DIFFUSION COEFFICIENT TO MOBILITY RATIO IN LOW-DIMENSIONAL NANOSTRUCTURES

ZAHARAH BINTI JOHARI

Submitted to the Faculty of Electrical Engineering
in partial fulfillment of the requirement of the degree of
Master of Engineering (Electrical-Electronics & Telecommunication)

Faculty of Electrical Engineering
Universiti Teknologi Malaysia

JUNE 2009

To my dearest

Father and Mother

Johari Bin Othman & Kamariah Binti Mohd Noordin

Brothers and Sisters

Maimunah Binti Johari

Salim Bin Johari

Atikah Binti Johari

Muhammad Bin Johari

Hakimi Bin Johari

ACKNOWLEDGEMENT

Praise to Allah S.W.T the most merciful and the most compassionate for the guidance and knowledge bestowed upon me, for without it I would not have been able to come this far. Peace is upon him, Muhammad the messenger of God

I wish to express my sincere appreciation to my supervisor, Prof Dr. Vijay K. Arora for his encouragements, guidance and motivations throughout the year and opened my view to the interesting world of Modeling in Nanoelectronics and Semiconductor. I would like to thank Professor Arora for his willingness to spend his time in explaining all the theories and knowledge behind this project.

My sincere appreciation also extends to all my colleagues and lab members who have provided assistance at various occasions. I believed we have spent a great years in UTM and experiencing lots in finishing the Master project. Thank you for making my years in UTM such an enjoyable chapter in my life.

I would like to express my special gratitude to all my lecturers for teaching me. Last but not least to my parents' for their encouragement, motivation, financial support and passionate love.

ABSTRAK

Komponen elektrik semakin mengecil sehingga mencapai domain skala nanometer dimana pengubahsuian perlu dilakukan terhadap sifat-sifat komponen ini bagi memenuhi ciri-ciri sebelum pengubahsuain. Pemalar diffusiviti dan mobiliti adalah dua parameter penting untuk di analisis kerana ia menentukan pergerakan partikel dalam bahan bahan separa pengalir. Peningkatan baru dalam bidang bahan separa pengalir ini telah membawa kepada pengecelian dimensi komponen dari 3-D kepada 2-D dan pengecilan seterusnye oleh satu atau lebih arah cartersian membawa kepada 1-D komponen. Dalam komponen berdimensi rendah, arus diffusiviti tidak boleh di abaikan sepertimana dalam komponen biasa. Dalam komponen yg berketumpatan tinggi, dengan kehadiran kecerunan berketumpatan terhadap komponen itu arus diffusiviti menjadi ketara. Penurunan mobility dan pemalar diffusiviti dalam kedua-dua komponen berketumpatan tinggi dan rendah beserta kehadiran tenga kuantum dan tanpa tenaga kuantum dibincangkan dengan terperinci. Nisbah Einstein yang bersamaan dengan voltan termal V_t bertukar dalam penghampiran berketumpatan tinggi. Dalam bahan berketumpatan tinggi ia adalah dalam sebutan η_d begantung kepada dimensi tertentu. Pada keadaan tenaga elektrik yang tinggi, nisbah ini didarabkan dengan faktor modulator untuk setiap dimensi. Secara kesimpulannya, projek ini telah membuat formulasi terdahap nisbah pemalar diffusiviti kepada penurunan mobiliti untuk kedua-dua bahan berketumpatan tinggi dan rendah dalam keadaan tenaga electric yang rendah dan tinggi.

ABSTRACT

The devices are moving towards nanometer domain where modification to it conventional properties need to be made to fit the modification. Diffusion coefficient and mobility are two important parameters to be analyzed as it determine how well particle moves in a semiconductor. New improvement in semiconductors technology have brought to the shrinking of device dimensions from bulk (3-D) to 2-D nanostructures and further reduction of one or more Cartesian direction to nanoscale results in 1-D nanowire. In low dimensional devices the diffusion current cannot be neglected as it does for conventional devices. In degenerate regime, the diffusion coefficient becoming more important as the concentration gradient is emphasized. The degradation of mobility and diffusion coefficient of both nondegenerate and degenerately-doped low dimensional nanostructure with and without quantum emission is elaborated. The Einstein ratio that was established to be equal to the thermal voltage V_t alter in degenerate approximation which shown to be a function of η_d depending on it dimensionalities. At higher electric field where quantum emission is present, the ratio is modified by the modulating factor. Present project has obtained extensions for the diffusion coefficient to the degraded mobility for both nondegenerate and degenerately-doped nanostructure with varying dimensionalities subjected to low and high electric field.

