Design and Development of a Simulator for Modelling Carbon Nanotube

S Farhana, Z Alam, S Motakabber and S Khan
Department of Electrical and Computer Engineering
Faculty of Engineering, International Islamic University Malaysia

E-mail: farhana.engineer@ieee.org

Abstract. In this paper, a Matlab simulator is developed for modelling of carbon Nanotubes (CNTs). First electronics structure is derived and discussed to facilitate the analysis and modelling of the simulator. Then a calculation is done for electron energy dispersion relations for single-wall zigzag CNTs with different tube indexes. From the analysis of energy dispersion relation, it is derived an analytical models for CNT parameters such as the mobility and the intrinsic carrier concentration. Once obtain the CNT parameters, and then import them to the developed simulator. The simulator is based on the semiconductor equations and quantum effects. Finally the simulator produces the result for optimum modelling of CNT for electronic device application.

1. Introduction
As roadmap, investigators are exploring new paradigms for electronic devices. Carbon nanotubes (CNTs) are being explored as a structure that may play leading role in future electronic systems [1-4]. Carbon nanotubes (CNTs) are sheets of graphite which formed into cylinders. A nanotube with one layer of carbon atoms is single-wall carbon nanotube (SWCNT), and a CNT with multiple layers of carbon atoms is multi-wall carbon nanotube (MWCNT). SWCNT has the ability to act as a conductor (metal) and as a semiconductor as well [5,6]. However, a self-detecting cantilevered CNT-gated FET consisting of a single-walled CNT (SWNT) channel with a multi-walled CNT (MWNT) cantilever functioning as a gate. With this device, the resonance of an MWNT cantilever was detected for the first time as the change in drain current toward the future application of CNT cantilevers to the mass measurement of biological molecules. Theory indicates that CNTs can be metallic or semiconducting according to the fundamental tube indexes (Im) with bandgap of the semiconducting tube depending on the CNT diameter [7].

Low-dimensional carbon, such as single-walled carbon nanotubes (SWNTs) [8-9], graphene [10,11] and hydrogen passivity diamond surface [12,13] has remarkable electronic properties for high frequency electronics. These unusual electronic properties originate from the unique crystal and electronic band structure which provides extremely high carrier mobilities [14,15]. Owing to the high charge mobility of SWNTs and low geometric capacitance, carriers on the tubes can respond to an external electric field in a picoseconds time scale [16]. This very fast response time opens new prospects for high frequency device applications. These drawbacks make single-tube devices
impractical for high frequency electronics. Dense arrays of SWNTs, however, increase the total gate capacitance and the contribution of the fringe capacitance becomes smaller. This paper describes the modelling of the simulator for designing the electronic structure, energy dispersion relation and intrinsic carrier concentration in the following sections.

2. CNT Electronic Structure

Carbon nanotubes (CNTs) which have unique electronic properties are being considered for various next generation device applications like field effect transistors or sensing elements. Due to the tiny radius of carbon nanotubes, the quantization of wavevectors to be quantized in the circumferential direction. Moreover, the thinness of the nanotube's cylindrical shell obviously yields an even shorter length of confinement in the radial direction, thus making the material virtually one-dimensional as far as electron transport is concerned.

2.1. Reciprocal lattice

The primitive cell of a carbon nanotube can be described in the unit vectors:

\[ \mathbf{R}_1 = \frac{a}{2} \left( \sqrt{3} \mathbf{x} + \mathbf{y} \right) \quad \text{and} \quad \mathbf{R}_2 = \frac{a}{2} \left( \sqrt{3} \mathbf{x} - \mathbf{y} \right) \]  

where, \( a = 2.49 \text{ Å} \) is the carbon to carbon atom distance between two carbon atoms.

