Mater. Res. Soc. Symp. Proc. Vol. 1018 © 2007 Materials Research Society 1018-EE10-17

Modeling and Simulation of n-Type Carbon Nanotube Field Effect Transistors Using Ca as Contact Electrodes

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ABSTRACT

In this research work, a model has been proposed in view of the recent experimental demonstration using Calcium (Ca) as a contact metal to realize the n-type carbon nanotube field effect transistors (CNTFET). In order to fully optimize this proposed device model, effects of different parameters like the work function, oxide thickness, the oxide capacitance and the source velocity limits were studied. Among all the parameters, the work function of the contact metal plays an important role for controlling the flow of carriers through the carbon nanotube channel and to reduce the threshold voltage. A semi-classical simulation of the proposed n-type CNTFET has been performed. Results show an excellent subthreshold swing value of 62.91 mV/decade, close to the International Technology Roadmap for Semiconductor (ITRS) specifications.

INTRODUCTION

Recently, carbon nanotubes have emerged as promising candidates for nanoscale field effect transistors. The carbon nanotube field effect transistors (CNTFETs) are excellent candidates for the current microelectronic technology that exhibits improved performance in nanometer-regime. Intense research is in progress to study the transport properties of carbon nanotube based field effect transistors. Due to the ability of ballistic transport, CNTFETs have been studied in recent years as a potential alternative to CMOS devices [1, 2]. It is shown that these CNTFETs can be made with ohmic or Schottky type contacts [3, 4]. The operation of Schottky contact CNTFETs is by modulating the transmission coefficient of the barriers at the contact between the metal and the CNT [5]. It has been observed that ambipolar conduction (both holes and electron conduction) is the matter on which to focus in these type of devices. Due to the ambipolar conduction of Schottky barrier CNTFETs, the I_{on}/I_{off} ratio is limited.

Recently, fabrication of an n-type carbon nanotube field effect transistor was reported [6-8] where Nosho et al. used a smaller work function contact metal rather than the large work function contact metal commonly used in carbon nanotube transistors (CNTs). Here, an n-type CNTFET is fabricated by selecting a contact metal. A recent study explains the operation mechanism of the nanotube FETs by a Schottky barriers modulation model in which the gating action is dominated by the Schottky barriers formed at the contact between the nanotube and the source metal. Javey et al. [9] reported that electrode / nanotube contact resistance can be reduced by using 'Pd' as the contact metal in p-type nanotube FETs. Since the work function of 'Pd' metal is larger than the pristine (pure) SWNT (w_f = 4.8 eV), the Schottky barrier height for holes is low. In a similar way, Nosho et al. has fabricated nanotube FETs where the contact electrodes of smaller work function (i.e. Ca, w_f = 2.8eV) than nanotube is used, which reduces the Schottky barrier height for electrons. In this case, the electrons are injected from contact electrodes into the nanotube, and n-type nanotube FETs are realized. This recent experimental development in the field of carbon nanotube-based FET would be another step of development in Nanotechnology. In this work a model based on A. Rahman et al. theory is been proposed to perform simulations of the above described n-type CNTFET where the effect of scaling different parameters are studied. The online simulator FETToy 2.0 [10] is being used in order to perform these simulations. FETToy 2.0 is a semi-classical "top of the barrier simulator." It assumes a one-point channel for which we can specify the top of the barrier for electron injection. The carriers are injected from the source, and the transport is ballistic. For nanotube MOSFETs, it assumes a cylindrical geometry where the gate is wrapped around the channel.

DEVICE MODEL

In the proposed device model shown in Figure 1 'Ca' is used as contact metal having a smaller work function than the nanotube. A channel length of 10nm is assumed; a zigzag nanotube with a diameter of 1nm and a ZrO_2 gate oxide of 2nm is also assumed having a dielectric constant of $k = 25$.