TABLE OF CONTENTS

CHAPTER	TITLE		PAGE
	DECLARATION		**ii**
	DEDICATION		**iii**
	ACKNOWLEDGEMENT		**iv**
	ABSTRACT		**v**
	ABSTRAK		**vi**
	TABLE OF CONTENT		**vii**
	LIST OF FIGURES		**xi**
	LIST OF ABBREVIATIONS		**xii**
	LIST OF SYMBOLS		**xiv**
1	**INTRODUCTION**		**1**
	1.1	Overview	1
	1.2	Background of Study	1
	1.3	Problem Statement	3
	1.4	Objectives	4
	1.5	Scope of Study	4
	1.6	Research Methodology	5
2	**LITERATURE REVIEW AND THEORY**		**6**
	2.1	Overview	6
	2.2	Three, Two and One Dimensional System	7
	2.3	Carrier Statistic for Low Dimensions and Fermi-Dirac Integral	11
	2.4	Effect of Quantum Emission	17

3	**CARRIER TRANSPORT**		**19**
	3.1	Overview	19
	3.2	Drift and Diffusion	19
	3.3	Mobility Degradation	23
	3.4	Diffusion Coefficient Degradation	27
4	**DIFFUSION COEFFICIENT TO MOBILITY RATIO**		**30**
	4.1	Overview	30
	4.2	Diffusion Coefficient to Mobility Ration in Non-Degenerately-doped	31
	4.3	Diffusion Coefficient to Mobility Ration in Degenerately-doped	32
	4.4	High Field Effect in Degenerately-Doped	36
5	**CONCLUSION AND FUTURE STUDY**		**40**
	5.1	Conclusion	40
	5.2	Future Study	41
REFERENCE			**42**
Appendices A - C			43-61

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE
2.1	The Quasi Low Dimensional System with dimensionalities 3, 2 and 1: (a) Q-3D System, (b) Q-2D System, and (c) Q-1D System	7
2.2	The energy band diagram for a Q-3D system	8
2.3	The energy band diagram for a Q-2D system	9
2.4	The energy band diagram for a Q-1D system	11
2.5	The plot of Fermi versus η for a 3-D System	14
2.6	The plot of Fermi versus η for a 2-D System	15
2.7	The plot of Fermi versus η for a 1-D System	16
3.1	Partially streamlined electron on a titled band diagram in an electric field.	22
3.2	Normalized Mobility to Normalized Electric Field in Non-Degenerate Low Dimensional Nanostructure	25
3.3	Normalized Mobility to Normalized Electric field in Degenerate Low Dimensional Nanostructure	27
3.4	Normalized Diffusion Coefficient to Normalized Electric Field for 1-, 2- and 3-D in Non-degenerate system	29
3.5	Normalized Diffusion Coefficient to Normalized Electric Field for 1-, 2- and 3-D in Degenerate system	30
4.1	Einstein Ratio vs. Normalized Electric Field for Non-degenerate 1-, 2 and 3-dimensional system	32
4.2	Einstein Ratio vs. reduces Fermi energy, η (3-, 2- and 1-D)	35
4. 3	Modulating factor approximation	37
4.4	Diffusivity to Mobility ration for degenerately-doped Nanostructure	39

LIST OF ABBREVIATIONS

CNT	-	Carbon Nanotubes
Q-3D	-	Quasi-Three Dimensional
Q-2D	-	Quasi-Two Dimensional
Q-1D	-	Quasi-One Dimensional
3-D	-	3-Dimensional
2-D	-	2-Dimensional
1-D	-	1-Dimensional

