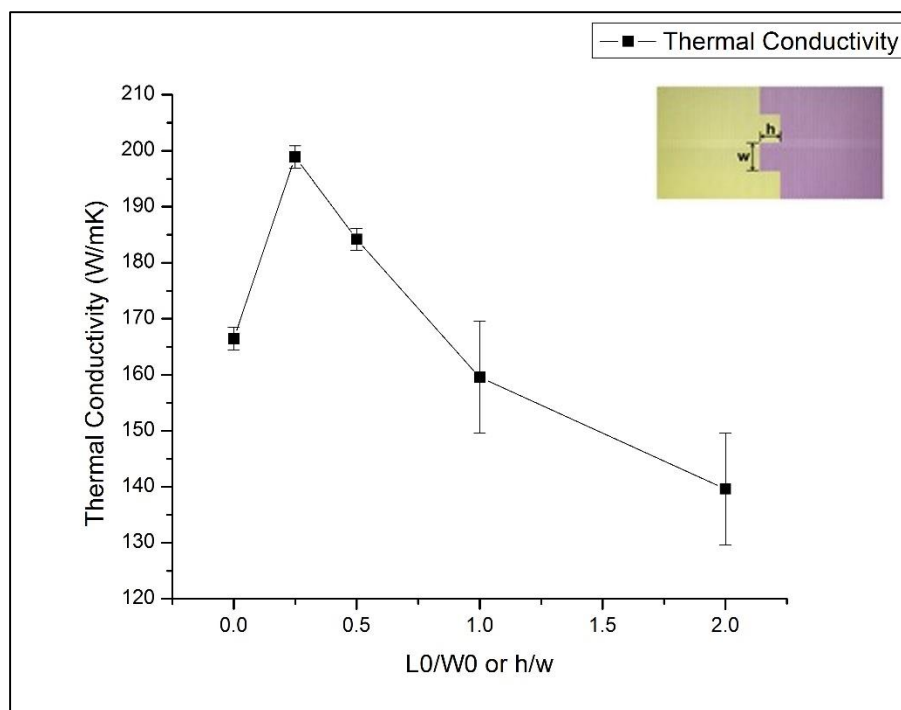


Figure 3-3: Relation thermal conductivity w.r.t h/w or $L0/W0$ in a case symbolic of single interface system.

This is very similar to having a single interface and calculating the effect of teeth in the interface on the thermal conductivity. The peak of 198.91 W/mK is reached in the case of $L0$ being 2.5\AA and $W0$ being 20\AA . Since $W0$ refers to the distance between two consecutive teeth, it would be equal to $2*w$ as shown in the figure 3-3. Hence the highest point of 198.91 W/mK is reached at a ratio of 0.25. Comparing the above figure 3-3 showing results from this research with a figure 3-4 worked on by my colleague Zuyuan Wang from the same research group but using NEMD on a truly single layer setup:

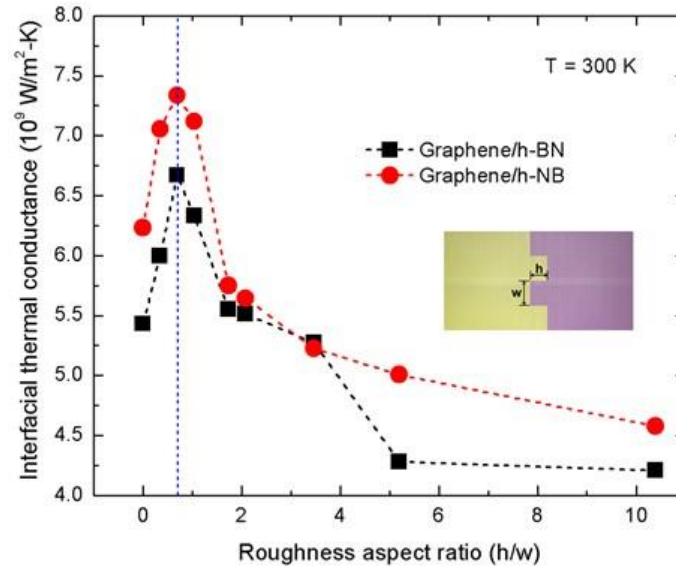


Figure 3-4: Effect of teeth on thermal conductivity of a Single Interface. Figure by Zuyuan Wang.

