MODELING AND SIMULATION OF BILAYER GRAPHENE NANORIBBON FIELD EFFECT TRANSISTOR

SEYED MAHDI MOUSAVI

UNIVERSITI TEKNOLOGI MALAYSIA

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SEYED MAHDI MOUSAVI

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Dedicated, in thankful appreciation for support, and encouragement to my beloved parents, sisters and my wife and my son.

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ABSTRACT

The unique structure and electronic properties of Bilayer Graphene Nanoribbon (BLG) such as long mean free path, ballistic transport and symmetrical band structure, promise a new device application in the future. Improving the modeling of BLG Field Effect Transistor (FET) devices, based on the quantum confinement effect, is the primary objective of this research. It presents an analytical and numerical model for evaluating electrical properties of BLG devices in equilibrium (temperature is constant) and non-equilibrium states (for different temperatures). By developing the carrier statistic and carrier transport model, the current-voltage model of a BLG FET is established and evaluated. Using an analytical model, BLG carrier concentration and conductance in degenerate and non-degenerate limits are explored. The carrier mobility and drain current (as a mean parameter of FET characteristic) are also being investigated. This research also presents a numerical implementation of the developed model. These models provide one with the chance to perform simulation in a reasonable amount of time, which is required for large-scale applications of device optimisations. MATLAB software is used in the numerical methods which have been extensively applied for the study of BLG FET behaviour. Comparison study of conductance, mobility and current-voltage with published experimental data is presented and good agreements with the proposed models are reported. The presented model can be used in Technology Computer Aided Design tools to improve the performance of next generation nano-devices.

ABSTRAK

Struktur yang unik dan sifat-sifat elektronik *Bilayer Graphene Nanoribbon (BLG)* seperti pergerakan bebas, pengangkutan balistik dan struktur jalur simetri menjadikan bahan tersebut mempunyai potensi yang luas dalam applikasi peranti baru di masa hadapan. Memperbaiki model peranti BLG Transistor Kesan Medan (FET) berdasarkan kesan penghadan kuantum adalah objektif utama dalam penyelidikan ini. Ia mempunyai model analisis dan berangka untuk menilai sifat elektrik peranti BLG dalam keadaan keseimbangan (suhu adalah malar) dan ketidakseimbangan (untuk suhu yang berbeza). Dengan membangunkan pembawa statistik dan pembawa pengangkutan model, model arus voltan FET BLG dihasilkan dan diuji. Menggunakan model analitikal, BLG kepekatan pembawa dan kealiran dalam had merosot dan bukan merosot akan dikaji. Kebolehgerakan pembawa dan arus saliran semasa juga sedang disiasat. Kajian ini juga membentangkan pelaksanaan berangka model yang dibangunkan. Model-model ini menyediakan satu peluang untuk melaksanakan simulasi dalam jumlah masa yang munasabah, yang diperlukan dalam aplikasi besar-besaran bagi meningkatkan kualiti peranti secara optimum disamping mempunyai saiz yang kecil. MATLAB adalah perisian digunakan dalam kaedah berangka yang telah digunakan secara meluas untuk kajian BLG tingkah laku FET. Kajian perbandingan kealiran, kebolehgerakan dan voltan semasa dengan data eksperimen yang diterbitkan menunjukkan persamaan dan penyesuaian yang baik dengan model yang dihasilkan. Model ini boleh digunakan dalam *Technology Computer Aided Design* untuk meningkatkan prestasi peranti nano untuk generasi akan datang.

