Effect of Metal and Carbon Nanotube Interface on Carbon Nanotube Field Effect Transistors (CN-FETs)

H. Arabshahi and G. R. Ebrahimi

1Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran
2Department of Metallurgy, Sabzevar Tarbiat Moallem University, Sabzevar, Iran
Email: g.rebrahimi@yahoo.com

ABSTRACT

A computational model for studying the metal and nanotube interface layer properties in Carbon nanotube field effect transistors (CNT-FETs) has been carried out. The CNT-FETs can be fabricated both with Ohmic and Schottky contacts. Here we have focused on Schottky barrier which operate by modulating the transmission coefficient of carriers through the Schottky barrier. The behavior of the devices has been studied by using Landauer-Buttiker formalism. Finally the variation of current versus channel properties, voltage and other properties has been calculated via our model. The ambipolar behavior was explained based on the Schottky-barrier-controlled transistor model, where the transistor action occurs primarily by changing the Schottky contact resistance by the gate voltage. The calculation results show a fair agreement with other theoretical and experimental results.

KEYWORDS: Carbon nanotube; transmission coefficient; Landauer-Buttiker.

INTRODUCTION

Carbon nanotube field effect transistors (CNT-FETs) have been studied in recent years as potential alternatives to CMOS devices. A CNT can be viewed as a rolled-up sheet of graphene with a diameter of a few nano-meters. Depending on the chiral angle the CNT can be either metallic or semiconducting. Semiconducting CNTs can be used as channels for transistors. The non-equilibrium Green’s function (NEGF) method has been successfully utilized to investigate the characteristics of nano-scale silicon transistors [1], CNT-FETs [2], and molecular devices [3]. To extend our previous works [4,5], the NEGF formalism is employed to study the effect of inelastic electron-phonon interaction on the on-current and gate delay time of CNT-FETs in more detail. In CNT-Fets metallic electrodes act as source and drain and CNT between them is a channel for passing carriers. In this research we have chosen a zigzag CNT which has semiconductor properties. With regard to characteristics of CNTs and their similarity to quantum wire, we consider them as a one dimension system that carriers can not dispersion in it and their transportation will be in ballistic form [7-9].

Contacts between metals and CNT lead to form Schottky barrier which its potential is about half of the band gap energy. In this research we import the Schottky barrier height as a variation parameter. Temperature is the other variation parameter which has been considered in our calculation. Our model can be used for all types of semi-conducting Carbon nanotubes. This paper is organized as follows. Details of the employed simulation model is presented in section 2 and the results of transient electron transport properties carried out on CNT-FETs structures are interpreted in section 3.

SIMULATION MODEL

Band diagram of a CNT-FETs with zigzag channel is shown in figure 1. As it can be seen there is three regions, two regions at the ends of nanotube and intermediate region where ballistic electron transport accuse.

Energy band diagram in left and right is calculated by solving one dimensional Laplace equation along the transport direction as

$$\nabla^2 V = 0 \Rightarrow \frac{\partial^2 V(\rho,z)}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial V(\rho,z)}{\partial \rho} + \frac{\partial^2 V(\rho,z)}{\partial z^2} = 0$$

(1)
With considering the region close to the source we can write

$$V_S(z) = \varphi_{SB} - (V_{GS} - V_{FB}) \left[ 1 - e^{-\frac{2Z}{t_{ox}}} \right]$$  \hspace{1cm} (2)$$

where $\varphi_{SB}$ is the Schottky barrier height, $V_{FB}$ is the flat band voltage, $t_{ox}$ is the insulator thickness and $L$ is the length of the nanotube. Passing current through channel is calculated by the Landauer Buttiker formula. In this way, current is calculated versus probability of passing carriers through conduction region.