The reciprocal lattice vectors are of the form [15,16]:

\[ \mathbf{b}_1 = \frac{2\pi}{a} \left( \frac{1}{\sqrt{3}} \mathbf{x} + \mathbf{y} \right) \quad \text{and} \quad \mathbf{b}_2 = \frac{2\pi}{a} \left( \frac{1}{\sqrt{3}} \mathbf{x} - \mathbf{y} \right) \]

2.2. Electronics properties

Armchair tubes: Simple zone folding predicts that if the difference of the \( n, m \): chiral indices is divisible by 3, and then the \( (n, m) \) nanotube is metallic. We shall refer to these nanotubes as "zone folding metallic", or shortly, ZF-M tubes.

Using the following equations to obtain calculate different nanotube.

The chiral vector of the nanotube is defined in (2),

\[ \mathbf{C}_h = n \mathbf{a}_1 + m \mathbf{a}_2 \]  

Length of the chiral vector is the peripheral length of the nanotube:

\[ L = |\mathbf{C}_h| = a \sqrt{n^2 + nm + m^2} \]  

The tube diameter is then given by,

\[ d_t = \frac{L}{\pi} = \frac{a}{\pi} \sqrt{n^2 + nm + m^2} \]  

The bandgap of a single wall nanotube (SWNT) is given by,

\[ E_g = \frac{2\gamma_0 a_{cc}}{d_t} \quad \text{and} \quad d = \gcd(n, m) \]  

if \( (n-m) \) is divisible by 3 then \( dr = 3d \) otherwise, \( dr = d \).

\[ N_{at} = 4 \times \frac{n^2 + m^2 + nm}{dr} \]
3. CNT Simulator

3.1. Energy Dispersion Relation
To account for the CNT-related quantum effects in the CNT-MOSFET channel, we need to determine the band-structure of the CNTs. Due to confinement, the band structure splits into a system of subbands when graphene is wrapped into a CNT. Each of the subbands has a characteristic effective mass, mobility, and band energy minima. We determine the energy levels of CNTs by applying zone-folding methods to graphene [14]. From the two-dimensional (2-D) graphene band diagram, we cut 1-D slices, whose numbers and locations are set by the fundamental tube indexes. The resulting band structure is given in figure 1. We use the bandgap of the CNT and the electron affinity of the graphite to obtain the electron affinities of CNTs. We then calculate CNT affinities by subtracting half the bandgap value of the lowest subband of the CNT from the electron affinity of graphite.

In order to examine the conductivity properties of the nanotube, it is necessary to derive its k relation. This is done by starting from the equivalent relation of a two dimensional graphene lattice. The energy dispersion for carbon nanotubes can be calculated from the electronic structure of graphene. The energy dispersion of graphene is:

\[
E_{2D}(K) = \pm \frac{V_{pp}}{\pi} \left\{ 3 + 2\cos(KR_1) + 2\cos(KR_2) + 2\cos(K(R_1 - R_2)) \right\}^{1/2}
\]

where \( V_{pp} \) is the nearest neighbour transfer integral, \( R_1 \) and \( R_2 \) are the unit cell vectors of a carbon nanotube given in equation (8). The 3d view of energy dispersion relation [17] is shown in figure 1.

![Energy Bandgap in Conduction & Valence Band for (5,3)](image)

**Figure 1.** Plot of the Energy dispersion relation between valence and conduction band

3.2. Density Of States
The allowed k-vectors in momentum space depend on vectors \( K_1 \) and \( K_2 \) as shown in figure 2. It is possible to represent the area in momentum space for a single state as, \( A_{\text{p-state}}^1 = \frac{h^2}{2} |K_1||K_2|/2 \) and a differential area as, \( A_p = \frac{h^2}{2} |K_1| |dk| \), where \( dk \) is in the direction of \( K_2 \) and \( h \) is the Planck’s constant divided by 2\( \pi \). Therefore, the density of states per unit energy can be defined as follows [18]:

\[
D(E) dE = 2 \frac{dA}{A_{\text{p-state}}} = 4 \frac{h^2}{h^2 |K_1||K_2|} |K_1| \frac{d|K_1|}{dE} = \frac{2 |T|}{\pi} \left( \frac{dE}{dk} \right)^{-1}
\]