LIST OF SYMBOLS

$k_{x,y,z}$	-	Wave Vector Component
λ_D	-	De Broglie Wavelength
ℓ_o	-	Mean Free Path
V_t	-	Thermal Voltage
η_d	-	Eta depends on Dimensionality
E_f	-	Fermi Energy depends on Dimensionality
ε	-	Electric Field
ε_c	-	Critical Electric Field
μ_d	-	Mobility depends on Dimensionality
μ_{od}	-	Low Field Ohmic Mobility depends on Dimensionality
D_d	-	Diffusion Coefficient depends on Dimensionality
D_{od}	-	Low Field Ohmic Diffusion Coefficient depends on Dimensionality
$\frac{\varepsilon}{\varepsilon_c}$	-	Normalized Electric Field
$\frac{\mu_d}{\mu_{od}}$	-	Normalized Mobility
$\frac{D_d}{D_{od}}$	-	Normalized Diffusion Coefficient
$\hbar\omega_o$	-	Quantum Emission Energy
$\Im_j$	-	Fermi Integral of order j
v_{th}	-	Thermal Velocity

v_{id}	-	Intrinsic Velocity depends on Dimensionality
V_t	-	Thermal Voltage
$\mathfrak{L}(\delta)$	-	Langevin Function
$\frac{I_1(\delta)}{I_o(\delta)}$	-	Bessel Function
q	-	Electron charge

LIST OF APPENDICES

APPENDIX	TITLE	PAGE
A	Gamma Function	42
B	Fermi-Dirac Integral	43
C1.	The program written to plot the degradation of mobility Non-Degenerate system	45
C2.	The program written to plot the degradation of mobility Degenerate system	49
C3.	The program written to plot the degradation of Mobility Degenerate system	51
C4.	The program written to plot the degradation of Diffusion Coefficient Degenerate system	53
C6.	The program to plot Modulating Factor Approximation	55
C5.	The program to plot Diffusion Coefficient to Mobility Ratio In Non-degenerate System	56
C7.	The program to plot Diffusion Coefficient to Mobility Ratio Degenerate System Subjected to a High Electric field	58

CHAPTER 1

INTRODUCTION

1.1 OVERVIEW

This chapter will briefly discuss about the background of studying the diffusivity to mobility ratio in 1-D, 2-D and 3-D. As many devices now are in degenerately-doped, the generalization of Einstein relation is important. The problem statement, objectives and scope of the study will also be discussed later in this chapter.

1.2 BACKGROUND OF STUDY

Nanotechnology is gaining its importance in today's industry where it is widely being discussed and researched by engineers as well as scientists. Nanotechnology has a great potential to be implemented in the biomedicine and semiconductor industry where devices are being scaled down to the nanometer scale. Electronic transport in semiconductors has received considerable attention since the arrival of transistor in 1947. During the last couple of decades, a lot of research has been carried out in this area. This is due to the presence of high electric field in a scale down dimensions where we are now in a sub-100nm regime. New improvement in semiconductors technology has brought to the shrinking of devices dimensions from bulk (3D) to 2D nanostructures where further reduction of one more Cartesian direction to nanoscale results in 1D nanowire. The presence of these low dimensional quantum states with their modified scattering characteristics are giving new problem and new opportunities in the development of new architectures of integrated nano-system.

The velocity, momentum and energy in bulk (3-D) samples are analog quantities that can have any value. When one dimensions is of nanoscale, quantum effects digitize velocity, momentum and energy. This downscaling transform 3D structures to 2-D structures and finally to 1-D nanowire. The presence of quantum waves or state in the design of electronic devices refers to quantum engineering. As explain in [1], the wavelength of a quantum waves described by de Broglie relation falls within the nanometer range. The effect of quantum waves becomes dominant when one or more of the three Cartesian directions are of nanometer regime. With presence of digital character of the electronic in quantum well, it allows a quantum of energy to be emitted when an electron make a transition from exited state to a ground state.

In many solid state device the band structure parameters, doping profiles degenerate or nondegenerate, and ambient temperatures play a variety of roles in determining performance behavior. The outcome that the higher mobility leads to higher saturation is not supported by experimental observations [4]. It has been confirmed in a number of works that the low-field mobility is a function of quantum confinement [1-10]. Mobility and diffusion coefficient is two important parameters in determining carriers transport. In bulk devices, the diffusion parameter might be neglected due to numbers of electrons diffuse is much smaller than the drift. In contrary with low dimensional devices, the diffusion parameter must be taken into account as it is now limited by its size. As many devices now are in degenerately doped, diffusion coefficient is important as it now a function of concentration.