If we consider chemical potential of source and drain as $\mu_L$ and $\mu_R$, and with considering just occupancy of one sub-band and back scattering of electrons in the left region of the source, the transmission current from the channel region can be written as

$$I = \frac{4q}{h} \int_{-\infty}^{\infty} \left[ f(E - \mu_L) - f(E - \mu_R) \right] T(E) dE$$  \hspace{1cm} (3)$$

where $f$ is a Fermi-Dirac function. By choosing $\mu_L = \mu + \delta \mu$ and $\mu_R = \mu$ and supposing $\delta \mu \ll \mu$ and using Tylor expansion we can write

$$I = \frac{4q}{h} \int_{-\infty}^{\infty} \left[ - \frac{\partial f(E, \mu)}{\partial E} T(E) dE \right] \delta \mu$$  \hspace{1cm} (4)$$

In this equation carrier tunneling has important rule. This transmission probability from Schottky barrier is calculated using WKB approximation as

$$T_{n,s}(E) = e^{-\frac{1}{\hbar} \int_{z_i}^{z_f} K(z) dz}$$

Where $z_i$ and $z_f$ are turning point. $K_z(Z)$ is the momentum carriers in nanotube direction where

$$K_z(z) = -k_n \sqrt{\frac{4}{9d^2V_{pp}k_n^2}} \left[ E - \left( \varphi_{SB} - V_{SD} \right) - \left( V_{GS} - V_{FB} \right) \left[ 1 - e^{-\frac{2Z}{t_{ox}}} \right] \right] - 1$$

$$R = \frac{d}{2\pi} \sqrt{3(n_1^2 + n_2^2 + n_1n_2)} \hspace{1cm} n = \frac{3n_1 - n_1 + n_2}{3R}$$

Where $R$ and $K_n$ are the nanotube characteristics. We begin by considering the effect of the metal- CNT barrier height on the $I - V_{GS}$ characteristics.
RESULTS OF SIMULATION

Figure 2 shows that for different Schottky barrier height the current are decreased at the first and then with increasing gate-source bias it is increased.

![Figure 2: The current variation for different applied voltages and a comparison for different Schottky barrier height.](image)

The minimum currents occur when the voltage of the gate is about half of the drain voltage. Reducing the barrier height for electrodes to zero, increase the electron conduction current for $V_{GS} > \frac{V_{SD}}{2}$ and decreases the hole current for $V_{GS} < \frac{V_{SD}}{2}$. For the CNT-FET with the metal Fermi level at the middle of the band gap, electrons and holes have symmetric manner in the conduction. Generally the minimum current is depended on $\phi_{SB}$. Figure 3 is compared the current for transistor with $\phi_{SB} = 0.4$eV at different temperatures ($T_1 < T_2$).

![Figure 3: The dependence of drain current on different temperature.](image)

As it can be seen from figure 3 the output drain current is increased with increasing temperatures due to an increasing energy of carriers and a highest carrier tunneling probability.

In figure 4 the effect of nanotube diameter in output characteristics of the simulated CNT transistor has been shown.
Figure 4: The effect of nanotube diameter on output I-V characteristics.

It can be seen that a larger diameter will reduce the band gap, so the conduction and valance bands will be closed to each other. This causes to a better carrier transmission to the higher layers and therefore the output drain current is increased.

Finally, figure 5 shows the I-V characteristics versus different source-drain voltages. As it can be seen, with increasing source-drain voltages the output drain current is also increased which is due to an increasing force on carriers which causes the number of carriers in the channel region are increased too.

Figure 4: The I-V characteristics versus different source-drain voltages in simulated CNT transistor.

CONCLUSION
The output drain current computed by our model shows for different source-gate voltages the minimum point for current is occurred in $V_{GS}=V_{SD}/2$. For both kind of carriers the Shottky barrier height is the same.

Our results have also shown that for values of $V_{GS}>V_{SD}/2$, the highest of Shottky barrier cause to an increase of output drain current and for $V_{GS}<V_{SD}/2$ the reduced Shottky barrier cause to a increase of output drain current.

We have also shown that increasing temperature will be increased the current and the channel characteristics will be effect on the transmission current.

REFERENCES
(2002) 126801