Where,
\[ K_1 = \frac{(2n + m)b_1 + (2m + n)b_2}{Nd_R} \text{ and } K_2 = \frac{mb_1 - nb_2}{N} \]

\[ n_\text{cnt} = \int_{E_c}^{\infty} D(E)f(E)\,dE \quad (10) \]

where \( D(E) \) is the density of states, \( f(E) \) is the Fermi level, and \( E_c \) is the conduction band minima. Using equations (9), the carrier concentration becomes,

\[ n_\text{cnt} = \sum_{\text{All Bands}} \left[ \frac{4}{\pi V_{ppz} a \sqrt{3}} \int_{E_c}^{\infty} E(E^2 - E^2_{\text{cmin}})^{-1/2} + \left(1 + e^{\frac{E - E_{c}}{K T}}\right)^{-1} \,dE \right] \quad (11) \]

The equation (11) can be simplified using mathematical manipulations to arrive at the following expression:

\[ n_\text{cnt} = \frac{4}{\pi V_{ppz} a \sqrt{3}} \int_{0}^{\infty} (E + E_c)(E^2 + 2E_cE')^{-1/2} \left(1 + e^{\frac{E - E_{c} + E'}{K T}}\right)^{-1} \,dE' \quad (12) \]

The limits of integration have been changed by replacing the variable \( E \) in equation (8) with \( (E, - E) \), where \( E_c \) is the lowest conduction energy. Furthermore, the summation has also been dropped as the Fermi function becomes negligible for conduction energy-minimums beyond the first band.

The integral in equation (12) is still very difficult to solve analytically, nevertheless, by letting \( x = \frac{E_c - E}{K T} \),

\[ n_\text{cnt} = \frac{4 \sqrt{KT}}{\pi V_{ppz} a \sqrt{3}} \int_{0}^{\infty} (KTx + E_c)[x(KTx + 2E_c)]^{-1/2}(1 + e^{x-n})^{-1} \,dx \quad (13) \]

### Figure 2. Density of states plot for a CNT

#### 3.3. CNT Intrinsic Carrier Concentration

With the density of states calculated, it is possible to calculate the carrier concentration of carbon nanotubes. The carrier concentration in any semiconductor is given by [19],

\[ n_\text{cnt} = \int_{E_c}^{\infty} D(E)f(E)\,dE \]

The limits of integration have been changed by replacing the variable \( E \) in equation (8) with \( (E, - E) \), where \( E_c \) is the lowest conduction energy. Furthermore, the summation has also been dropped as the Fermi function becomes negligible for conduction energy-minimums beyond the first band.

The integral in equation (12) is still very difficult to solve analytically, nevertheless, by letting \( x = \frac{E_c - E}{K T} \),

\[ n_\text{cnt} = \frac{4 \sqrt{KT}}{\pi V_{ppz} a \sqrt{3}} \int_{0}^{\infty} (KTx + E_c)[x(KTx + 2E_c)]^{-1/2}(1 + e^{x-n})^{-1} \,dx \quad (13) \]
To investigate the effects of embedding a CNT into a MOSFET, we developed a novel device simulator. One of the fundamental quantities required by our CNT-MOSFET solver is the CNT intrinsic carrier concentration is shown in figure 3. Thus we develop a methodology to obtain the intrinsic concentrations of different tubes. We start from the parabolic energy dispersion approximation. The density of states for each subband is zero for energies less than the energy minimum of that particular subband, and becomes the following for energies greater than the subband energy minimum.

![Figure 3. CNT intrinsic carrier concentration](image)

4. Conclusion
A Matlab simulator is developed for the analysis of carbon Nanotubes (CNTs). A quantum method is derived to develop this simulator. The result shows that this simulator is capable to perform the modelling of CNT by exploring its properties such as energy dispersion relation, density of states and CNT intrinsic carrier concentration. Thus, we concluded that CNT employing higher mobility, lower bandgap carbon Nanotubes appear to exhibit improved capabilities and therefore may represent a new paradigm for devices in the 21st century.

