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## Study of Carbon NanoTube Field Effect Transistors for NEMS

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### 1. Introduction

The recent developments of Carbon NanoTube Field Effect Transistor (CNTFET) technology indicate the perspective of the Nanoelectromechanical systems (NEMS). Carbon nanotubes (CNT) are ideal candidates for NEMS due to their chemical and physical structures, low masses and exceptional stiffness. Study of NEMS devices in the light of quantum mechanics requires understanding the interplay between the physical, geometrical and electrical parameters of the system (Dang et al., 2006). An analytical representation of (CNT) based field effect transistor is developed for high frequency NEMS applications to examine the characteristics observed from the fabricated devices. The analytical models enable us to gain deep insights of the device performance and behavior. The developed analytical model of CNTFETs represents its viability into transistor applications for NEMS switches, RF circuits, memory cells, field emission displays, biomedical instruments etc (Polash & Huq, 2008).

The metal-nanotube contacts in the CNTFETs are treated as Schottky barriers and analyzed by means of a ballistic model (Natori et al., 2005). The famous Landauer formula is used to calculate the conductance of the tube by relating the energy dependant transmission probability within the tight binding approximation of the CNTFET (Datta, 2000). Transmission function of the CNT is expressed in terms of the Green's functions of the conductors and the coupling of the conductor leads. The Green's function is incorporated with the transfer Hamiltonian approach to calculate the tunneling currents. The non-equilibrium Green's function transport equation is solved iteratively along with a 2D Poisson equation to improve the numerical convergence. The charge density is calculated by integrating the 1D universal density-of-states along with the source-drain Fermi-Dirac distribution function over energy within the energy gap of the CNT. The calculations show that the proposed device can perform stable operation at high current levels ( $670 \mu\text{A}/\mu\text{m}$ ). Upper limits of device characteristics are considered for the model. Degradation in measured data is observed due to the limitations in device fabrication technology and imperfect contact placement on the CNT. Commercialization of CNTs NEMS/sensors is a great challenge due to the price and size of such measuring equipments (Fujita et al., 2007). When small bias current is used, resistance measurement of CNTs sensor becomes difficult and high accuracy current source and analogue to digital converter (ADC) are required to maintain a reasonable signal to noise ratio (SNR). Controlled growth of CNT is yet to be

mastered (Javey et al., 2005). In situ coupling of source/drain to CNT mechanism needs to be idealized for better approximating the NEMS performance. Replacing the metal-CNT SB contact with highly doped CNT source/drain (ohmic like) contact could improve the NEMS performance.

## 2. CNTFETs and NEMS

Carbon nanotubes are nano size ( $10^{-9}$ ) Carbon atom made tubes with nanostructure and are wrapped into the form of a cylinders with graphene sheet. There are two basic tube structures: SWNT-Single-Walled NanoTube and MWNT- Multi-Walled NanoTube (Reich et al., 2004). Carbon nanotubes are being used in day to day applications. Advances in medicine are being contributed to Carbon nanotubes in some way (Kam & Wong, 2005). One of the advances that researchers are working on, is CNT based devices such as nanoshells, NEMS, and quantum dots and their properties. Using these electronics devices such as NEMS (nano-electro-mechanical-systems); it will be possible to carry DNA to cancerous cells and destroy them with minimal damage to surrounding healthy cells through methods. CNT based FET devices propose that by working with smart NEMS, it is possible to destroy only cancerous cells leaving healthy untouched. This devices will be able to know and identify threats of cancer cells.

CNT based micro/nano objects or devices can be comprised of a range of miniature structures, including cantilevers and diaphragms, static structures, chemically sensitive surfaces and electrical devices (resistors and FETs). Devices used for NEMs are valves, mixers and pumps and CNTFET can act as an active valve or controlled switch.

Reasons for minaturization of NEMS using CNTFETs can be summerised as follows (i) reducing the sensor element to the scale of the target species and hence providing a higher sensitivity (ii) reduced reagent volumes and associated costs, (iii) reduced time to result due to small volumes resulting in higher effective concentrations, (iv) amenability of portability and miniaturization of the entire system (v) point-of-care diagnostic, (vi) Multi-agent detection capability (Gruner., 2006).

Materials requirements are different from NEMS to NEMS and it is even more important for CNTFET based-NEMS. Desired properties of NEMS materials shows biocompatible, chemically modifiable, easy to fabricate, economic and soft compliable. Because of their dimensions and the good electrical, mechanical, chemical and physical properties CNTFETs make great emitter of electrical fields. These devices exhibit a wide range of favorable electrical properties (Hoenlein et al., 2003); some of them are presented below:

- High transconductance. This property determines the performance of any FET. given that a higher transconductance results in greater gain or amplification.
- Superior threshold voltage.
- Superior subthreshold slope. This property is very important for low power applications.
- High mobility.
- Ballistic transport. This property results in high speed devices .
- High current density.
- High on / off current ratios.

Electrical applications are arising each day, and not only in integrated circuits but nanotubes are also being used in auto industry, medical science, mechanical system, electronics, and recreational purposes.

Researchers in nano technology have encounter barriers that slow down it's progress especially in the medical field. We have seen that this study could lead to a potential cure for cancer however studies have shown that the toxicity of carbon can be lethal to humans. According to an article publish in the U.S National Library of Medicine and the National Institute of Health, they examine the impact of CNTs under different conditions, nanotubes could cross membrane barrier and reach organs and could induce harmful effects as inflammatory and fibrotic reactions in vital organs (Kam & Nadine 2005).

### 3. CNTFETs device structure

Carbon nanotube field effect transistors (CNTFETs) exhibited promising characteristics through experiments, yet the underlying mechanism is not fully understood (Lin et al., 2005). Theoretical analysis of CNTFETs with Schottky barriers (SB) is represented by means of a ballistic transport within quantum transport regime (Hasan et al., 2006). Due to outstanding electrical and mechanical characteristics, high-speed operation of two terminals or three terminal CNTFET-NEMS switches have been demonstrated. They are expected to use in memory circuits or RF switches.