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LIST OF ABBREVIATIONS

BLG	-	Bilayer Graphene Nanoribbon
CNT	-	Carbon Nanotubes
DOS	-	Density of State
ECAD	-	Electrical Computer Aided Design
FET	-	Field Effect Transistor
GNR	-	Graphene Nanoribbon
IC	-	Integrated Circuit
ITRS	-	International Technology Roadmap for Semiconductor
3D	-	Three-Dimensional
2D	-	Two-Dimensional
1D	-	One-Dimensional
DIBL	-	Drain Induced Barrier Lowering
MOS	-	Metal Oxid Semiconductor
NEGF	-	Non-Equilibrium Green's Function
Q3D	-	Quasi Three-Dimension
Q2D	-	Quasi Two-Dimensional
Q1D	-	Quasi One-Dimensional
Q0D	-	Quasi Zero-Dimensional

RF	-	Radio Frequency
SEM	-	Scanning Electron Microscopy
SLG	-	Single Layer Graphene
S	-	Swing
SiC	-	Silicon Carbide
TB	-	Tight Binding

LIST OF SYMBOLS

a	-	Vector of Lattice
a_{c-c}	-	Carbon-Carbon (C-C) bond length
AC	-	Alternating-current
$\vec{C}$	-	Chiral vector
C°	-	Celsius
$D(E)$	-	Density of State
1D	-	1-Dimensional
2D	-	2-Dimensional
3D	-	3-Dimensional
E_c	-	Conduction band
E_f	-	Fermi energy level
E_g	-	Band gap energy
E_v	-	Valence band
eV	-	Electron-volt
$f(E)$	-	Fermi-Dirac integral
G	-	Conductance
h	-	Plank's Constant
I_D	-	Drain current in a MOSFET
k	-	Wave Vector

k_B	-	Boltzmann's Constant
L	-	Length of the nanoribbon
$m*$	-	Effective mass
N	-	Number of dimer lines
N_c	-	Effective Density of States
n	-	Carrier Concentration
η_f	-	Formalized Fermi energy
N_{1D}	-	Effective Density of State
Q	-	Charge
S	-	Swing
Si	-	Silicon
SiO_2	-	Silicon dioxide
t	-	C-C bonding Energy
T	-	Temperature
v_F	-	Fermi velocity
V_g	-	Gate voltage
V_{Ds}	-	Drain to source voltage
W	-	Effective or electrical channel width
Γ	-	Gamma function
σ	-	Conductivity
γ	-	Fitting parameter
τ	-	Mean collision time
ψ	-	Wavefunction
λ_D	-	De-Broglie wavelength

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CHAPTER 1

INTRODUCTION

1.1 Background

Based on the technology demand for smaller size, higher processing speeds and lower power consumption of metal-oxide-semiconductor field effect transistor (MOSFET) led to the downsizing of channel length. The downsizing of channel of MOSFET transistor has many limitations which severely affect the expected performance of these devices (Eduardo and Castro, 2010). Since 1965, Gordon Moore, one of the Intel co-founder predicted, the number of transistors in a die will approximately double every 24 months. This popular prediction was known as Moor's Low and it has been treated as a guide for the transistor manufacturing even until today. In fulfilling the Moore's law, industry for example Intel has actually exceeded the normal prediction (year 1965 actual data) in year 1970 as shown in Figure 1.1. They have gone beyond Moor‘s prophecy and are able to fabricate recent Core 2 Quad processor with only 45 nm channel length (Connor, 2007; Group, 2010). Figure 1.1 clearly shows that the numbers of transistors in Intel processor are exponentially increase with years.

International Technology Roadmap for semiconductor (ITRS) has pointed out some significant hurdles of these conventional MOSFET, including the leakage current, interconnect problems, power consumption and quantum effect (O'Connor et al, 2007). The MOSFET is expected to reach its channel length limits of 10 nm before year 2020.