References
[1] Lundstrom M 2003 A top-down look at bottom-up electronics in Symp. VLSI Tech. Dig. pp. 5–8.
[2] Wong H S P 2002 Field effect transistors from silicon MOSFETs to carbon nanotube FETs in Proc. MIEL vol. 1 pp. 103–107.
[3] Guo J, Datta S and Lundstrom M 2002 Assessment of silicon MOS and carbon nanotube FET performance limits using a general theory of ballistic transistors in IEDM Tech. Dig. pp. 29.3.1–29.3.4.
[4] Avouris P 2002 Molecular electronics with carbon nanotubes Acc. Chem. Res. vol. 35 pp. 1026–34.
[5] Navi K, Rashtian M, Hashemipour O, Khatir A, Keshavarzian P 2010 High speed capacitor-inverter based carbon nanotube full adder Nanoscale Research Letters 859:862.
[6] Navi K, Rad R, Moaiyeri M, Momeni A 2010 A low-voltage and energyefficient full adder cell based on carbon nanotube technology Nano Micro Letters 114:120.
[7] Naoyuki M, Takayuki A and Seiji A 2012 A Carbon Nanotube Field-Effect Transistor with a Cantilevered Carbon Nanotube Gate Applied Physics Express 5.
[8] Pennington G and Goldsman N 2003 *Semiclassical transport and phonon scattering on electrons in semiconducting carbon nanotubes* Phys. Rev. B, Condens Matter vol. 68 pp. 45 426-1–45 426-11.

[9] Pennington G and Goldsman N 2003 *Monte Carlo study of electron transport in a carbon nanotube* IEICE Trans. Elect. vol. E86-C, pp. 372–8.

[10] Lin Y M, Dimitrakopoulos C, Jenkins K A, Farmer D B, Chiu H Y, Grill A and Avouris P 2010 *100 GHz transistors from wafer-scale epitaxial graphene* Science 327 662.

[11] Xia F N, Mueller T, Lin Y M, Valdes-Garcia A and Avouris P 2009 *Ultrafast graphene photodetector* Nature Nanotechnol 4 839–43.

[12] Kasu M, Ueda K, Ye H, Yamauchi Y, Sasaki S and Makimoto T 2006 *High RF output power for H-terminated diamond FETs* Diamond Relat. Mater. 15 783–6.

[13] Ueda K, Kasu M, Yamauchi Y, Makimoto T, Schwitters M, Twitchen D J, Scarsbrook G A and Coe S E 2006 *Diamond FET using high-quality polycrystalline diamond with f(T) of 45 GHz and f(max) of 120 GHz* IEEE Electron Device Lett. 27 570–2.

[14] Zhou X J, Park J Y, Huang S M, Liu J and McEuen P L 2005 *Band structure, phonon scattering, and the performance limit of single-walled carbonnanotube transistors* Phys Rev. Lett. 95 146805.

[15] Jimenez D, Cartoixa X, Miranda E, Sune J, Chaves F A and Roche S 2007 *A simple drain current model for Schottky-barrier carbon nanotube field effecttransistors* Nanotechnology 18 025201.

[16] Zhong Z H, Gabor N M, Sharping J E, Gaeta A L and McEuen P L 2008 *Terahertz time-domain measurement of ballistic electron resonance in a single-walled carbon nanotube* Nature Nanotechnol. 3 201–5.

[17] Farhana, S., Alam, A. Z., Motakabber, S., & Khan, S. 2013 *Analysis of CNT electronics structure to design CNTFET* in Nanoelectronics Conference (INEC), 2013 IEEE 5th International (pp. 329-332). IEEE.

[18] Griffiths D. 1995 *Introduction to Quantum Mechanics* Prentice Hall, Inc., Upper Saddle River, NJ.

[19] Shur M. 1990 *Physics of Semiconductor Devices*, Prentice Hall.