Carbon nanotubes are single atomic layer thick sheet of graphite rolled into seamless cylinders with nanometer dimensions. Since the invention in 1991 by S. Iijima, CNTs have drawn great attention of researchers because of their extraordinary chemical, physical, and electrical properties. CNT can be metallic or semiconducting based on the direction of graphene sheet roll (Iijima et al., 1992). Understanding in detail the nature of the direction of graphene sheet roll is therefore an important ingredient in the development of reliable CNT NEMS. Minimal series resistance and quantum effects in CNT based NEMS switches govern the electron flow which causes ballistic transport.

The channel of the proposed device is formed with a (13, 0) CNT which has a diameter of 1nm and length is 15nm. Source and drain electrodes are placed at the ends of nanotube length while the gate electrode is co-axially placed along the tube axis. High- $\kappa$  (~25) dielectric zirconium oxide (ZrO<sub>2</sub>) is used for gate insulation. The drain is biased with external voltage source and the source is connected to the ground. The electronic properties of a nanotube derived from the dispersion relation of a graphite sheet with wave vectors ( $k_x$ ,  $k_y$ ) is given by (Khan et al., 2007);

$$E(k_x, k_y) = \pm \gamma \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)} \quad (1)$$

$\gamma$  is the nearest neighbor-hopping parameter and  $a$  is lattice constant.

$\gamma = 2.5 \sim 3.2$  from different measurements and  $a = 0.246$  nm.

Imposing boundary condition along the tube circumference quantizes the two dimensional wave vector

$$(k_x, k_y) \cdot \mathbf{C} = 2\pi q \quad (2)$$

$$\mathbf{C} = n\mathbf{a}_1 + m\mathbf{a}_2 \quad (3)$$

where **C** is the chiral vector of the nanotube having and *n,m,q* are integers. This leads to the condition at which metallic conductance occurs which is

$$(n - m) = 3q$$

(4)

The above condition suggests that 1/3rd of the tubes are metallic and 2/3rd are semi conducting. It has also been found that when *m*=0, the energy density of states is the highest which reveals the best semi conducting properties [Someya et al., 2003]. Figure 1 shows the schematic representation of a coaxially gated CNTFET with Non-equilibrium Green’s function (NEGF) quantities (Rahman et al., 2003).

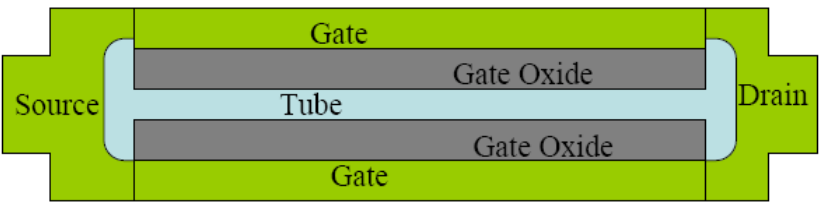


Fig. 1. Schematic representation of a coaxially gated CNTFET with NEGF quantities

4. Modelling of CNTFETs

Energy gap for a semiconducting nanotube is dependent on tube diameter and is given by

$$E_g = \frac{2d_{cc}\gamma}{D}$$

(5)

For a (13, 0) nanotube, the tube diameter is 1nm, *dcc* = 0.1421 nm and *γ* = 3.00 gives the energy gap of 0.8526 eV. It is reported that there exist characteristic end states at the end of single-wall CNTs. The parameters used in the proposed model and calculations are listed in Table 1.

Energy Gap	0.75 eV	Temperature	300K
Gate Oxide Thickness	2nm	Source Fermi level	-0.32eV
Gate Dielectric constant	25	Gate Control Parameter	0.88eV
CNT Diameter	1nm	Drain Control Parameter	0.035eV

Table 1. parameters of the proposed cntfet

Conductance between two leads source and drain is defined in terms of current and voltage: *I*=*G**V*.

Using Landauer formula, conductance is expressed by the following equations:

$$G = 2 q^2 T / h \quad (6)$$

Where  $q$  is the charge of electron and  $h$  is the Planck's constant.

$T$  is known as the transmission function in terms of energy that represents the probability of an electron injected at one end of a conductor will emit at the other end.  $T$  can be expressed as

$$T = \text{trace} (\Gamma_S G_0^r \Gamma_D G_0^a) \quad (7)$$

$G_0^r$   $G_0^a$  represents the retarded and advanced Green's function of the nanotube and  $\Gamma_{D,S}$  are the coupling of the CNT to the source and the drain. The retarded Green's function is calculated by NEGF formulation:

$$G_0^r = (EI - H - \Sigma_S - \Sigma_D)^{-1} \quad (8)$$

Where  $E$  is Fermi energy,  $I$  is the identity matrix,  $H$  is the Hamiltonian of the nanotube.  $\Sigma_{D,S}$  is the self energy terms at the source and drain coupling of the contacts are the calculated using the broadening function of the self energy terms at the source and drain:

$$\Gamma_{S,D} = i (\Sigma_{S,D} - \Sigma_{S,D}^+) \quad (9)$$

The nanotube behaves as the conducting channel in the CNTFET from the source to drain; it depends on the current density of the tube. The current density is a measure of the density of flow of an electric current per unit area across a section. The current density is an area density described by  $J$ . The current through an area  $A$  is simply the flux of the current density through that area as show below:

$$\bar{I} = \int \bar{J} \cdot d\bar{A}$$

If the flow of the current is through a uniform area  $I = JA$

Using the charge density within the device, the NEGF transport equation is solved iteratively with the poisson equation until self-consistent potential distribution is found. Finally the current is calculated using the Landauer Böttiker expression:

$$I_d = \frac{4d \int T(E) [f_S(E) - f_D(E)] dE}{h} \quad (10)$$

$T$  is the transmission probability across the source/drain;  $f_S$  and  $f_D$  are the source/drain Fermi-Dirac distribution functions consistent potential; The equation is solved simultaneously to evaluate and characterize the performance of these devices.