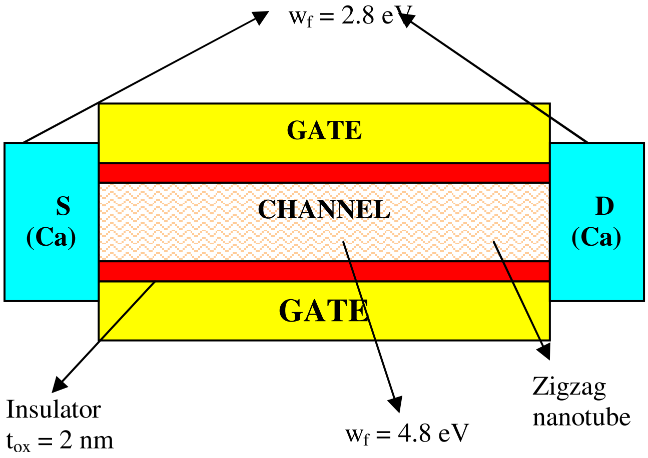


Figure 1: Schematic of proposed n-type CNTFET

The basic assumption here is MOSFET like CNTFET, where the Schottky barrier is assumed to be very low or even negative. The performance of the proposed device is based on Natori's theory [11] of ballistic FETs. Due to the fact operation in an aqueous environment and the absence of dangling bonds in a carbon nanotube structure (unlike in Si) facilitates the use of high-k gate dielectrics, it is possible to achieve larger gate insulator capacitance. Additionally, relatively low-density states of one-dimensional conductor reduce the quantum capacitances, thus the CNTFETs operate well in quantum capacitance limits.

EFFECT OF WORK FUNCTION

In order to analyze the performance of the proposed device, we perform simulations using FETToy 2.0, an online simulator discussed. Table 1 shows the specifications of the device being simulated.

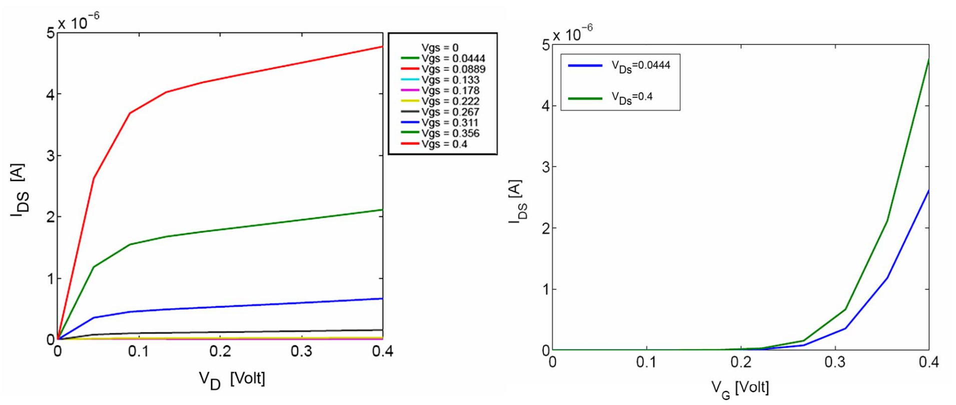
Table 1: The device specifications used for simulation.

Gate insulator thickness	2 nm
Dielectric Constant (k)	25
Channel Length (L)	10 nm
Diameter of Nanotube (d)	1 nm
Valley Degeneracy	2
Temperature (T)	300 K
Band Gap (E_g)	0.7 eV
Applied Voltage range (V)	0 - 0.4 V

Initially, we start our simulations by varying the source Fermi level 'E_f', which is effected by the work function of the contact metal. A smaller work function value would raise the Fermi level. Note the source Fermi level is used to set the threshold voltage (V_t) of the device. For a CNTFET, the band gap is given as Eg = 0.7/d eV, where'd' is the diameter of the nanotube. Using this relation, for our specifications of the device where a carbon nanotube of diameter 1nm is used, the obtained band gap is Eg = 0.7 eV. Thus, we start the simulation with the specifications shown in Table 2 and E_f = -0.35 eV. The obtained *I-V* characteristics with these specifications are as shown in Figure 2. Table 2 shows the obtained values at source Fermi level E_f= -0.35 eV.

Table 2: Values obtained with E_f= -0.35 eV.

Ion (μA/μm)	Ioff (μA/μm)	Subthreshold Swing S (mV/dec)	V_inj (m/s)
4.73×10^{-6}	9.22×10^{-12}	62.72	2.317×10^{5}