As you can see that the trend of the curve is exactly the same but the ratio at which the peak is reached in this figure 3-4 is approximately 0.8~1.0 whereas the ratio at which the peak was reached in figure 3-3 according to my results is 0.25. This might be due to the fact that our case is not strictly a single interface, having 3 to 4 interfaces to help the conductance.

3.5 Effect of Interfacial Roughness on Thermal Conductivity of System with Respect to the Length of the Teeth and Periodic Length.

In section 3.3 of this chapter, we discuss the importance of 5nm as the periodic length and how it's the critical period where a big chunk of phonons have their wavelengths and hence causes a drop in thermal conductivity. Now in that section we had simulated using

$PL = 50\text{\AA}$ and teeth length $L_0 = 2.5\text{\AA}$. Does that mean however rough the interface is the thermal conductivity will be greater than the one for the smooth interface case? To find out how the system behaves under different teeth length, the cases simulated were such that the width between consecutive teeth were kept constant at $W_0 = 20\text{\AA}$, the length of the system constant at 200\AA for all cases except for $PL = 100\text{\AA}$ and $PL = 200\text{\AA}$ for which the system length of 400\AA has been chosen. The cases have the following $PL = 20\text{\AA}$, 30\AA , 40\AA , 50\AA , 66\AA , 100\AA , and 200\AA . The conditions are similar to the ones shown in the initial results setup where the irregular periodicity was encountered. For this time, the revised MATLAB code was used to generate the coordinate files which will form the perfectly periodic system.