## 5. Simulation results

The nanoHUB is a rich, web-based resource for research, education and collaboration in nanotechnology. NanoHUB.org was created by the National Science Foundation and the funded the Network for Computational Nanotechnology (NCN). The NCN is a network of universities with a vision to pioneer the development of nanotechnology, from science to manufacturing through innovative theory, exploratory simulation, and novel cyber infrastructure. The research work goes from Nano-bio, nano-electromechanical systems, nano-electronics to special projects, providing information for nanoHUB to grow. This simulation tool is available at nanoHUB.org and creates a 3D image of the nanotube and gives the “Energy vs. Axial Wave Vector”, the “Lowest Sub-band” and the “Density of States (DOS) vs. Energy”.

### 5.1 I-V Characteristics

The FETToy is a tool that simulates the ballistic I-V characteristics of MOSFET. It simulates from single gate MOSFET to double gate MOSFET to Silicon Nanowire MOSFET and Carbon Nanotube MOSFET. Using the simulation tool the characteristics of CNTFET is investigated with different device structure and applied voltages.

The FETToy simulates the I-V characteristics under a certain biased condition where the Gate Control Parameter and the Drain Control Parameter should be less than or equal to 1. The simulation models the drain voltage  $V_D$  at 1 volt. The thickness of the oxide layer and the carbon nanotube diameter determine the performance of the CNTFETs. The thicker the oxide the less voltage will go through the insulator as well as the bigger the diameter the more current density it could develop.

The gate insulator is varied from 1.5nm to 4.5nm, the gate controlled parameter and drain control parameters are varied from 0 to 1 and the diameter of CNT is varied from 0.1nm to 10nm. If the gate control parameter and the drain control parameters are increased, the drain current increases significantly. This increases the drain current by 24.3uA. This current also depends on the thickness of the oxide layer. The current reduces by a factor of 6.7uA at the saturation region where the drain voltage is 1 volt. At a diameter of 0.1nm, the results show a very low drain current figure 2. At a diameter of 1nm, the current coming out of the drain is drastically changing from 3uA to approximately 28uA. The drain current reaches approximately 78uA at the diameter of 10 nm figure 3. The bigger diameter allows higher drain current. The fact is that the triode region and the saturation region are depending on the diameter, unlike the MOSFET depending of the channel pinch off.

### 5.2 Transconductance Behavior

In order to achieve a relatively large transconductance the CNT must have large diameter. The larger the transconductance, the greater the gain it will deliver. However the increase of  $g_m$  at larger  $V_{GS}$  has the disadvantage of reducing the allowable voltage signals swing at the drain. As the diameter gets smaller this reduces the carrier mobility, changing the transconductance. The transconductance behavior is obtained at 1nm diameter, with different gate and drain voltage. The transconductance varies by a factor of 10/V depending on the amount of voltage applied to the gate (figure 4,5). However, the increase of  $V_G$  will reduce the allowed voltage signal through the drain.