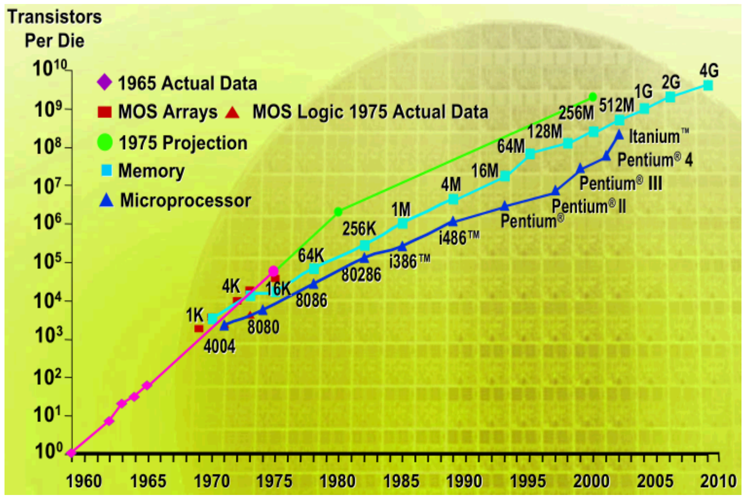

Figure 1.1 Exponential growth of the transistors in Intel processor per year, according to Moore's Law.

Group of researchers declared the first graphene-based field-effect transistor at the Manchester University in 2004 (Fal'ko and Geim 2007; Novoselov 2007). Graphene, the unzipped form of carbon nanotubes (CNT) is the recently discovered allotrope of carbon that has gained tremendous amount of scientific technological interests. The graphene nanoribbon (GNR) is a single graphene that has been developed as a substitute device possibility to replace the CNT chirality challenge and can be used as channel transport region with a narrow channel size in a FET-like device (Novoselov 2007). Theoretically, they are expected to show good electronic properties and very high electron or hole mobility, comparable to the properties observed in CNTs. Graphene is semimetal and does not have a band gap (band gap is zero), but with a narrow channel width (transverse direction) it can provide a band gap (Schwierz, 2010). Hence, there are two methods to explain the band gap and electronic properties in GNR. Material properties like the band gap (E_G) have an important role in graphene transistors. The new development in this transistor by using new material and fabrication method is able to complement or even replace the current silicon technology.

Bilayer graphene nanoribbon (BLG) including two layers graphene plate was developed, in 2006. Researchers observed a low energy band gap at the *k* point in BLG when an electric field is applied (Feng Wang, 2009). Yuanbo Zhang, also have described widely tunable band structure near Dirac point in double layer graphene (Novoselov, McCann et al. 2006; Yuanbo Zhang 2009). Creating a band gap in BLG is very important in FET transistors. BLG devices have a better performance with superior on-off ratio for future application. In 2010, Eduardo and Castro published electronic properties of BLGs (Castro, 2010). This led to the equation of energy band gap and density of state that have effect in the calculation of carrier statistic. They also studied edge properties (zigzag and armchair BLG) at zero energy and the Fermi level of the undoped system (Eduardo, 2010). In this research, we investigate theoretically double layer graphene nanoribbon model in field effect transistor.

1.2 Problem Statements

Conventional methods to improve metal oxide semiconductor (MOSFET) such as downsizing of the channel length have so far succeeded. Some aspects including the short channel effect, leakage current, interconnect difficulties, high power consumption and quantum effect are due to the downsizing of channel length in a planar MOSFET, (O'Connor et al, 2007). Hence, the modeling of conventional devices is no longer precise when the channel lengths get the nanometer scale because of the several unidentified parameters. BLGs have the unique electronic properties, for example, symmetrical band structures, ballistic transport, high current and so on. Therefore, we can enable the development of BLG FET. Our focus is on the modeling of carrier statistic, carrier velocity and mobility in BLG channel and to compare with experimental data. In summary, the problems in this research are:

a) The modeling of carrier concentration (degenerate and non-degenerate approximation) in BLG FET model.

We are used one-dimensional calculation for nanoscale devices. Most of the models calculated carrier concentration based on the Maxwell Boltzmann approximation (degenerate and non-degenerate regime).

b) The modeling of conductance in nanoscale BLG FET model for degenerate and non-degenerate regime.