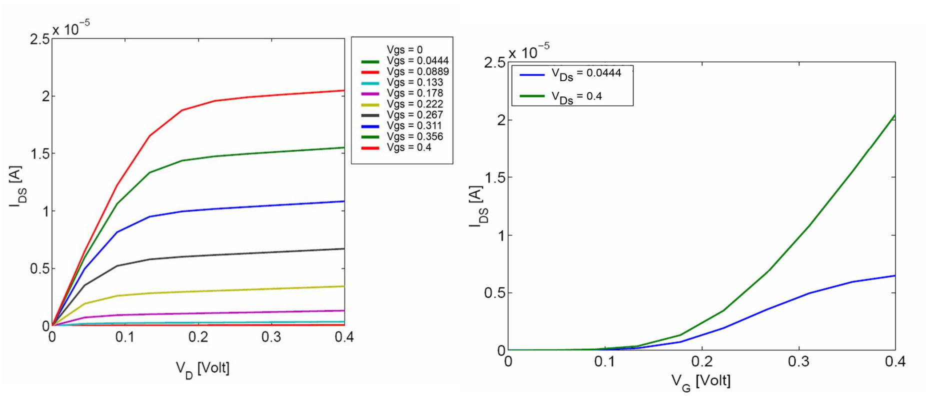
(a) (b)

Figure 2: The *I-V* characteristics obtained for E_f = -0.35 eV. (a) Shows the I_D vs.V_D for the proposed n-type CNTFET. (b) Shows the I_D vs.V_G for proposed n-type CNTFET.

As previously mentioned, the smaller work function will act as rise the source Fermi level, thus for the proposed device with a smaller 'w_f', we perform the simulation with an increased value of E_f= -0.20 eV and analyze the results obtained above. Figure 3 shows the *I-V* characteristics obtained for E_f = -0.20 eV. Table 3 shows the corresponding values.

Table 3: Values obtained with E_f = -0.20 eV.

Ion (μA/μm)	Ioff (μA/μm)	Subthreshold Swing (mV/dec)	V_inj (m/s)
20.48×10^{-6}	3.03×10^{-9}	62.91	3.61×10^{5}



(a) (b)

Figure 3: *I-V* characteristics obtained with E_f = -0.20 eV. (a) I_D vs. V_D for proposed n-type CNTFET. (b) I_D vs. V_G for proposed n-type CNTFET.

The I_{on}/I_{off} ratio obtained at two different values of source Fermi level i.e. at E_f = -0.35 eV and E_f = -0.20 eV are 0.51×10^{6} and 675.9×10^{5} respectively. Also the subthreshold swing (S) value obtained for E_f = -0.20 eV is 62.91 mV/dec close to the ITRS specifications [12] that ensures that for this value of source Fermi level the proposed device gives high Ion/Ioff ratio and better 'S' value. If we compare the plotted results obtained with different 'E_f' values, the graphs obtained with the E_f = -0.20 eV value show the threshold voltage is less compared to the one obtained with E_f = -0.35 eV (Figure 2). The current saturation with E_f = -0.20 eV takes place at a high gate and drain bias, as shown in Figure 3. Thus, the smaller work function metal contact raises the source Fermi level, giving a reduced threshold voltage.

DISCUSSION

As discussed earlier, the CNT-based FETs behave like Schottky types rather than Ohmic. The presence of these Schottky barriers severely limits the on-state conductance and reduces the current delivery capability. It is interesting to note that if the transparent electrical contact is made with the metallic SWNT, they behave as ballistic conductors. The carrier transport through the valence and conduction bands of a high-quality semiconducting SWNT could also be ballistic, giving an opportunity to realize a ballistic FET [13]. Table 5 shows the experimental values of a 'Pd' contacted short channel CNTFET where a nanotube with a diameter 1.7 nm, an oxide thickness of 67 nm having a dielectric constant of k = 30, and channel length L = 300nm is used.

Table 5: The experimental data obtained for 'Pd' contacted CNTFET [13].

Channel Length (L)	Dielectric constant (k)	Diameter (d)	Subthreshold Swing (S)	Oxide thickness (t_{ox})	On current (I_{on})
300 nm	30	1.7 nm	170 mV/decade	67 nm	30 a

The subthreshold swing of 170 mV/decade was achieved by giving an on-current value of 30 μA, which is 20% more than the experimental ballistic current limit of 25 μA. The current value obtained here can be explained based on the work function of 'Pd.' The work function of 'Pd' contact metal is ϕ_{pd} =5.1 eV, which is reduced when exposed to Hydrogen gas [13]. Due to a reduced work function, the Schottky barrier height for holes ncreases and decreases for electrons. The pure Pd-contacted SWNT-FET exhibits metallic behavior for p-channel conduction.

