A computational Analysis of Interaction between Inorganic Semiconductor Nanowire and partial charge Molecules for DNA Sensor Application

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A thesis submitted
In fulfillment of the requirements for the degree of
Doctor of Philosophy

INSTITUTE OF NANO ELECTRONIC ENGINEERING
UNIVERSITY MALAYSIA PERLIS

2015

UNIVERSITI MALAYSIA PERLIS

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Academic Session : 2015/2016

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ACKNOWLEDGEMENT

بسم الله الرحمن الرحيم

First of all, thanks to God (ﷲ) for giving me both physical and mental health. Indeed, I would proudly express my deep gratitude and sincere thanks to my main supervisor, Prof. Dr. Uda Hashim, for his great support, professional guidance, and positive encouragement. In fact, he spent his valuable time providing me with invaluable and critical comments during my Ph.D progress. Without his help, I would not have been able to gain what I have achieved. More importantly, he encouraged me to participate in international conferences and write research papers for publications in international journals and related research activities. Besides that, he gave me valuable advice whenever I have difficulties in both my academic and personal life, which had a positive impact on my life.

I specially thank my parents for their supports and generosity towards me all through my life especially during this research period. I would like to also thank Dr. Majnur my co-supervisor who assisted me in the simulation of my research work and with frequent advices. Finally, then, I would like to express my sincere thanks to all those who have contributed to the success of my study. In fact, Nanostructure biosensor Group, my friends' help and my family's supports, I would not have completed my Ph.D thesis. God bless you all. Indeed

Abdul Mohaimen W Fagri

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LIST OF ABBREVIATIONS

CD	Charge distribution
PC	Partial charge
SC	Surface charge
Se-NW	Semiconducting nanowires
Si-NW	Silicon Nanowires
SOI	Semiconductor on insulator
C M	COMOSL Multiphysics simulation
MD	Molecular dynamics
VMD	Visual Molecular Dynamics
PDB	Protein data bank
F_n	Functional layer
EC	External charge
SsDNA	Single strand DNA
FES	Field effect sensor
SNS	Silicon nanowire sensor
TC	thermal conductivity
K-SiNW	Kinks silicon nanowire
El	Electrolyte
PH	Ph solution
MOSFET	Field effect transistor
PLV	pulsed laser vaporization
µm	Micrometer
I_{on} and I_{off}	Function of the length
Poly-Si	Poly-silicon
SiO_2	Silicon dioxide

LIST OF SYMBOLS

u	Potential	V
L	Length	m
R	Radius	m
f	Thickness of functional layer	m
Si	Silicon	
ε	Relative permittivity	F m^{-1}
c	Ion concentration	mol / l
σ	Surface charge	σ
σ_{12}	Surface charge of Si	σ_{12}
σ_{23}	Surface charge of oxide	σ_{23}
σ_{34}	Surface charge of functional	σ_{34}
(κ)	Thermal conductivity	
x, y, z	Cartesian coordinates	m
r,ϕ, z	Cylindrical coordinates	m
G	Conductance	S
$\boldsymbol{R}_{\Omega}$	Resistance	Ω
J	Current density	A m^{-2}
$\boldsymbol{\sigma_{con}}$	Conductivity	Sm^{-1}
E	Electric field	V m^{-1}
I	Current	A
$\boldsymbol{l}$	Thickness of electrolyte	m
$\boldsymbol{\sigma}$	Surface charge	C m^{-2}
n_0	Initial electron concentration	Cm^{-3}

p_0	Initial hole concentration	Cm^{-3}
n	Electron concentration	Cm^{-3}
p	Hole concentration	Cm^{-3}
$\mathrm{k_b}$	Boltzmann Constant	J k^{-1}
T	T Temperature	K
$\mathrm{N_A}$	Acceptor concentration	C m^{-3}
$\mathrm{N_D}$	Donor concentration	Cm^{-3}
L_1	Silicon nanowire layer	
L_2	Oxide layer	
L_3	Functional layer	
L_4	Electrolyte layer	

Analisis pengiraan interaksi antara semikonduktor inorganik nanowire dengan molekul caj separa untuk aplikasi sensor DNA