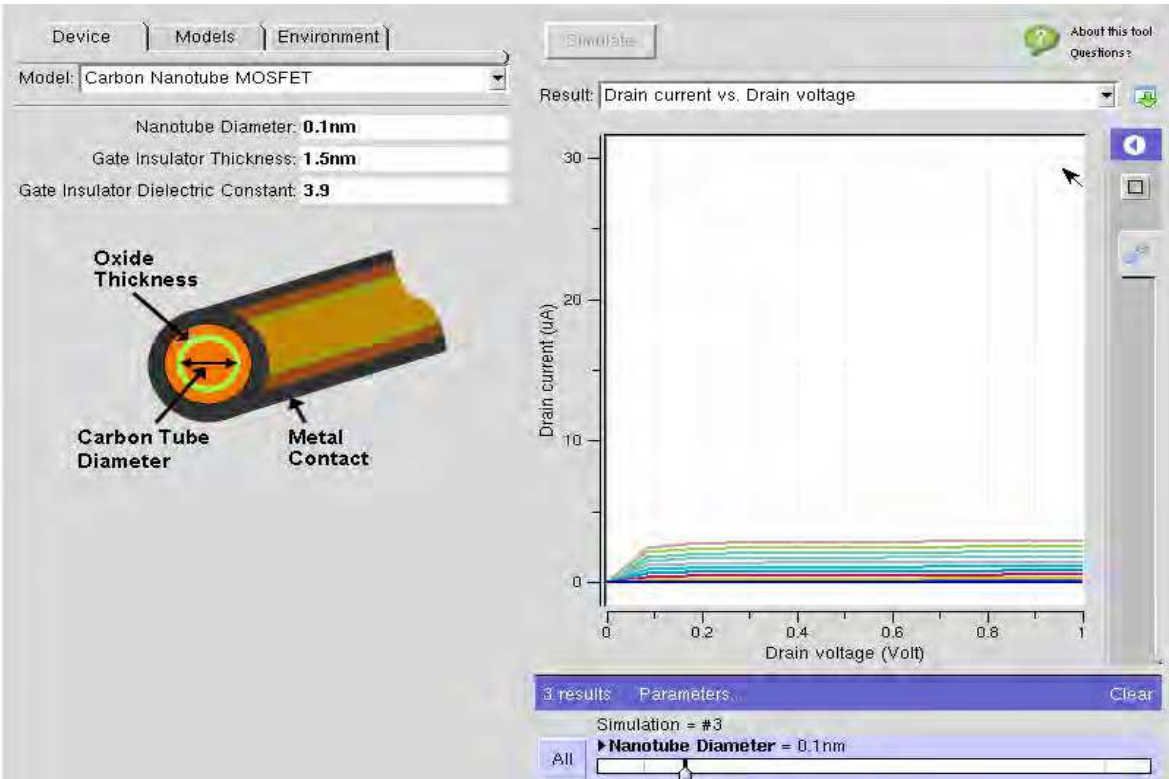


Fig. 2. I-V charecteristics of CNTFET at a diameter of 0.1nm

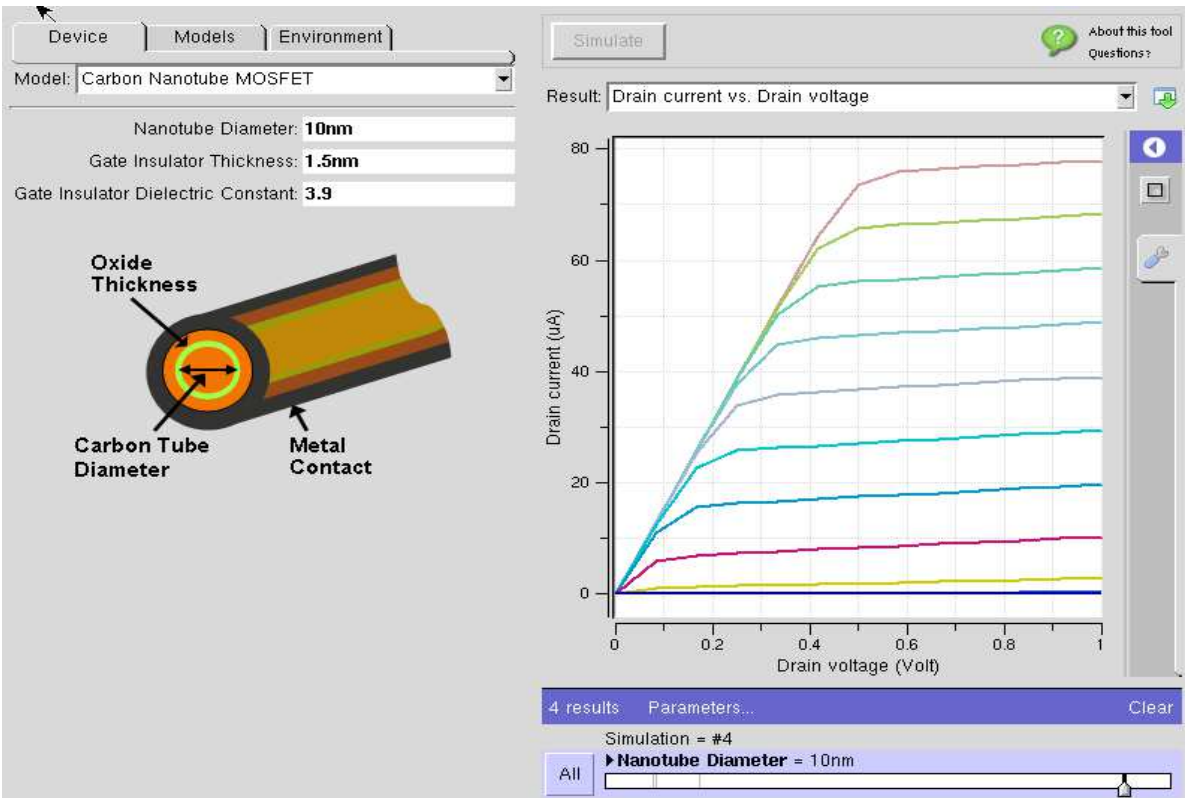


Fig. 3. I-V charecteristics of CNTFET at a diameter of 10 nm



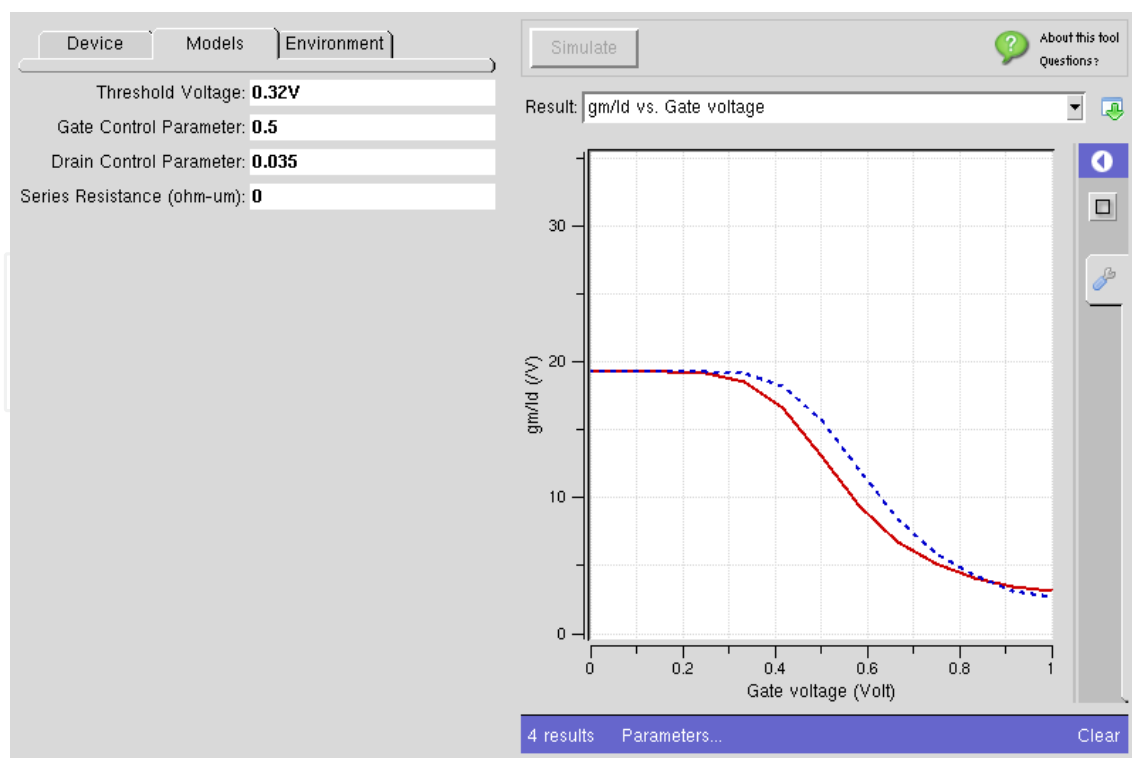


Fig. 4. Transconductance behavior of CNTFET (  $V_D= 0.5V$ )