Only in the Lundstrom work we see the conductance approach for the nanoscale transistor modeling. But their work based on the Maxwell Boltzmann approximation (non-degenerate regime). On the other hand, nanoscale devices operate in degenerate regime. We are investigated the conductance approach in nanoscale BLG FET modeling for both degenerate and non-degenerate regime.

c) Ballistic carrier transport model for BLG FET structure is used in degenerate regime by improving these published charge-based BLG FET models.

Since the carrier transport properties in channel MOSFET model are no longer capable of characteristic the carrier transport truly even for sub-100 nm MOSFETs. Nanoscale transistors operate in quasi-ballistic transport regime.

1.3 Research objectives

This research focused on the modeling and simulating of bilayer graphene nanoribbon FET as a one dimensional device. It included modeling carrier concentration, ballistic conductance, electronic transport properties and current-voltage in BLG FET. Semi-empirical model as a platform of the modeling technique based on device physics formulation is employed. The MATLAB software is used as a main platform to model in BLG field effect transistor. Combined with a Circuit Simulator, it will demonstrate the ultimate application of the full transistors design. The Electronic and Electrical Computer Aided Design (ECAD) tools will be able to assess this model to optimize transistor performance through multiple process and design variations. The objectives of this research are:

a) To analytically model the carrier concentration in degenerate and non-degenerate regime for BLG.

b) To investigate an analytical model for ballistic conductance of BLG in degenerate and non-degenerate limits.

c) To formulate analytical model for carrier transport in BLG FET.

d) To investigate an analytical and semi-empirical model of BLG FET for current-voltage in the linear (Ohmic) region.

e) To compare the numerical results and analytical models with experimental data in terms of their physical structure for BLG FET.

f) To present model can be used through Technology Computer Aided Design (TCAD) tools to improve the performance of next generation devices.

1.4 Research Scopes

In this study, the literature review aids to understand the GNR physic. The scope of research is the development of an analytical BLG FET model in the areas:

a) The development the modeling of BLG FET devices, based on the carrier statistic in degenerate and non-degenerate limit.

b) The enhancement of carrier transport, conductance in degenerate and non-degenerate limit and current-voltage model for BLG.

c) Comparison of the numerical modeled and simulated device with experimental data in terms of their physical structure for BLG FET.

d) MATLAB software is used as the numerical platforms to establish the model development.

1.5 Research Activities

In this research we have investigated the model of double layer graphene nanoribbon field effect transistor. This included the study and development of energy band structure, carrier concentration, ballistic conductance, electronic transport properties and current-voltage in 1D BLG model. The physical phenomena of the model are described with improved Fermi-Dirac function and partial differential equations via simulation of the physical process using MATLAB software. The predefined modeling template can be modified to suit specific applications through equation-based modeling capabilities. The calculated data will be generated via MATLAB to be compared and validated against the experimental data measured from BLG devices published. Basically, the activities require for this research can be divided into four categories which are:

a) Literature review.

b) Modeling the carrier concentration, ballistic conductance, carrier transport and current-voltage (*I-V* characteristic) of BLG transistor.

c) Numerical simulation works: adoption of theoretical developed for BLG transistor using MATLAB software.

d) Comparison study between modeling and experimental data to validate the transistor model.

1.6 Research Flowchart

Two main parts of the work is shown in the flowchart, (Figure 1.2).