ABSTRAK

Penyelidikan kini adalah untuk menyiasat kesan caj separa yang diakibatkan penghibridan DNA pada kealiran daripada nanowire silikon melalui pengiraan unsur oleh terhingga. Satu biosensor direka dengan nanowire silikon dengan berdiameter 15nm dari pusat yang dikelilingi oleh lapisan 2nm SiO_2 ketebalan dragon. Lapisan oksida tersebut dikelilingi oleh lapsian bio-interface yang berukuran 5nm dan keseluruhan sistem ini telah tenggelam dalam suatu elektrolit yang berjejari 80nm. Untuk tujuan pemodelan dan simulasi, setiap satu daripada lapisan berkenaan dianggap sebagai satu medium kontinum dicirikan oleh pemalar dielektrik yang sepadan. Untuk mencari kesan penghibridan pada kealiran nanowire, pengagihan potensi elektrostatik dalam nanowire dan lapisan yang lain telah dikira dengan menggunakan persamaan Poisson dengan statistik Boltzmann tanpa menambah sasaran DNA dalam lapisan elektrolit. Kealiran daripada nanowire dalam keadaan ini dikirakan walaupun mengintegrasikan kesan potensi pada pembawa cas dalam nanowire itu. Kemudian, pengedaran potensi sekali lagi dikira dengan sasaran DNA dalam elektrolit dan kealiran daripada nanowire itu dikira semula. Pengiraan unsur terhingga menunjukkan bahawa kealiran nanowire bergantung pada secara nonlinear atas cas luaran (cas separa) pada bio-interface disebabkan oleh penghibridan sasaran DNA dengan probe DNA dalam lapisan berfungsi. Cas separa diakibatkan penghibridan di antara probe dan sasaran DNA telah dikira menggunakan simulasi dinamik molekul. Oleh itu, simulasi unsure terhingga menunjukkan bahawa penghibridan sasaran DNA dengan probe DNA dikaitkan dengan satu cas dalam kealiran nanowire itu. Jika perbezaan potensi luaran digunakan antara dua terminal nanowire itu, perubahan dalam kealiran nanowire akan dikesan sebagai perubahan dan diukur sebagai arus elektrik. Kepekaan relatif nanowire disebabkan oleh penghibridan molekul DNA siasatan dan sasaran dianggarkan melalui simulasi. Dalam simulasi ini, kepekaan relatif dianggarkan 75% iaitu lebih tinggi daripada sensitiviti dilaporkan sebelum ini. Oleh itu, ia boleh disimpulkan bahawa kajian ini mencadangkan satu sistem nanowire biosensor penghibridan berdasarkan dengan kepekaan cukup tinggi bagi negeri-of-the-art penyelidikan. . Kepekaan relatif nanowire disebabkan oleh penghibridan molekul DNA siasatan dan sasaran dianggarkan melalui simulasi. Dalam simulasi ini, kepekaan relatif dianggarkan 75% iaitu lebih tinggi daripada sensitiviti dilaporkan sebelum ini. Oleh itu, ia boleh disimpulkan bahawa kajian ini mencadangkan satu sistem nanowire biosensor penghibridan berdasarkan dengan kepekaan cukup tinggi bagi “state-of-the-art” penyelidikan.

A Computational Analysis of Interaction between Inorganic Semiconductor Nanowire and Molecular Partial Charge for DNA Sensor Application

ABSTRACT

This research aimed to investigate the effects of partial charge due to DNA hybridization on the conductance of the silicon nanowire through finite element calculations. A biosensor was designed with the silicon nanowire of 15 nm radius at the core and surrounded by a silicon dioxide (SiO_2) layer of 2 nm thickness. The oxide layer was surrounded by a 5 nm thick functional bio-interface layer incorporating probe ssDNA and this whole system was immersed in an electrolyte of 80 nm radius. For the purpose of modeling and simulation, each of this layers was treated as a continuum medium characterized by the corresponding dielectric constant. In order to determine the effects of hybridization on nanowire conductance, the distribution of the electrostatic potential in the nanowire and other layers were first computed using Poisson equation with Boltzmann statistics without adding target DNA in the electrolyte layer. The conductance of the nanowire in this condition was computed by integrating the effect of the potential charge carriers within the nanowire and partial charge due to probe ssDNA. Then, the potential distribution was again calculated with the target DNA in the electrolyte and the conductance of the nanowire was re-calculated. Partial charge due to hybridization between probe and target DNAs was first computed using molecular dynamics simulation and integrated into the finite element calculation. The Finite element calculations showed that the nanowire conductance depended nonlinearly on the external charge (partial charge) of the bio-interface due to the hybridization of the target DNA with probe DNA in the functional layer. That is, the hybridization of target DNA with probe DNA is associated with a change in the nanowire conductance. If an external potential difference is applied between two terminals of the nanowire, this change in the nanowire conductance would be detected as a change in the measured current. The relative sensitivity of the nanowire due to the hybridization of the probe and target DNA molecules was estimated through simulation. In this simulation, the relative sensitivity was estimated to be 75% which is higher than the previously reported sensitivity. Thus it may be concluded that the present research proposed a hybridization based nanowire bio-sensor system with a significantly high sensitivity for the state-of-the-art of research.

