SENSING PROPERTIES OF DEFORMED GRAPHENE NANORIBBON THROUGH WARPING

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A thesis submitted in fulfilment of the
requirements for the award of the degree of
Master of Philosophy

Faculty of Electrical Engineering
Universiti Teknologi Malaysia

DECEMBER 2017

Specially dedication to my parents, siblings and friends for their love and respect

ACKNOWLEDGEMENT

Alhamdulillah - praise to Allah for all His blessing and compassion I was able to complete my master project entitled “Sensing Properties of Deformed Graphene Nanoribbon Through Warping” although have gone through some difficulties along the way however managed to complete this project.

First and foremost, I would like to express my gratitude to my supervisor Dr. Zaharah Johari and Dr. Nurul Ezaila Alias for their valuable comment, advice and utmost patience and dedication for guiding me to complete this project. I appreciate all their time spend for me and resources that she has provided in support of my research and education. I would also like to thank them for helping in getting additional information for the project. Not to forget, my parent and siblings for their support, concern, encouragement and understanding me through out the year.

Finally I would also like to thanks who have contributed directly or indirectly to succeed this project who I might not mentioned their name specifically. Without them, this project would not be successful.

ABSTRACT

Semiconductor materials have become the fundamental building block in the design of gas sensor. Previous researchers work on gas sensor that recognized its limitations such as low binding energy, low sensitivity and poor selectivity. As an alternative, considerable interests have generated in carbon based material like graphene to improve the sensing device performance. The purpose of this study is to investigate the sensing behaviour of deformed armchair graphene nanoribbon (AGNR) through warping using Extended-Huckel Theory (EHT) coupled with Non-Equilibrium Green Function (NEGF). The AGNR are warped upward and inward at angles of 180^o, 270^o and 360^o. The sensing properties are measured for oxygen (O_2) and ammonia (NH_3) molecules, particularly on their binding energy, charge transfer and sensitivity. Generally, inward warped AGNR shows better performance compared to upward deformation. Three AGNR configurations have been investigated; 3m, 3m+1 and 3m+2, where m known as an integer. Performance of each AGNR configuration behaves differently with the applied warping. Simulation results have indicated that for upward 3m configuration, the warping AGNR exhibit 98% enhancement in binding energy when warped at 360^o for NH_3 molecule. While for 3m+1 and 3m+2 the binding energy exhibit 72% and 64% improvement respectively. The same trend of observation is achieved for O_2 molecules. The results obtained also discovered a chemisorption in 3m, 3m+1 and 3m+2 configuration for both O_2 and NH_3. For 3m and 3m+1 configurations, the sensitivity has been observed at two-order of magnitude for higher warping angles, which most previous studies have not achieved. Meanwhile, negative sensitivity is observed in 3m+2 configuration. The marked improvement of the warped AGNR sensing properties is attributed from the combination of strain and curvature effect. The warping can also be an alternative method to minimize drawbacks in traditional gas sensors. The sensitivity of gas sensor could be enhanced by introducing the warped AGNR.