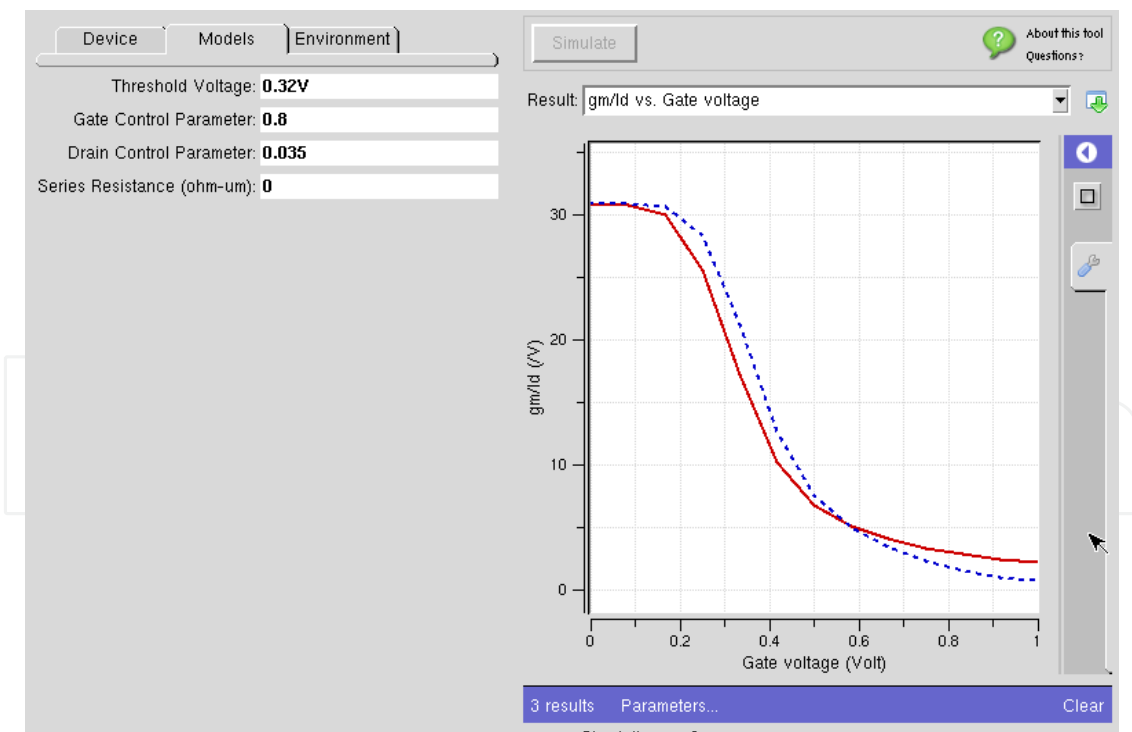


Fig. 5. Transconductance behavior of CNTFET (  $V_D= 0.8V$ )

6. Results analysis

Figure 6 shows the density of state (DOS) of different types of nanotubes with respect to energy gap. The simulation is done by using ‘CNTbands 2.0’ available from [www.nanohub.org](http://www.nanohub.org). The simulated end states are within the energy gap of semiconducting CNTs, implying that the end states are a 1-D analogy with conventional surface states. At metal-semiconductor (M-S) CNT junctions, however, no interface state was experimentally manifested, whereas some electronic states of semiconducting CNT diffuse into the metallic CNT across an M-S CNT. The calculated band gaps are in good agreement with those calculated within local density approximation. The band gaps of CNTs are small (from 0.2 to 2.0 eV), so CNTs are either metallic or semiconductive. The energy band structures of carbon atom C provides an occupied energy level in the band gap depending upon the DOS and types of CNT. The (13, 0) nanotube acts as semi conducting material since it has energy gap between conduction and valence band. The (10, 10) nanotube and the (10, 5) nanotube act as conducting material as the valance and conduction bands are overlapping. The electron can be excited more easily from valance band level to conducting band than that from filled band. This excited electron leads this kind of nanotube to be conductive as that of N-type semiconductor. The energy gap of this kind of CNT is small, so the valance level can easily provide electrons to the conducting band. Therefore, it is the energy gap, DOS and types of CNT that determines the conductivity of the material. The FETToy tool available in the website [www.nanohub.org](http://www.nanohub.org) is useful to observe the characteristics of carbon nanotube FET, which is considered having cylindrical geometry. Using the simulation tool the different characteristics of the CNTFET are obtained.