CHAPTER 1

INTRODUCTION

1.0 Introduction

A biosensor is widely defined as a device consisting of a biological recognition system, often called a bioreceptor, and a transducer (Vo-Dinhn, T, 2006). In general, a biochip has an array of individual sample that can be individually monitored and is widely used for the analysis of multiple analytes. The interaction of the analyte with the bioreceptor is designed to have an effect measured by the transducer, which converts information into a measurable output, such as an electrical signal. Moreover, there are several classification schemes. Biosensors and biochips can be classified either by their bioreceptor or transducer type (Vo-Dinhn, T, 2006). A bioreceptor is a biological molecule including antibody, enzyme, protein, or nucleic acid or a living biological system; for example, cell, tissue, or the whole system utilizes a biochemical mechanism for recognition. The sampling component of a biosensor contains a bio-sensitive layer. The layer can either contain bioreceptors or be made of bioreceptors covalently attached to the transducer. The most common forms of bioreceptors used in biosensing are based on 1) antibody/antigen interaction, 2) nucleic acid interaction, 3) enzymatic interaction, 4) cellular interaction and 5) interactions using biomimetic materials such as synthetic bioreceptors. For transducer classification, the conventional techniques include: 1) optical measurements such as luminescence, surface plasmon resonance, etc., 2) electrochemical and 3) mass-sensitive measurements (i.e. surface acoustic wave, microbalance) (Tuan, 2008). The development of biosensors was first reported in the early 1960s. Today, Biosensors have drawn much attention of many researchers and are widely used in various applications, especially in two major areas: biological monitoring and environmental sensing applications (Vo-Dinhn, T, 2006). Moreover, the interaction of silicon nanowire (Si--NW) and partial charge DNA hybirdization is the interaction between DNA molecules, which is required to activate the Si--NW between DNA and inorganic nanowire surface functional group. It is necessary to gain insights into various techniques to investigate the bases of the binding chemistry between these two materials (Romancová, 2013). Indeed, another approach is required to discover the mechanism of the interaction between the two molecules (Chemie, 2012) because DNA is possible to carry genetic information and involves the most cellular processes.

On the other hand, Biosensors can be classified either by the type of biological signaling mechanism they utilize or by the type of signal transduction employed. Transduction can be accomplished via a variety of methods (Touhami, A, 2015). Most forms of transduction can be categorized into three main classes including electrochemical detection, optical detection and mass detection methods. However, new types of transducers are constantly being developed for use in biosensors. Each of these three main classes contains different subclasses, creating a nearly infinite number of possible transduction methods or a combination of other methods. All those methods can be performed using Si--NW (Touhami, A, 2015).

Silicon nanowire (Si-NW) is a promising device structure in the field of semiconductor with many advantages. Nanowire biosensors are a class of nanobiosensors, of which the major sensing components are made of nanowires coated by biological molecules such as DNA molecules, polypeptides, etc. A nanowire is an one-dimensional fibril like nanostructure, with the diameter constrained to tens of nanometers or less. Since their surface properties can be easily modified, nanowires have been decorated virtually with any potential chemical or biological molecular recognition unit, making the wires themselves analyse independently. Moreover, nanowires can be used for both efficient transport of electrons and optical excitation, these two factors make them critical to the function and integration of nanoscale devices.

1.1 Background of This Study

1.1.1 Nanotechnology

The term 'nano' originated from the Greek word, which means an extremely small size or dwarf. This term has almost become a standard since 1960, and it is currently being used in science and engineering field. The term 'nano size' corresponds to one billionth of a meter or also factor 10^{-9}. There are a large number of examples with regard to nanotechnology that shows how to image the small size of Nano. The small size of nano-scale resulted from the fact that one has to take one part of 10000 parts of human hair to get a nanometer scale (Hunt & Mehta, 2006).

Nanoscience and nanotechnology are defined in different ways. In fact, they have different scopes and contexts for a specific application (Al-mufti, A.W et al., 2013). However, the Royal Society of the UK differentiates between nanoscience and nanotechnology. According to them, the former includes the investigation and manipulation of nanoscale materials and systems; whereas the second one is concerned with the design, development and characterization of nanomaterial for Nano devices and systems.

Nevertheless, research and development activities in both of these fields focus on the scales of atoms, molecules, or macromolecules. In fact, some of these structures in biology and chemistry can be seen as tiny machines (Ghindilis et al., 2009). Examples include adenosine triphosphate (ATP) synthase, which is responsible for the catalysis of molecule synthesis. There are other examples of enzymes which catalyze other molecular reactions. Due to their advantages, the nanomaterials and nanostructures have made tremendous contributions to futuristic technologies including material engineering sensor, medical, and biotechnology applications.