ABSTRAK

Bahan semikonduktor telah menjadi asas pembangunan dalam reka bentuk sensor gas. Penyelidikan sebelum ini ke atas sensor gas mendapati kelemahan seperti tenaga ikatan yang lemah, kurang sensitif dan kepilihan. Sebagai alternatif, bahan berasaskan karbon seperti grafin digunakan untuk meningkatkan prestasi peranti penderiaan. Tujuan kajian ini adalah untuk mengkaji tingkah laku penderiaan dengan mengunakan *armchair graphene nanoribbon* (AGNR) yang telah diubah bentuk dengan penggunaan *Extended-Huckel Theory* (EHT) serta *Non-Equilibrium Green Function* (NEGF). AGNR diledingkan ke atas and ke bawah dengan sudut 180^o, 270^o dan 360^o. Sifat-sifat penderiaan diukur untuk mengkaji gas oksigen (O_2) dan ammonia (NH_3) kursusnya pada tenaga ikatan, pemindahan cas dan sensitiviti. Umumnya, AGNR yang meleding ke bawah menunjukkan prestasi penderiaan yang lebih baik berbanding dengan meleding ke atas. Tiga AGNR konfigurasi telah disiasat; 3m, 3m+1 dan 3m+2, di mana m adalah integer. Prestasi setiap AGNR konfigurasi bertindak berbeza dengan ledingan. Keputusan, simulasi menunjukkan bahawa konfigurasi 3m meleding ke atas, mempamerkan peningkatan 98% dalam tenaga ikatan ketika leding pada sudut 360^o untuk molekul NH_3. Sementara, 3m+1 dan 3m+2 menunjukkan peningkatan tenaga ikatan masing-masing 72% dan 64%. Trend yang sama dicapai untuk molekul O_2. Hasil yang diperoleh juga menemui pengkimierapan bagi konfigurasi 3m, 3m+1 dan 3m+2 untuk kedua-dua O_2 and NH_3. Untuk konfigurasi 3m dan 3m+1, sensitiviti telah diperhatikan pada dua tertib magnitud untuk sudut meleding yang lebih tinggi, di mana tidak dicapai dalam kebanyakan kajian sebelum ini. Sementara itu, sensitiviti negatif diperhatikan dalam konfigurasi 3m+2 untuk molekul O_2. Penambahbaikan yang ketara diperolehi dalam prestasi penderian daripada AGNR yang meleding dan ini adalah kesan daripada gabungan antara ketegangan dan keledingan. Keledingan ini juga boleh menjadi salah satu kaedah untuk meminimumkan kelemahan dalam sensor gas tradisional. Sensitiviti sensor gas dapat ditingkatkan dengan memperkenalkan ledingan pada AGNR

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LIST OF ABBREVIATIONS

1D	-	One-dimensional
2D	-	Two-dimensional
AGNR	-	Armchair Graphene Nanoribbon
ATK	-	Atomistic ToolKit
CNT	-	Carbon Nanotube
DFT	-	Density Functional Theory
DOS	-	Density of state
EHT	-	Extended Huckel Theory
GGA	-	Generalized Gradient Approximation
GNRFET	-	Graphene Nanoribbon Field Effect Transistor
MOS	-	Metal oxide semiconductor
NEGF	-	Non Equilibrium Green Function
SCF	-	Self-consistency calculation
SV	-	Single Vacancy
SW	-	Stone-Wales
TB	-	Tight Binding
TS	-	Transmission Spectrum
VDW	-	Van der Waals
ZGNR	-	Zigzag Graphene Nanoribbon

LIST OF SYMBOLS

CO	-	Carbon monoxide
CO_2	-	Carbon dioxide
E_a	-	Binding energy
NH_3	-	Ammonia
NiO	-	Nickel oxide
NO_2	-	Nitrogen dioxide
O_2	-	Oxygen
S	-	Sensitivity
SnO_2	-	Tin dioxide
TiO_2	-	Titanium dioxide
WO_3	-	Tungsten trioxide
ϵ	-	Strain
Γ	-	Gamma Function
π	-	Band Energy

CHAPTER 1

INTRODUCTION

1.1 Background Study

Gas sensor is a device which detects the presence of various gases in a particular area. It has received much attention recently in both domestic and industrial application [1]. Sensing devices have wide application in various fields such as industrial, medical diagnosis, agricultural, chemical process and environmental monitoring safety. Based on studies done, the suitable competitor for the development of gas sensor for this wide range of application is solid state gas sensor [1, 2]. This solid state gas sensor owns its popularity based on its small size, high sensitivity for low concentration range of parts-per-million (ppm), low power consumption and cost. Besides that, it is also shown that solid state gas sensor has reversible interaction of gas with solid state material used [3]. These advantages have captured great interest of scientists and industries. In addition, this type of gas sensor has been used widely for chemical sensor. However, it suffers from stability for long term and measurement accuracy [1].

Capone *et al.* [1] discussed that semiconductor gas sensor is usually based on metal oxide semiconductor (MOS) such as tin dioxide (SnO_2), titanium dioxide (TiO_2), tungsten trioxide (WO_3) and nickel oxide (NiO). The MOS gas sensor has advantages in cost due to the simplicity in the architecture. This is desirable for the manufacturer to build MOS sensor. However, the disadvantages are that this MOS sensor has issue in power consumption and sensitivity to react with gas molecules. Using conventional material silicon has finally reached its limits and hence researchers are actively exploring other advanced material to replace silicon for better performance[4, 5]. By employing nanotechnology it provides enhanced solid state gas sensor performance, for example ultra-high sensitivity, fast response time and recovery and high specificity [6, 7].