Next, we obtained the above parameters for our proposed n-type CNTFET using 'Ca' as the contact metal. The values are as shown in Table 6. The simulations were carried out using TiO_2 as an insulating material with a thickness 2 nm and a dielectric constant of k = 40. Simulations were repeated by changing the diameter value from 1 nm to 2.5 nm; the on-current values obtained are 23 μA and 27 μA; respectively. The on-current value with respect to 1 nm is still higher than what was obtained with ZrO_2 as an insulating material as shown in Table 6, where it is 20 μA. The reason for this is the high-k material. Table 6 shows the simulated on-current value for the proposed device is 27 μA, which is higher than the experimental on-current value (i.e. 25 μA).The Ion value is 10% more than the experimental value, so we can suggest the proposed n-type CNTFET can give on-current value higher than the experimental value. These simulations were completed at the oxide thickness of 2 nm, a very good value for designing a transistor. The subthreshold swing value obtained for the proposed model is 62.82 mV/decade, significantly less than the experimental value of S = 170 mV/decade [13]. Yet the subthreshold value for the proposed device in this work is very close to 60 mV/decade, the specification given by the ITRS, the reason for this is the assumption of complete gate control on the channel. This can be observed from the simulator where the gate control parameter 'a_g' value is 0.95 that is close to 1.

Table 6: The simulation result data obtained for CNTFET with 'Ca' as contact metal in this study.

Dielectric constant (k)	Diameter (d)	Subthreshold Swing (S)	DIBL	Oxide thickness (tox)	On current (Ion)
40	2.5 nm	62.82 mV/decade	52.59 mV/V	2 nm	27 μA

CONCLUSIONS

In this study a model has been proposed to realize the performance of n-type CNTFET. We performed the simulation of such a device where the behavior of the proposed model of the device under the influence of various parameters was observed The effect of the work function, which in turn reduces the source Fermi level, is being observed and helps to achieve the high on-current for the proposed device. It shows that when source Fermi level is increased, the threshold voltage of the device is reduced giving high switching speed for the proposed device. The subthreshold swing of the proposed model is 62.91 mV/decade, which is an excellent value for any device as per the ITRS specifications. The I_{on}/I_{off} ratio of 10^6 is achieved, which is close to the expected value for the short channel device. The proposed device model is also well in agreement with the experimental values in the literature.

REFERENCES

1. K. Horiuchi, T. Kato, S. Hashii, A. Hashimoto, T. Sasaki, N. Aoki, Y. Ochiai, Appl. Phys. Lett., 2005, 86, 153108.
2. M. Pourfath, E. Ungersböck, A. Gehring, B.-H. Cheong, W. Park, H. Kosina, S. Selberherr, proceeding of the 34th European Solid-State Device Research Conference," Institute of Electrical and Electronics Engineers, 2004, 429.
3. R. Martel, V. Derycke, C. Lavoie, J. Appenzeller, K. Chan, J. Tersoff and P. Avouris, "Ambipolar electrical transport in semiconducting single-wall carbon nanotubes," Phys. Rev. Lett., vol. 87, no. 25, pp. 256807, 2001.
4. J. Appenzeller, J. Knoch, V. Derycke, R. Martel, S. Wind, and P. Avouris, Phys. Rev. Lett., 2002, 89, 126801.
5. Z. Ren, Ph. D. Thesis, Purdue University, West Lafayette, IN, Dec. 2001.
6. J. Gou and M. Lundstrom, IEEE Trans. On Electron Devices, vol. 49, issue 11, pp. 1897-1902, 2002.
7. Y. Nosho, Y. Ohno, S. Kishimoto, and T. Mizutani , Appl. Phys. Lett., vol. 86, pp. 073105, Feb. 2005.
8. H. Ishii, Sugiyama, E. Ito and K. SekiAdv. Mater. (Weinheim, Ger.), vol. 11, pp. 605, 1999.
9. A. Javey, J. Gou, D. B. Farmer, Q. Wang, D. Wang, R. G. Gordon, M. Lundstom, and H. Dai, Nano letter, vol. 4, no. 3, pp. 447-450, 2004.
10. FETToy2.0 tool information, http://www.nanohub.org/simulation_tools/fettoy_tool_information," 10/03/2005.
11. K. Natori, J. Applied Phys., vol. 76, no. 8, 15 Oct., 1994.
12. International Technology Roadmap for Semiconductor, 2001 Edition, Semiconductor Industry Association, "www.itrs.net," 10/03/2005.
13. A. Javey, J. Gou, Q. Wang, M. Lundstrom, H. Dai, Nature, 2003, 424, 654.