ELETRONIC PROPERTIES OF BORON NITRIDE NANORIBBONS WITH SINGLE VACANCY DEFECT

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ELECTRONIC PROPERTIES OF BORON NITRIDE NANORIBBONS WITH SINGLE VACANCY DEFECT

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DEDICATION

This project report is dedicated to my father, who taught me that the best kind of knowledge to have is that which is learned for its own sake. It is also dedicated to my mother, who taught me that even the largest task can be accomplished if it is done one step at a time.

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ABSTRACT

Hexagonal boron nitride (h-BN), also known as Boron Nitride Nanoribbons (BNNRs), is an electrical insulator with high thermal stability suitable to make as an excellent thermal conductor, including high-temperature equipment. BNNRs is a wide bandgap semiconductor within the range of 5eV until 6eV. In this work, two models of BNNRs with single vacancy defect used included Armchair BNNRs and Zigzag BNNRs to investigate its electronic properties. Nearest-neighbour tight-binding model and numerical method are used to simulate the electronic properties of BNNRs with single vacancy, including band structure and local density of states. This simulation work is done by generating a script using numerical computational methods in MATLAB software. The alpha and beta matrix used in the script are modified accordingly when the boron or nitrogen atom is missing. Besides, small perturbation effect is applied into the model to study the effects of impurities at the edges of BNNRs. The simulation result from this work is compared with a pristine BNNRs to study the impact of single vacancy of BNNRs to electronic properties of BNNRs. The comparison results showed that the band structure and local density of state for both ABNNRs and ZBNNRs with single vacancy defect is distorted when compared to pristine model. Besides, the effect of edge perturbation is symmetrical when compared to previous research.

ABSTRAK

Boron nitrida heksagon (h-BN), juga dikenali sebagai reben-nano Boron Nitrida (BNNRs) adalah penebat elektrik dengan kestabilan haba yang tinggi, ciri ini sesuai untuk dibuat sebagai konduktor termal yang sangat baik, termasuk peralatan suhu tinggi. BNNRs ialah semikonduktor dengan jalur yang lebar dalam lingkungan julat 5eV hingga 6eV. Dalam karya ini, dua model BNNR dengan kekosongan satu atom digunakan termasuk lengan-kerusi BNNRs dan zigzag BNNRs untuk menyiasat sifat elektroniknya. Model ikatan ketat terdekat (NNTB) dan kaedah berangka adalah digunakan untuk mensimulasikan sifat elektronik BNNRs dengan kekosongan satu atom, termasuk struktur pita dan ketumpatan keadaan (DOS). Kerja simulasi ini dilakukan dengan menghasilkan skrip menggunakan kaedah pengiraan berangka dalam perisian MATLAB. Matriks alfa dan beta yang digunakan dalam skrip diubah suai sewajarnya apabila atom boron atau nitrogen hilang. Hasil simulasi daripada kerja ini dibandingkan dengan BNNR asli untuk mengkaji kesan kekosongan tunggal BNNR kepada sifat elektronik BNNR. Hasil perbandingan menunjukkan bahawa sktruktur jalur dan ketumpatan tempatan bagi kedua-dua ABNNR dan ZBNNR dengan kekosongan tunggal diherotkan jika dibandingkan dengan model tulen. Selain itu, kesan gangguan tepi adalah simetri jika dibandingkan dengan penyelidikan terdahulu.

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LIST OF ABBREVIATIONS

h-BN	-	Hexagonal Boron Nitride
2D	-	Two-Dimensional
ABNNRs	-	Armchair Boron Nitride Nanoribbons
BN	-	Boron Nitride
BNNRs	-	Boron Nitride Nanoribbons
GNRs	-	Graphene Nanoribbons
MATLAB	-	Matrix Laboratory
DOS	-	Density of States
DFT	-	Density Functional Theory
1D	-	One-Dimensional
UTM	-	Universiti Teknologi Malaysia
NEGF	-	Non-equilibrium Green's Function
ZBNNRs	-	Zigzag Boron Nitride Nanoribbons
NNTB	-	Nearest-neighbor tight-binding

LIST OF SYMBOLS

α	-	Alpha
β	-	Beta
N	-	Width of BNNRs
l	-	Length of BNNRs
ε	-	Self-interacting energy
t	-	Interaction energy between unit cells
H	-	Hamiltonian matrix