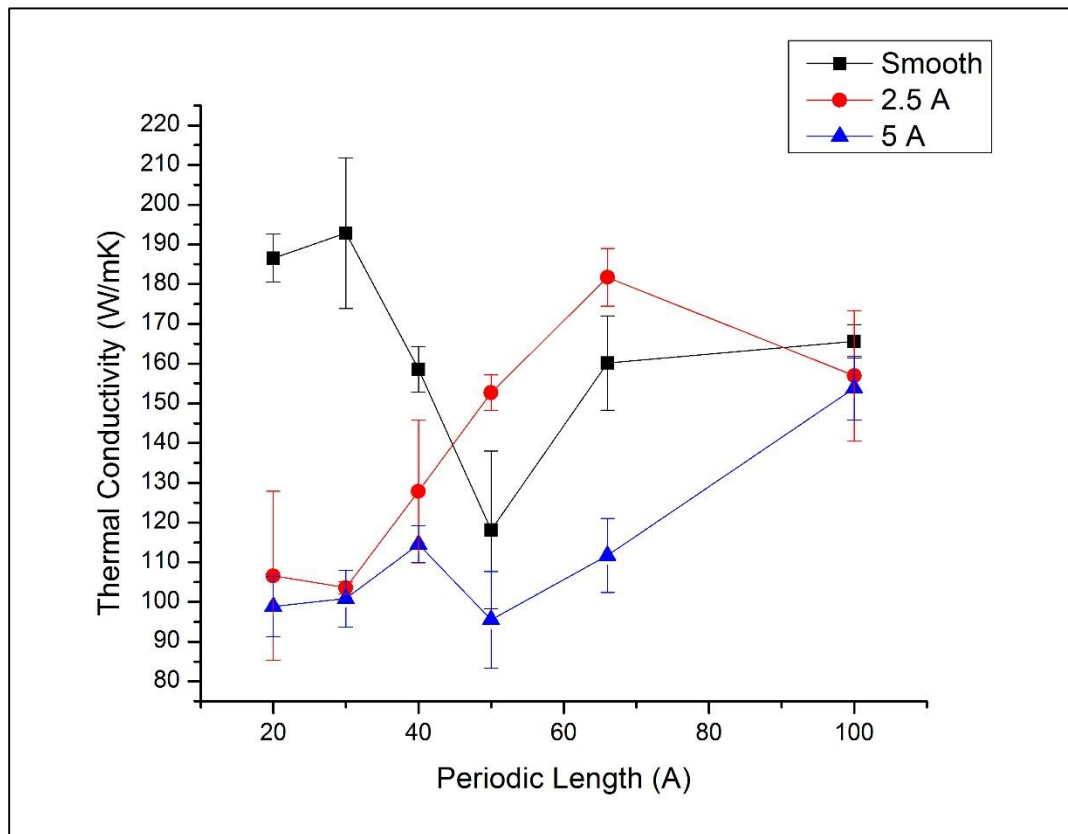


Figure 3-5: Effect of interfacial roughness on thermal conductivity of system with respect to the length of the teeth and periodic length.

In figure 3-5 above the graph in black refers to the thermal conductivity of the system with smooth interfaces, the blue graph refers to the thermal conductivity values of the system with teeth 5\AA in length and the red graph refers to the thermal conductivity values of the system with teeth 2.5\AA in length.

Starting from the left of the graph we can see that for very small periodic lengths such as $PL = 20\text{\AA}$, 30\AA and 40\AA the system with the smooth interfaces have a considerably higher thermal conductivity as the interfaces with the teeth would be very close to each other due to the small period length and this would provide for a lot of scattering and hence loss in thermal conductivity.

Before, we tackle what happens between $PL=50\text{\AA}$ and $PL = 100\text{\AA}$, we see that at $PL = 100\text{\AA}$ the smooth interface system has once again become the system with highest

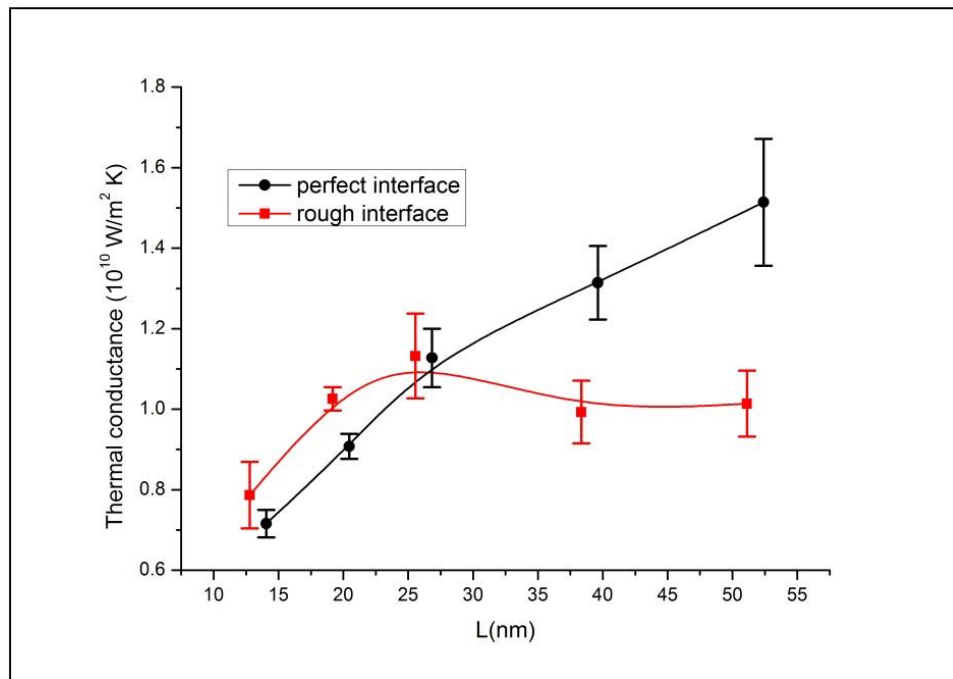


Figure 3-6: Size Effect showing that the thermal conductivity of a system will keep increasing for the smooth interface system and plateau off for the system with the rough interface.

thermal conductivity as expected. They will continue to rise from there on as the size of the system keeps increasing, this is known as size effect. It has been shown by my colleague Tianli Feng that as the size of the system keeps increasing the thermal conductivity of the system with the smooth interface will continue to rise while the system with the rough interface tapers off. Refer figure 3-6 for this discussion.