Today's main focus in gas sensing aims to obtain high selectivity, sensitivity and low recovery time. Numerous studies have been established using carbon nanotubes (CNT) [8, 9], graphene [10, 11], graphene nanoribon (GNR) [12, 13] which allow detection of various types of gases. Low-dimensional carbon structures have been the focus of extensive research since the discovery of fullerenes and (CNTs) [14]. These novel forms of carbon present unique opportunities to study low-dimensional physical phenomena. Depending on their chirality and diameter, CNT can behave as semiconducting or metallic. They are also known to have high chemical reactivity due to the strain present in their curved lattice. However, it has been found that the presence of chirality in CNT causes difficulty in the fabrication process. This is due to the fact that CNT is highly reactive, which easily reacts with other unintentionally contaminant that causes difficulty in the fabrication process.

Graphene is a planar allotrope of carbon where all of the carbon atoms form a covalent bond in a single plane. Its two-dimensional (2D) crystal with a large surface to volume ratio maximizes the effect of sensing [6, 15]. Any detection method is to accomplish a level of sensitivity that individual quanta of a measured entity can be resolved. In the case of chemical sensors, the quantum is one atom or molecule. Such resolution is beyond the reach of any detection technique, including solid-state gas sensors. Nano sensors that is made from graphene is competent of detecting individual events when a gas molecule binds or unbinds from the graphene's surface. The changes in current conductivity is due to the bind molecules that change the conductance in graphene one by one with electron. The achieved sensitivity is due to the fact that graphene is an exceptionally low-noise material electronically, which makes it a promising candidate for chemical sensor [8].

Though the potential of graphene as gas sensor has been demonstrated, additional modification still needs to be done in order to fully utilize this material. Graphene is known as zero band gap [16]. Therefore, graphene sensing properties are currently significantly lower than CNT and this has been shown to be directly linked to the low sensitivity [2]. Despite the fact, GNR has a finite band gap depending on the types of edge. There are two types of GNR which are called armchair GNR (AGNR) and zigzag GNR (ZGNR) as illustrated in Figure 1.1. AGNR has zigzag cross section at the edges of width, while ZGNR has armchair cross section. There are three types of dimer lines for AGNR know as 3m, 3m+1 and 3m+2, where m is a positive integer. Earlier theoretical studies based on tight-binding (TB) approximation [17], found that GNRs are a relatively new class of nanomaterials that can behave as metallic or semiconducting character. ZGNR are all known as metallic regardless of

their widths. Meanwhile, for AGNR 3m+2 is metallic otherwise it is semiconducting [17, 18]. Thus, it is expected that gas molecule binding will have a higher effect on modifying the electronic properties of GNRs then graphene. They are currently being investigated to outstanding electrical, mechanical, thermal, optical, and quantum-mechanical properties [19].