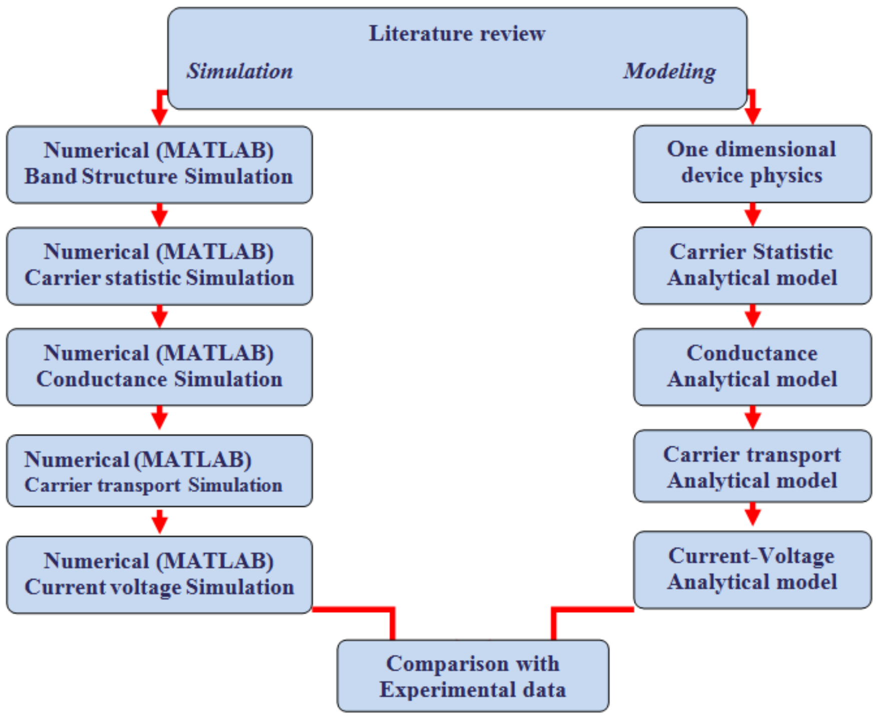

Figure 1.2 Research flow chart

The literature review of one dimensional device included the study in the modeling part and simulation part using MATLAB software. We began with band structure study of bilayer graphene nanoribbon as a basic point of physical view. Then, we are investigated the carrier statistic, ballistic conductance, carrier mobility and current-voltage analytical model in BLG FET. Understanding of band energy helps to find carrier density of states and carrier concentration. We employed these equations in ballistic conductance calculation and then our mobility model is completed by using conductance, and mobility approach for *I-V* characteristic of a BLG FET. In simulation part parallel to the modeling study, MATLAB software programming is used extensively.

1.7 Modeling of BLG

The main assumption taken into explanation for this model is the streamlined ballistic conductance in BLG FET. The effective density of state and carrier concentration in BLG channel was directly affected by conductance. This is due to the type of metal being chosen to be the contacts, which will indeed influences the resistance at the channel-contact interface and thus carrier concentration in the channel. The mobility model in BLG FET is a function of BLG channel length, phonon scattering mean free path and Fermi level of metal electrode. Finally, all the models developed were applied in the *I-V* model to obtain the output characteristics of BLG FET. The comparison between the developed *I-V* model and experimental data will be carried out in order to verify this model.

1.8 Software

1.8.1 MATLAB

In this research, MATLAB software has an important role as the platform for data analysis, processing, and organizing for display into graphs. In order to compare the developed BLG FET model with the experimental data, software such as MATLAB was needed. A few comparisons have carried out in carrier statistic and conductance model for both degenerate and non-degenerate regime. Some parameters such as gate voltage, drain voltage, BLG dimensions, and so on, were taken to be same as the experimental data in order to obtain a fair comparison.

1.9 Outline of Thesis

In this research we are considered the essential physics of quasi-1 dimensional BLG FET. To model an analytical bilayer graphene nanoribbon as well as compare with experimental data. In chapter 2, the literature review on the theory of graphene nanoribbon, one-dimensional concept and some structure device are discussed. Chapter 3 explained the basic concepts of semiconductors that are needed in nanotransistors. There is some new establish on one-dimension physics which is provided a foundation to the rest of the thesis. In chapter 4, the modeling and simulation of BLG including the band structure, carrier statistic, carrier transport, ballistic conductance and current-voltage modeling are presented. Finally, the results, expected outcomes and research works are demonstrated. Then, the comparison between the established BLG FET model and experimental data are carried out in order to validate the proposed equation. The MATLAB modeling on BLG results were reported.

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