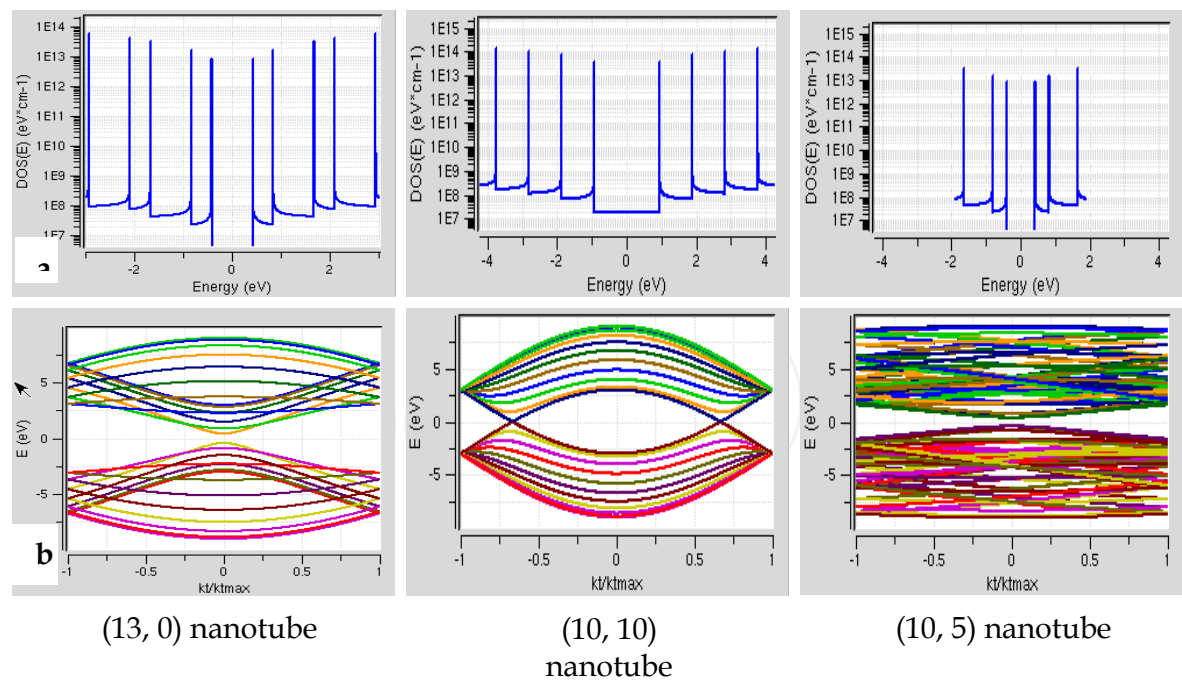


Fig. 6. (a): Energy Density of state (DOS); (b): Energy gap of different types of nanotubes  
The input parameters used in the simulation are presented in Table 2. Figure 7(a) shows the output characteristics of the CNTFET. The output characteristics indicate MOSFET like behavior. The channel allows the current flow when the gate voltage is greater than 0.26V.

As a result, the on-current is  $9.660\text{e-}05\text{ A}$  at  $V_g=1.20\text{V}$  and  $V_d=1.20\text{V}$ , and the off-current is  $8.665\text{e-}11\text{ A}$  at  $V_g=0.00\text{V}$  and  $V_d=1.20\text{V}$ . The FETToy tool also produced six more different plots which are useful to understand the behavior of this transistor. Figure 7(b) presents the average velocity versus the gate voltage at saturation region. Figure 8(a) show the mobile charge behavior as a function of gate voltage. In Figure 8 (b) the mobile charge versus the drain voltage is shown at different gate voltages. It is noticed that increasing the drain voltage beyond a specific value has no longer an effect on the shape of the curves since the mobile charge remains constant. It is also observed that low drain voltage produces higher mobile charge and high drain voltage produces lower mobile charge. Figure 9 (a) shows the quantum capacitance versus the gate voltage at different drain voltages. It is noted that a higher quantum capacitance can be reached at a gate voltage greater than  $0.3\text{V}$ . Lower drain voltage shows significant capacitance effect. Figure 9 (b) shows the transconductance behavior as a function of the gate voltage with different drain voltages.

Gate insulator thickness:	2e-09 (m)	Temperature:	300 (K)
Insulator dielectric constant:	25	Initial gate voltage:	0 (eV)
Threshold voltage:	0.32	Final gate voltage:	1.2 (eV)
Gate control parameter:	0.88	Number of bias points (gate):	15
Drain control parameter:	0.035	Initial drain voltage:	0 (eV)
Series Resistance:	0 (ohms)	Final drain voltage:	1.2 (eV)
NT diameter:	1e-09 (m)	Number of bias points (drain):	30

Table 2. input parameters for simulation

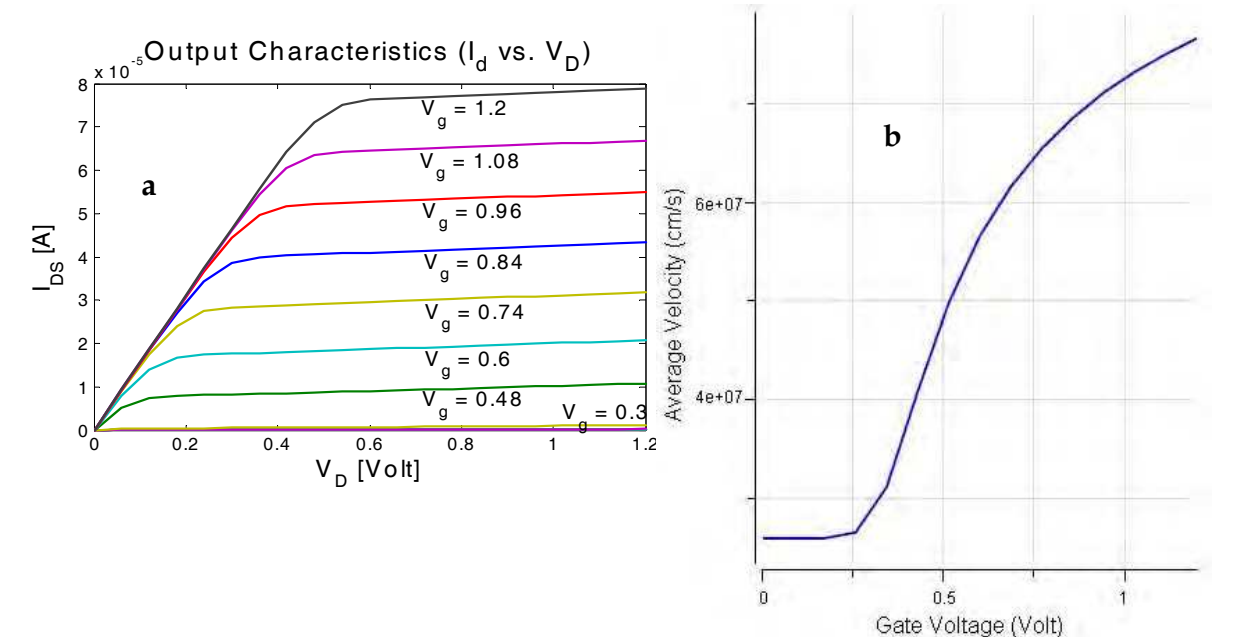


Fig. 7. (a): Output characteristics indicate MOSFET like behavior; (b): Average velocity vs. Gate voltage

