

HIGH FIELD TRANSPORT IN CARBON NANOTUBE

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HIGH FIELD TRANSPORT IN CARBON NANOTUBE

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I declare that this project report entitled “*High Field Transport in Carbon Nanotube*” is the result of my research except as cited in the references. The project report has not been accepted for any degree and is not currently submitted in candidature of any other degree.



Signature :

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To my esteemed and cherished family, friends and all those who have contributed in this project for their continuous support, encouragement and motivation

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ABSTRACT

Projected to be a material of scientific legend, carbon nanotubes (CNTs) exhibit a variety of intriguing electronic properties such as metallic and semiconducting behaviour due to the quantum confinement of electrons in the circumferential direction. The steady-state electronic transport properties of carbon nanotube, including phonon scattering are investigated. High Field Transport spanning the complete landscape of equilibrium to nonequilibrium regimes are examined. The role of chirality in the evaluation of the electronic band structure of CNTs, and the zone folding of graphene, an important precursor for CNT formation are studied. The electron energy dispersion relations are obtained by applying the zone folding technique to the dispersion relation of graphene, which are calculated using the tight binding formalism. Nonequilibrium Arora Distribution Function (NEADF), which is a natural extension of Fermi Dirac distribution function by inclusion of energy gained / absorbed in the mean free part (mfp) forms the strong foundation for analysis, from theoretical perspective.

ABSTRAK

Dijangka menjadi bahan legenda saintifik, karbon nanotubes (CNTs) mempamerkan pelbagai ciri-ciri menarik elektronik seperti logam dan tingkah laku semikonduktor kerana pantang kuantum elektron dalam arah lilitan. Sifat-sifat pengangkutan elektronik keadaan mantap karbon tiub nano, termasuk fonon penyerakan disiasat. Pengangkutan bidang tinggi merangkumi landskap lengkap keseimbangan kepada rejim tak seimbang diteliti. Peranan chirality dalam penilaian struktur elektronik jalur CNTs, dan lipatan zon daripada graphene, seorang pelopor penting untuk pembentukan CNT dikaji. Hubungan serakan tenaga elektron diperolehi dengan menggunakan teknik lipatan zon untuk hubungan sebaran daripada graphene, yang dikira menggunakan formalisme mengikat ketat. Fungsi taburan tak seimbang Arora (NEADF), yang merupakan lanjutan daripada fungsi taburan Fermi Dirac oleh kemasukan tenaga diperolehi / diserap dalam min sebahagian percuma (mfp) membentuk asas yang kukuh untuk analisis, dari perspektif teori.

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LIST OF ABBREVIATIONS

AFM	-	Atomic Force Microscope
BTE	-	Boltzmann Transport Equation
CNT	-	Carbon Nanotube
CNTFET	-	Carbon Nanotube Field Effect Transistor
DNA	-	Deoxyribonucleic Acid
1D	-	One Dimensional
2D	-	Two Dimensional
3D	-	Three Dimensional
I-V	-	Current-Voltage
MATLAB	-	Matrix Laboratory
MFP	-	Mean Free Path
MWCNT	-	Multi-wall Carbon Nanotube
NASA	-	National American Space Agency
NEADF	-	Nonequilibrium Arora Distribution Function
NEGF	-	Nonequilibrium Green Function
NEMS	-	Nano-electromechanical Systems
NNTB	-	Near neighbour Tight Binding
RF	-	Radio Frequency
RFID	-	Radio Frequency Identification
SEM	-	Scanning Electron Microscope
STM	-	Scanning Tunnelling Microscope
SWCNT	-	Single-wall Carbon Nanotube

Tanh	-	Hyperbolic Tan
TEM	-	Transmission Electron Microscope
ULSI	-	Ultra-large Scale Integrated circuit

LIST OF SYMBOLS

\mathcal{E}	-	Electric field
V_{th}	-	Thermal Voltage
L	-	Length
μ	-	Mobility
ℓ	-	Mean Free Path
\hbar	-	Plank Constant divided by 2π (\hbar - bar)
v_{id}	-	Intrinsic Velocity
d	-	Dimensionality
\mathfrak{F}	-	Fermi Dirac Integral Function
μ_{∞}	-	Mobility at low Electric field and long channel
\mathcal{E}_c	-	Critical Electric Field
T_{ud}	-	Unidirectional Temperature
k_B	-	Boltzmann Constant
E	-	Energy
q	-	Charge
λ_D	-	de Broglie Wavelength
τ_t	-	Transit Time
τ_c	-	Collision Time

v_{inj}	-	Injection Velocity
N_o	-	Bose-Einstein Distribution
E_F	-	Fermi Energy
E_c	-	Conduction Band
E_v	-	Valence Band
$I_o(\delta)$	-	Modified Bessel Function of order zero
$n_d(\delta)$	-	Normalized Electrochemical potential
$\mathcal{L}(\delta)$	-	Langevin Function
v_{sat}	-	Saturation Velocity
ℓ_B	-	Ballistic Mean Free path
E_Q	-	Quantum Energy
R	-	Resistance
R_Q	-	Resistance quantum
Γ	-	Gamma Function
$M(\delta)$	-	Modulating Function
m	-	Mass
m^*	-	Effective mass
m_o	-	Electron rest mass
ε	-	Permittivity
E_g	-	Energy Bandgap
g_v	-	Valley Degeneracy