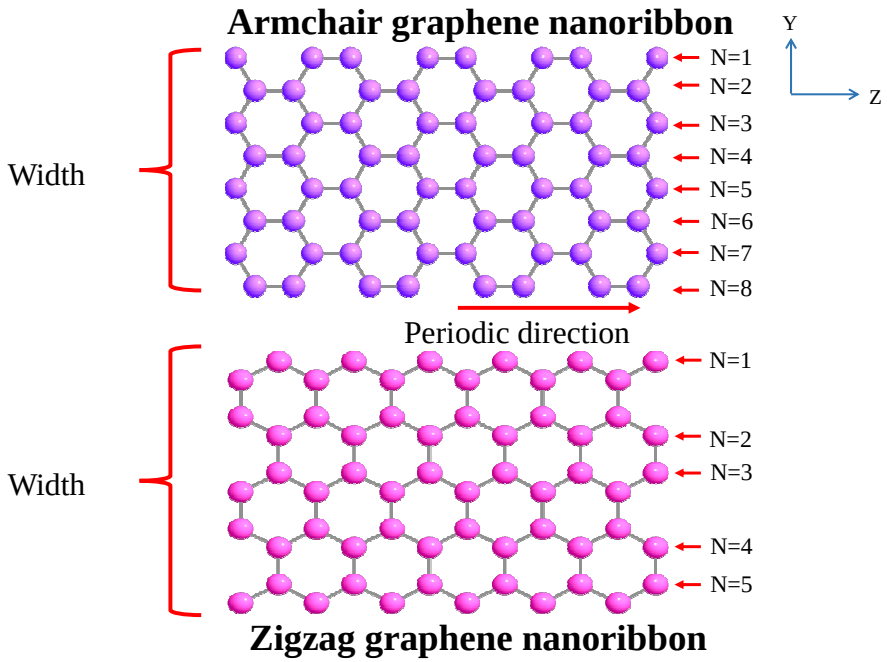

Figure 1.1: A illustration of GNR with AGNR (top) and ZGNR (bottom)

Recently, another promising approach has been introduced by using mechanical strain that has a substantial effect on the electronic band structure of AGNR [20, 21]. Due to the low reactivity of graphene, it requires harsh chemical treatment to allow functionalization to occur. Using conventional mechanical stress applied under uniaxial strain to the AGNR, the lattice becomes distorted and Dirac points relative to the allowed wavevector line in k-lines leading to the modulation of the electronic properties of AGNR [22]. Moreover, if the carbons are located in plane of graphene are generally expected to be relatively chemically inert due to the conjugation. Therefore, another technique such as non-planar deformation of graphene is initiated. This deformation includes scrolling, twisting, warping and buckling [23, 24]. This kind of deformation changes the AGNR to cylindrically geometry and

bond stretch is introduced by its own motion [25]. Although AGNR with various architectures and geometries have largely been successful, additional work is needed to address the deformation effects like warping on AGNR, which has been shown in Figure 1.2.

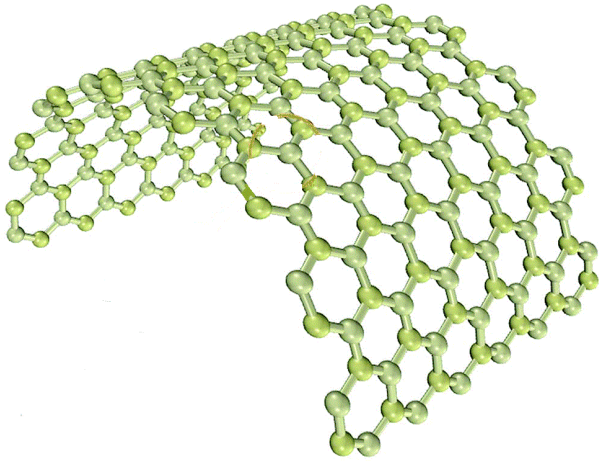

Figure 1.2: A Schematic Representation of Warping Graphene

The interesting combination of graphene and CNT behaviour in warping can give a rise to peculiar electronic properties [23]. This technique has been predicted to enhance the chemical reactivity as the carbon atoms are residing on the highly curved surface due to the diminished electronic delocalization [26]. It predicts that higher internal strain energy results in the formation of curvature in the device. In addition, warping deformation has more stable energy than planar structure and an extremely large surface to volume ratio, which favours the binding of gases on the structure and can probably further improve a sensor performance in sensitivity because the interaction between the gas molecule and material is higher [27]. This in turn can greatly manipulate its chemical reactivity allowing the tuning of sensing properties as needed. The effect of chemical functionalization on the mechanical properties of GNR still remain unexplored, although it is especially important for gas sensor application. It is a great interest to see the performance of warping AGNR as a gas sensor. The enhancement in gas sensing performance using warping is promising and its demand further studies. Therefore, it is important for future studies to understand the sensing performance of warping AGNR. It is worth studying since warping is a combination of graphene and CNT, which have originated from the same carbon material.

1.2 Problem Statement

Significant efforts have been made in using conventional material in gas sensor devices. Low selectivity, less sensitivity and high power consumption was observed in conventional material. Therefore, advanced carbon material is introduced such as CNT and graphene. A number of studies have demonstrated that low power consumption and high selectivity can be observed using this carbon material [5]. However, the sensitivity of graphene is less significant as compared to the sensitivity of CNT. Therefore, it has limited graphene application in sensing application.