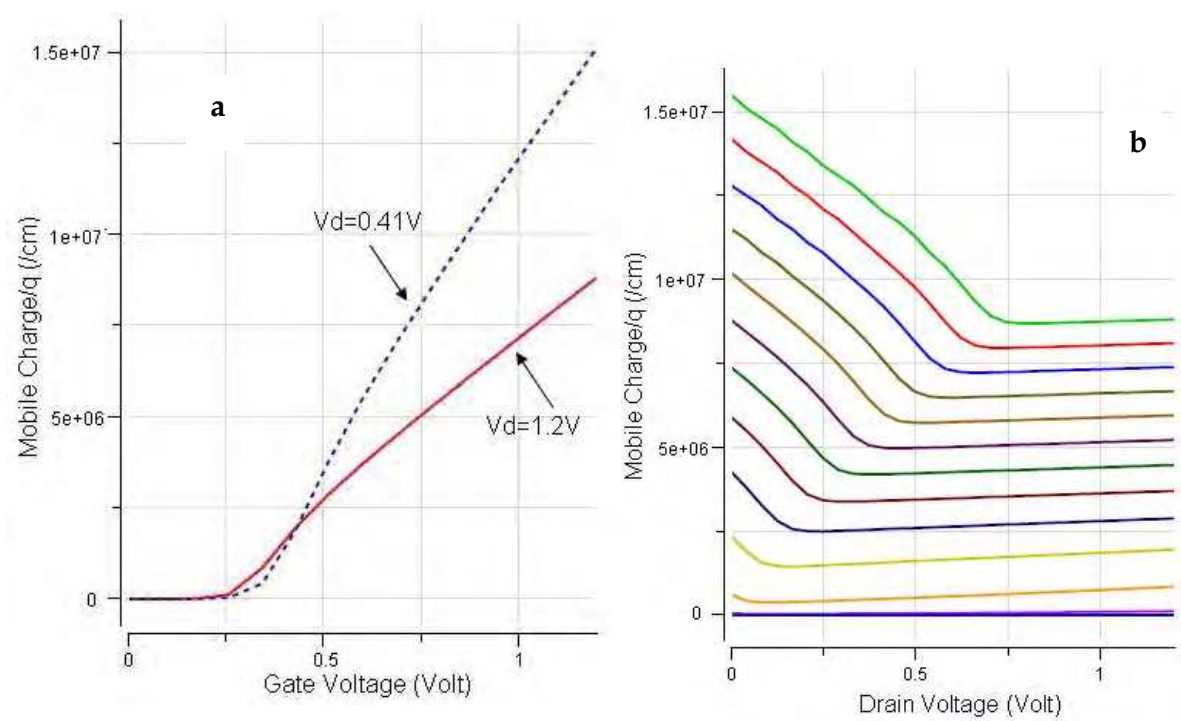


Fig. 8. (a): Mobile charge vs. Gate voltage; (b): Mobile charge vs. Drain voltage

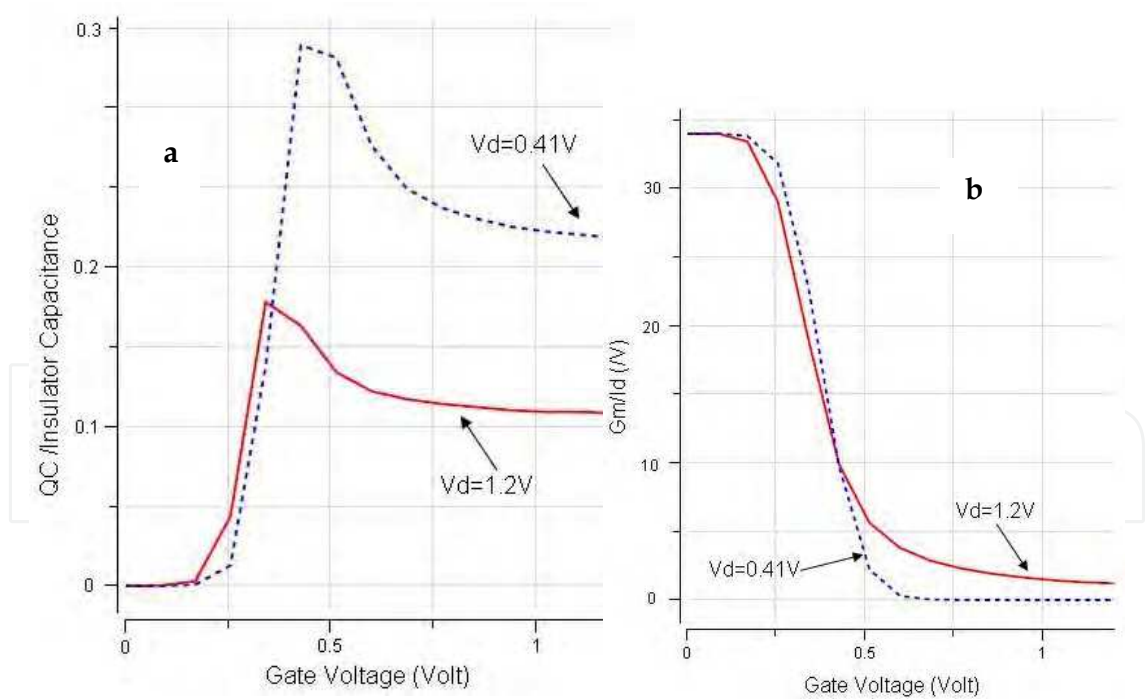


Fig. 9. (a): QC/Insulator Capacitance vs. Gate voltage; (b): Transconductance behavior as a function of Gate voltage