E_{ac}	-	Energy dispersion for Armchair Nanotube
eV	-	Electron Volts

CHAPTER 1

INTRODUCTION

1.1 Introduction

Carbon nanotubes have remarkable potential in nanoscale electronic devices. They are often configured in field effect transistor structures. The important factors that determine the transport properties of CNTs include the wire diameter, which is important for both classical and quantum size effects, material composition, surface conditions, crystal quality, and crystallographic orientation along the wire axis for materials [1]

The determination of the transport properties of a material, namely the response of the electrons in the material to the application of an external electromagnetic field, or a temperature gradient, is the most useful way to classify material properties [2]. The dc conductivity can be used to describe the material as metallic, insulating or semiconducting. But the thermal transport and the effects of a magnetic field can be also important properties to measure [2]. From theoretical perspective, we would like to calculate the relevant transport coefficients in the linear-response regime, where the effect of perturbing fields is taken into account.

The nature of transport in nanodevices in general is dependent on the characteristic length scales of the active region of the device. Electronic transport in low dimensional systems can be categorized into two types-ballistic transport and diffusive transport. The transport is said to be in the diffusive regime if the scattering events are frequent as carriers traverse the active region of the device. In this case, the

transport becomes reasonably approximated by the semiclassical Boltzmann transport equation (BTE). Energy dissipation occurs throughout the device, and the contacts are simply injectors and extractors of carriers near equilibrium. On the other hand, transport is ballistic if no scattering occurs from source to drain, and the wave nature of charge carriers becomes important in terms of quantum mechanical reflection and interference from the structure itself, and the overall description of the transport is in terms of quantum mechanical fluxes and transmission, with energy dissipated in the contact themselves rather than active region of the device [3]

Though the literature has not shown any concrete consistency in the identifiers for high field initiated saturation of drift velocity and current in a nano channel [4], conventional wisdom suggests that a higher mobility leads to a higher saturation velocity. However, this general perception is punctured by a series of experimental observations and theoretical studies [5][6][7][8]. According to Thornber [9], saturation velocity is invariant under scaling of the magnitude of the scattering rates, which brings about alteration in mobility. Similarly, the mobility is invariant under the scaling of the magnitude of momentum, which alters the saturation velocity. Non-equilibrium Arora distribution function [6] (NEADF) is a theoretical formalism that covers very well the landscape from low to high electric field, from nondegenerate to degenerate state, and converging to low dimensional nanosemble.[10]. The crux of NEADF is the realignment of stochastic velocity vectors in equilibrium to unidirectional one, ultimately leading to saturation. NEADF is much simpler than the nonequilibrium Green function (NEGF) [11] that requires extensive numerical computation.

1.2 Problem Statement

High field transport spanning a wide range of temperatures from degenerate to nondegenerate regimes poses great challenge when under experimental and explorative study.

Continuous device scaling going into nanoscale creates new opportunities and new problems for applications in the ultra large scale integrated circuits (ULSI). In the scaled down regime, circuit devices experience substantial departure from the inherent characteristics.

Where possible, the model is compared with experimental data. There is the possibility of arriving at inconclusive result when analysis is based on a single and independent data.

1.3 Objectives

The objectives of this projects are:

1. To explore quantum conductance in carbon nanotubes as electrons transit from a low field to a high field regime.
2. To investigate mobility in a collision-free ballistic transport in a carbon nanotube channel.
3. To explore nonequilibrium Arora Distribution Function with the goal of understanding the saturation velocity that forms the backbone of current-voltage characteristics in metallic CNTs
4. To investigate the novel properties of CNTs that make them suitable for assortment of interesting applications

1.4 Scope

The project is restricted within the following scope:

1. One dimensional (1D) carbon nanotubes form the focus of our study. 2D and 3D nanoparticles such thin films, nanoribbons are not considered
2. The review of band structure of CNTs factors in on graphene as it is fundamental to the formation of CNTs via the roll up process.
3. Metallic CNTs with zero bandgap is the focus for comparison with experimental data from the published literature, although semiconducting modes will be discussed in brief.
4. MATLAB[®] (R2013 version) is used is used as a vehicle for computational work, drawing graphs and possible simulations

1.5 Research Methodology

First and foremost, the literature review of CNTs is carried out, with the goal of discovering the unique properties of CNTs that make candidates for high field transport. This is followed by gathering experimental data from the published literature.

The simulated theoretical model is then compared with the experimental data in order to discover consistency or otherwise of previous work on high transport in CNTs, which will eventually lead to direction for future work

The theoretical frame work is based on nonequilibrium Arora's distribution function, while high field characterization is the direct outcome of the construction of the appropriate MATLAB[®] functions.

1.6 Organisation of the Project

Chapter 2 deals with literature review of CNT band structure. It is divided into three sections. The first section deals with some fundamentals of CNT. Chirality is instrumental to understanding the basic structure of carbon nanotubes. It also discusses CNT lattice structure. The second section considers CNT band structure, particularly, the band structure of arm chair, and zig-zag nanotubes are discussed. The last section of this chapter is devoted to the determination of CNT Brillouin zone.

Chapter 3 looks into the concept of high field distribution in carbon nanotubes. In this chapter, tilted band diagrams and velocity response to electric field are examined. Ballistic mobility and quantum emission are also discussed. It also looks into high field distribution function, concluding with the treatment of degenerate and nondegenerate responses. In chapter 4 applications to CNT are examined. And finally, the conclusion and future recommendations on the project are discussed in chapter 5.

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