The core concept of nanotechnology topic was suggested by Richard Feynman, who won Nobel Prize in Physics. In terms of the characterization of nano size particles, the name of Richard Adolf Zsigmondy, an Austrian chemist, was recognized in the field of nanotechnology by research community in 1914 (Santamaria, 2012). Also, Norio Taniguchi, Tokyo University Sciencetist, was the first person to define nanotechnology in 1974 (Taniguchi, 1974). As a part of history, John Bardeen and Walter Brattain (Grundmann, 2011) built transistor for the first time in 1974. Moreover, Gordon Moore predicted that transistors density in an integrated circuit will double up approximately each two years (Moore, 1965). This is known as Moore's law in the field of information technology. This trend has been a practical assistance in study during the last 50 years. Kim Eric Drexler (an American engineer) made a significant contribution to popularizing nanotechnology in 1980's (Eric, 1986). He prophesized that it would be possible to create devices like robots, or even computers to a few nanometers wide scale which is similar to that of DNA.

It is the fact that the most current studies focus on the synthesis and simulation of nanomaterial. The synthesis processes can be divided into two main classes: bottom-up and top-down methods. Moreover, the investigation into the existing literature on the nanoscale topics showed that this goal was achieved through proposing a variety of methods. In the top-down approach, bulk materials are tailored through casting, sawing or maching into custom nanoscale products. Some well-known methods in this category include ball milling, mechanochemical processing, solution based chemistry, etching, and physical and chemical vapor deposition techniques. However, the top-down is a bigger size of material into nano size material through a lithography process or crushing. Moreover, this top-down method is mostly used in the fabrication of the current computer processors.

In the second method, named bottom-up approach, nanomaterials are created by manipulating material at the atomic and molecular level. In this sense, this approach is similar to the processes in which DNA molecules of living cells are formed through the patterned organization of atoms. The main success and useful application of nanotechnology would be availability of tools and process for controlled placement individual atoms in order to develop an intricate material of a great complexity at nanoscale. It would provide opportunities for a huge flexibility to produce any devices through engineering atoms and molecules. Finally, it is expected that some judicious blend of top-down and bottom-up approaches will lead to a new era of innovative nanotechnology.

1.1.2 Nanostructure

A material can be called a nanostructure if its length scale is in the range of ~ 1-100 nm in one or more dimensions. The electrons in the nanostructure cannot move freely in nanoscale dimension(s), that is, they are confined in those dimensions, whereas the electrons are free to move in the other dimension(s). Nanostructures can be classified based on the number of dimensions in which free electrons are possible to move. Thus, nanostructures can be classified into three categories, namely, quantum dots, quantum wires and quantum wells. A nanostructure behaves differently both from individual atoms or molecules at the smaller scale and from bulk material at the bigger scale. As they are between these two far away scales, they are referred to as mesoscopic structures as well. Nanoscience research deals with the unique properties of the nanoscale materials and structures that do not generally exist in other scales such as atomic and bulk material scales.

1.1.3 Nanomaterial

Nanomaterials are very useful and become the keystones of nanotechnology and nanoscience. However, nanostructure science has been a wide and multi-topics of research and improvement activity during the last years. It is potential for changing the ways, in which the products and materials are made in a variety and the environment of functionalities. Moreover, it is a promising material for making money in the future (Chemie A, 2012).

However, a material with one dimension at least is less than 100 nanometres approximately, which is a well-defined nanoscale material. Nanomaterial unique properties are optical and electrical properties. More especially, the occurrence of additional properties makes it more interesting in a high scale dynamic response. Furthermore, all these improved properties are extremely potential in electronics, medicine, and other fields.

Although, a number of nano materials exist naturally, engineered nano materials (ENM) are of a particular interest. ENMs have already been designed for a number of commercial processes and used for different commercial products. Their implications can be found in different areas such as cosmetics, sports materials, electronics and many daily items as well as in medicine, diagnosis and imaging etc.

Moreover, Synthesis DNA is a resource designed for the DNA level to take more benefits due to their tiny size and properties of molecules, which are normally not seen in conventional, bulk counterparts. It can be interpreted that materials with a high scale and various properties are increasingly required a relative surface area regarding the new quantum effects. Furthermore, at the nano scale, as the result of the quantum effects, the characteristics of materials characteristics as well as their properties are determined, which leads to novel optical and electrical behaviours.

1.2 Problem Statement

One of the major problems of biosensor is the inadequate sensitivity of devices. Indeed, a suitable nanowire size leads to a higher sensitivity. Therefore, it is vital to increase sensitivity by improving other aspects of the design.

The possible problem to be resolved in this research is to explore the effects of DNA hybridization partial charge on the conductance of silicon nanowire. Previous studies showed the selection of proper size as a main problem in the design. The use of certain size leads to a good performance of nanowire High sensitivity needed for a biosensor; therefore, it is necessary to determine a suitable nanowire size leading to higher sensitivity.

In addition, other problems were found in previous studies in which sensitivity is insufficient for the conductance of the silicon nanowire connected with different sizes of nanowire with high sensitivity. Si-NW was designed with 15 nm, which can affect the