The feasibility of using graphene deformation in the enhancement of graphene sensing behaviour is promising and demanding for further study as it is still in its early stage as compared to dopant and defect [12, 28, 29]. Although introducing dopant and defect improves the sensing performance, this technique deteriorates the crystallization and intrinsic of the graphene. There are many ways to deform graphene where one of the method is by warping [24, 30]. Most theoretical work on deformation graphene focuses on the electronic properties such as band structure, density of states, and thermal conductivity behaviour [30, 31]. There have been a few reports on the sensing capabilities such as binding energy, charge transfer and sensitivity. It is necessary to determine the binding energy because it determines how strongly the molecules bind with the material which later its affect charge transfer and sensitivity.

Motivated by these, this study aims to extend the idea to study the deformed AGNR on sensing properties through warping. As the warping will indirectly stretch the layers to form curvature which is almost similar in CNT. It is believed that the presence of curvature and bond stretch on the graphene layer will enhance its chemical reactivity. Therefore, the merit of using warping technique to form curvature and stretch on AGNR by varying warping angle is studied and is aimed to enhance the sensing properties. These fundamental properties deserve a closer look to fully exploit deformed graphene in electronic devices. Thus, this will be looked upon by means of computational study in this study.

1.3 Research Objective

This study focuses on the analysis of sensing behaviour of warping AGNR by computational study using Atomistic ToolKit (ATK) version of 2015.1. The objectives

are as follow:

1. To form deformed AGNR through warping method and to determine the sensing properties in term of binding energy, charge transfer and sensitivity.
2. To analyze and evaluate the sensing performance of inward and upward warping AGNR by the combination of curvature and strain effect
3. To investigate the gate biasing effect at highest warping angle between inward and upward warped AGNR.

1.4 Research Scope

1. This study will be conducted using ATK software version 2015.1 with three AGNR configurations which are 3m, 3m+1 and 3m+2.
2. Properties evaluation include:
   (a) Sensing properties :
      i. Binding Energy, to obtain the binding capacity between analyte and substrate.
      ii. Charge Transfer, to determine whether the analyte acts as donor or acceptor.
      iii. Sensitivity, to measure how fast the material detect molecules.
   (b) Electronic properties :
      i. Band Structure, to obtain the energy gap of device either it behaves as semiconducting or metallic behavior even after warping is applied.
      ii. Density of State (DOS), to determine whether the characteristic of unwarped device is sustained.
      iii. Total Energy, to be used to calculate binding energy.
   (c) Transport properties :
      i. Current-voltage (I-V) characteristic, to observe the current conductivity is increase or decrease after warping applied and to use to obtain sensitivity.
      ii. Transmission Spectrum (TS), to observe the pathway of electron flow.

3. AGNR deformation are limited to two types of warping which are inward and upward warping. While the warping angle of 180^o, 270^o and 360^o are used where the curvature increase with the warping angle.

4. Two types of gas molecules are chosen such as

   (a) Ammonia (NH_3): Ammonia is a toxic gas. Therefore, ammonia sensor is needed to prevent early possible leakage especially in industry.

   (b) Oxygen (O_2): Oxygen sensors are used in oxygen analysers which find a lot of use in medical applications such as anaesthesia monitors, respirators and oxygen concentration.

1.5 Research Contribution

The outcome of this study has two major contributions. The first contribution is the study of deformed AGNR through warping which are inward and upward at higher warping angle. This study investigate on three types of sensing properties which are binding energy, charge transfer and sensitivity. The second contribution is through simulation. It found that the sensing performance was enhanced in term of binding energy and sensitivity especially using 3m+1 AGNR configuration. The binding energy was improved by more than two fold while the sensitivity was enhanced by ten fold. Besides that, this study has been performed using computational simulation, which could help other experimental researcher to uncover critical areas in the fabrication process as well as optimize their time on designing.

1.6 Thesis Organization

This thesis begins with the introduction of gas sensor using advanced materials and background of the research study as outline in Chapter 1. Review study of gas sensing properties and deformation of GNR's electronic and mechanical properties which provides the foundation of the thesis has been presented in Chapter 2. In Chapter 3, computational details of the study have been presented. In addition details of warping behaviour, electronic and transport properties of warping AGNR have been also elaborated. The results achieved are shown in Chapter 4. Finally, a summary of this study with few recommendations for future study are presented in Chapter 5.

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