As expected, in figure 3-5 we see a big drop at $PL = 50\text{\AA}$ for the black graph, which is due to the fact that at 5nm you have a critical period where many medium wavelength phonons begin to scatter at the interface causing sudden dip in thermal conductivity. When we look at what happens to the other two graphs at $PL = 50\text{\AA}$, it becomes very interesting. Both having the same number of teeth separated by the same distance, the only difference being one having teeth that is 2.5\AA and another having teeth that is 5\AA long. The thermal conductivity for the system with teeth length = 2.5\AA rises steeply and at $PL = 50\text{\AA}$ has the highest thermal conductivity of all the systems. On the other hand the system with teeth length = 5\AA has thermal conductivity less than its smooth counterpart despite the sharp drop for the smooth interface system.

This behavior tells us that there is such a thing as optimum roughness. At teeth length = 5\AA it seems like the teeth are disrupting the phonons at the interface causing a dip in the thermal conductivity. On the other hand the system with teeth length = 2.5\AA which is denoted as the red graph is benefiting from the teeth which are essentially one unit cell thick and are increasing the area over which the phonons are being transmitted to the next material without disrupting the phonon flow. Not only does the added area help the thermal conductivity, but research show that the thermal conductance is much higher in an angled bond between Graphene and Boron Nitride compared to an arm-chair bond which is

horizontal [31]. And since the teeth is only 2.5\AA there are a whole lot of bonds between graphene and boron nitride which help in increasing the thermal conductivity of the system.

Additionally, as shown in figure 3-4, it does matter if the atoms linked are Carbon to Nitrogen or Carbon to Boron, and they play a part in deciding the amount of thermal transport taking place.

CHAPTER 4. CONCLUSION AND FUTURE WORK

4.1 Conclusion

The turn of the nano-technology age has brought a plethora of challenges for mankind to solve. As we go towards the age of faster and faster computing, thermal management will become one of the world top challenges and solving the world's thermal management problems start with the research that goes into the new materials or to find methods to tune upcoming materials.

Graphene and Boron Nitride are materials that have excellent properties with which a very potent superlattice can be formed. The most crucial part about this is superlattice is that the qualities and its properties can be completely tunable.

Through this thesis project we have tried to get a better understanding of the impact of interfacial roughness on a single interface and superlattice of Graphene Boron Nitride. We have delved into using Equilibrium Molecular Dynamics Green Kubo method to simulate this superlattice. Through this thesis project we have been able to gather understanding about the challenges facing research in thermoelectrics as well as get a better understanding of how the different parameters such as periodic length, teeth length, teeth width, or roughness in general affects the thermal conductivity of a superlattice. I hope this

knowledge is a small step in taking this line of work forward and making an impact on the world.

In conclusion, due to the wonderful properties of Graphene and Boron Nitride, the thermal transport can be tuned to cater one's need. It is important to understand the different properties of this system as it has tremendous potential to become the material of the future especially for the semi-conductor industry. This thesis has pursued deeper understanding of the unusual thermal transport in Graphene Boron Nitride in single interface and superlattice tuned by interfacial roughness.

4.2 Future Work

The future for this stream is going to be based on getting a full grasp on these materials enough to tune them to incredible accuracy. Immediate future work could include trying to mesh the concept of interfacial mixing and interfacial roughness to enhance the properties being sought out.

The future lies in harnessing any form of heat to put it to our use. Maybe the future holds building made out of thermos electric materials which only let in sun's heat come in and none to go out during frigid winters. As for now, this is a step towards a more prosperous world. As they say, "All you can do is the best you can do", I hope all of us keep striving to achieve the best we can achieve and no doubt the world would be filled with wonders.

Finally, I would like to once again thank Prof. Ruan for guiding me on this extremely fulfilling and interesting project and to all those who have guided me and inspired me along the way!

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