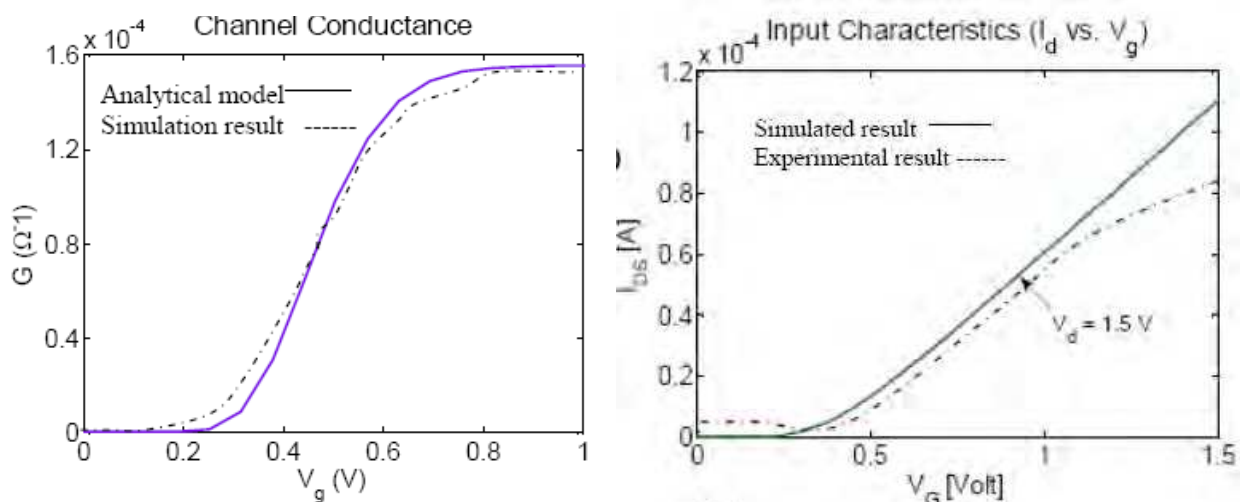


Fig. 10. (a): Channel conductance is saturated after certain gate voltage; (b): Transfer characteristics of the CNTFET shows on current for small bias voltage

Preliminary results from the analytical model and the measured data at room temperature presented in (Someya et al., 2003) demonstrate the feasibility of the developed model. The channel transconductance behaviors as a function of gate voltage are presented in Figure 10(a). The simulated results are compared with the analytical model. The transfer current voltage characteristics are compared with the experimental data in Figure 10(b) at room temperature. The channel conductance approaches the quantum conductance  $4q^2/h$  ( $1.5 \times 10^{-4}$  S) indicates the ballistic transport in the channel. The conductance is largely controlled by the electric field at the contact rather than the electrostatic potential. The SB height is determined by the metal work function which governs the current flow in the channel. Current saturates slower for a larger SB height. The device saturates at a small bias voltage. CNTFET model input characteristics indicates that the transistor is *n*-type. The device becomes *p*-type in presence of oxygen as the Fermi level at the metal-nanotube interface is shifted toward the valence band, allowing for hole conduction. If the same device annealed in vacuum, the Fermi level shifts toward the conduction band and favors electron injection, thus producing an *n*-type FET. Analytical formulation of CNTFET properties using ballistic transport properties with SB is presented. The calculations show that the proposed device can perform stable operation at high current levels ( $\sim 70 \mu\text{A}$ ). Upper limits of device characteristics are considered for the model. Degradation in measured data is observed due to the limitations in device fabrication technology and imperfect contact placement on the CNT.

## 7. Conclusion

The development and the dimensions of carbon nanotubes make the transistor a challenge to develop and to control the aspects of it, such as threshold voltage, maximum drain current, maximum transconductance. The investigated characteristics of CNTFETs represent its viability into transistor applications for NEMS switches, memory cells, field emission displays, biomedical instruments etc (Singh, 2005). Even with pessimistic assumptions,



CNTFET nanoelectronics can achieve significantly greater performance at a fraction of resource than of silicon technology. The understanding of CNTFET device physics should prove useful in optimizing device designs (Javey et al., 2002). The electronic conductivity and the thermal conductivity of CNTs are as good as or even better than those of noble metals (Mizutani et al., 2008). The mechanical strength of CNTs is extremely high. Significant system benefits are anticipated from CNT based electronics devices; however, there are many technological and material challenges for them. Localized oxidation on the CNT is critical for developing such devices (Tsang, 2003). Controlled growth of CNT is yet to be mastered. In situ coupling of source/drain to CNT mechanism needs to be idealized for better approximating the device performance. Replacing the metal-CNT SB contact with highly doped CNT source/drain (ohmic like) contact could improve the device performance (Javey et al., 2002).

It is possible to explore CNTFETs, especially in the area of optoelectronic devices, where electron and holes carriers are being recombined in a variety of different mechanisms. CNTs are direct-gap material and, as such, they directly absorb and emit light, thus possibly enabling a future optoelectronics technology based on SWCNTs. (Tenne, 2008); so it can be used as light emitters or a light detector depending on the biasing. The American Institute of Physics states that the ambipolar behavior of CNTFETs, even though tends to create a current leakage, if modified can lead to be recombined and give off the recombination energy in the form of light.

Silicon contains dangling bonds. These bonds are defects that affect the flow of electrons, however, carbon does not have surface dangling bonds as silicon does and so there is no need to use silicon dioxide as the gate insulator, the electrons will flow from the source to the gate without dangling bonds; this shows better performance in CNTFETs. CNTFET involves no doping and also allows control of the emission intensity and the position of the emitting spot.

Although major research is needed to achieve the goal of modifying the behavior of CNTFET, the progress made up to this date envisions a future for CNT based electronics (Singh et al., 2005). The different characteristics that carbon nanotubes have by altering their coefficient are amazing. The armchair characterizes lead to a metallic conductive tube, however the flexibility of the Zig-zag and chiral could be defined as both with respect to the different  $n$  and  $m$ . The nanoHUB community creates friendly user simulation environment that are not only makes it easy to use but makes the student learn by altering the different outcomes to deal with during the simulation.

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This book has been outlined as follows: A review on the literature and increasing research interests in the field of carbon nanotubes. Fabrication techniques followed by an analysis on the physical properties of carbon nanotubes. The device physics of implemented carbon nanotubes applications along with proposed models in an effort to describe their behavior in circuits and interconnects. And ultimately, the book pursues a significant amount of work in applications of carbon nanotubes in sensors, nanoparticles and nanostructures, and biotechnology. Readers of this book should have a strong background on physical electronics and semiconductor device physics. Philanthropists and readers with strong background in quantum transport physics and semiconductors materials could definitely benefit from the results presented in the chapters of this book. Especially, those with research interests in the areas of nanoparticles and nanotechnology.

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