Concentration gradient in degenerately doped in higher than the nondegenerate. Mobility is found to be degraded in high electric field [4, 6].

1.3 PROBLEM STATEMENT

New improvement in semiconductors technology has brought to the shrinking of devices dimensions from bulk (3-D) to 2-D nanostructures where further reduction of one more Cartesian direction to nanoscale results in 1-D nanowire. The presence of these low dimensional quantum states with their modified scattering characteristics are giving new problem and new opportunities in the development of new architectures of integrated nano-system. In extremely high electric field, the distribution of electrons with velocity vectors is favored for those moving against the electric field and disfavoured for those in its direction. That sets the streaming of the electrons with unidirectional velocity vectors giving the velocity that is the intrinsic velocity that is the ultimate saturation velocity and limits the current. The traditional scattering-limited mobility $\mu = v_d / \mathcal{E}$ with constant slope of v_d-E characteristics is to be distinguished from the differential (or signal) mobility $\mu_d = dv_d / d\mathcal{E}$ when v_d-E characteristics are nonlinear. In equilibrium, there is equal a priori probability of electron going in either direction and hence net drift is zero. This equilibrium is perturbed as the bands tilt in a high electric field [1]. The electric dipoles $qE\ell$ of an electron tend to align opposite (antiparallel) to the electric field. The probability enhances by exp $(qE\ell/k_BT)$ in the antiparallel direction and decreases by $\exp(-qE\ell/k_BT)$ in the parallel direction.

The establish Einstein Relation gives diffusion coefficient to mobility ratio equal to the thermal voltage $Vt = 0.0259eV$ at room temperature for nondegenerate semiconductor in a low electric field. In nondegenerately doped, the ratio alters in high electric field where quantum emission is presence. As most devices moved to degenerately doped as well as low dimensional nanostructures, the diffusion coefficient is related to the concentration gradient whereby concentration gradient is higher in degenerately-doped. Mobility is also limited by the dimension of the devices. Thus, the present study have look into the diffusion to mobility ratio in degenerately doped low dimensional nanostructures subjected to both high and low electric field.

1.4 OBJECTIVES

The objectives of the research are as follows:

1.4.1 To assess the quantum factors that transform mobility and diffusion coefficients in 3-, 2-, and 1-dimensional nanostructures.

1.4.2 To investigate the diffusion coefficient to mobility ratio in 3-, 2-, and 1-dimensional nanostructures subjected to a high electric field.

1.4.3 To embrace the relation for degenerately doped low dimensional nanostructure and establish connection with the Einstein ratio that is equal to the thermal voltage.

1.5 SCOPE OF THE STUDY

1.5.1 This research project will first involve the study on the characteristic of low dimensional nanostructures system including the change in the energy band diagram, the change in the density of states as well as in the Fermi-Dirac Distribution function.

1.5.2 The research will then study on a nondegenerate and degenerate-doped for low dimensional nanostructure subjected to both low and high electric field.

1.5.3 Lastly, the diffusion to mobility ratio for degenerately-doped low dimensional nanostructure with the connection with conventional Einstein Relation is formulized.

1.5.4 MATLAB will be the platform for data analysis, processing and organizing for display into graphs.

1.5 RESEARCH METHODOLOGY

The velocity, momentum and energy in bulk (3-D) samples are analog quantities that can have any value. When one of the dimensions is of nanometre scale, quantum effects digitize velocity, momentum and energy. This downscaling transforms 3-D structure to 2-D nanostructure. A further reduction of one more Cartesian direction to nanoscale results in a 1-D nanowire. The diffusion coefficient to mobility ratio for both nondegenerate and degenerate system is delineated. The conventional Einstein ratio will be extended to embrace the degenerate statistic and see how it will enhance with the present of high electric field. One expression for diffusion coefficient to mobility ratio is formulized both for nondegenerate and degenerate system taking into account the high electric field effect. The result will be simulated and presented using MATLAB.