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Boron Nitride (BN) is a typical III-V group compound with a stoichiometry of boron and nitrogen being 1:1 [1]. BN is similar to carbon in any lattice structure where it consists of zero-dimensional cage, one-dimensional nanotube, two-dimensional monolayer and three-dimensional diamond-like crystal structure [1]. A hexagonal boron nitride (h-BN) sheet is analogous to graphene since it is isoelectronic and isomorphic to the graphene honeycomb lattice [2]. By cutting a straight line, hexagonal boron nitride can be constructed into two type of boron nitride nanoribbons (BNNRs): armchair boron nitride nanoribbons (ABNNRs) and zigzag boron nitride nanoribbons (ZBNNRs) [3]. BNNRs possess higher thermal stability, oxidation stability up to eight hundred degree Celsius, chemical inertness [4], and excellent optical properties. In the BN structure, the boron atom and nitrogen atom connected with a strong covalent bond. However, the interlayer between BN layers held together with weak Van der Waals force [5]. Lai Kien Wei has done a study on pristine BNNRs and introduced edge perturbation to get the electronic properties of BNNRs [6]. Edge perturbation is a process to make disturbance on a regular structure to change its motion. Edge perturbation is a method to create an "imperfect structure" on BNNRs [7]. Edge perturbation is able to decrease the large energy bandgap of BN and become more semiconducting [6].

Solutions of Schrödinger's equation, either by using first-principles, or semi-empirical methods, are the basis for most quantum transport models, for example, the popular Non-Equailibrium Green's Function (NEGF) formalism and also the Usuki method. Solving Schrödinger's equation is a complicated task due to it involves the solution of the integral for each energy state existing in the whole system. The mathematical analysis of the Schrödinger's equation is more complicated than

involving a small system if it is enlarged. Longer time and more effort are needed to study Schrödinger's equation, including the theory part and the calculation part. Many researchers are using Schrödinger's equation to investigate the band structure and electronic properties of BNNRs.

In this research, the pristine BNNRs will be modified to a single vacancy defect BNNRs. One of the nitrogen or boron atom will be removed from BNNRs when constructing Hamiltonian equation. The *t* term and energy on site of boron and nitrogen in alpha and beta will be modified accordingly when boron or nitrogen is removed. The *t* term will become zero and energy on site of boron and nitrogen will changes to an infinite value [8].

1.2 Problem Background

BN is a potential material that can be used in nanotechnology due to its uniqueness, including electronic properties. Schrödinger's equation in semi-classical physics is analogue to Newton's second law in a physical class. Schrödinger's equation widely used as the fundamental equation for describing quantum mechanical behaviour. Schrödinger's equation always deals with the probability of quantum mechanics. Hence it is a linear partial differential equation. Solving Schrödinger's equation is a complicated task due to it involves the solutions of the integral for each energy state existing in the whole system. The mathematical analysis of the Schrödinger's equation is more complicated than involving a small system if it is enlarged. Longer time and more effort needed to study Schrödinger's equation, including the theory part and the calculation part. Many researchers are using Schrödinger's equation to investigate the band structure and electronic properties of BNNRs.

This bottom approach of BN allows a more accurate description of carrier transport phenomena. Non-equilibrium Green's Function (NEGF) approach is used to preserve the wave characteristics transport electron.

1.3 Problem Statement

Various h-BN materials have been widely used for many technological fields. The defect of BNNRs during fabrication is difficult to avoid and will give impacts to the industries. Atomic-scale defect such as vacancies and dislocations will change the chemical properties of BNNRs [9]. Various methods have been developed by researcher to fabricate h-BN such as mechanical exfoliation, chemical exfoliation, chemical vapor deposition and others [1]. The fabrication process is improving, but it still can't avoid the defect during fabrication process. Thus, the modelling of BNNRs with single vacancy defect is to study the non-idealities effects.

Previous researchers used other methods to compute the electronic properties of BNNRs with single vacancy such as density functional theory (DFT) and first-principle calculation. These methods need a large system that is computationally difficult and time consumed. In this research, the nearest-neighbour tight-binding (NNTB) model and numerical method are used to compute the band structure, bandgap energy and local DOS of BNNRs. These two methods are used due to they are computationally efficient and accessible by applying assumptions on the BNNRs model.

1.4 Research Objectives

The objectives of the research are:

(a) To compute and compare the electronic properties such as bandgap energy and local density of state of ABNNRs and ZBNNRs with single vacancy and edge perturbation

(b) To develop the numerical nearest-neighbour tight binding Hamiltonian operator matrix model of ABNNRs and ZBNNRs with single vacancy for the simulation of electronic properties.

1.5 Research Scope

This work focused on the computational modelling of ecteronic properties of BNNRs with single vacancy. The onsite energy of boron atom and nitrogen atom is modified to infinite value when the atom is missing. Besides, the *t* term that used in Hamiltonian equation is changes to zero when there is no connection between the atoms. All simulations of the electronic properties of BNNRs is done using Matrix Laboratory (MATLAB) software.

1.6 Organization of Report

This report contains four chapters. Chapter 1 introduces the introduction, problem background, problem statement, research objectives and the scope of this project. Chapter 2 will discuss about the literature review based on information gathered from studying articles and journals. Chapter 3 covers the research methodology of this project where the function of the materials and devices used in this project are introduced. Chapter 4 discusses the preliminary result of ABNNRs and ZBNNRs with single vacancy defect.

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