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11

Numerical Modeling of the I-V Characteristics of Carbon Nanotube Field Effect Transistors

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1. Introduction

Carbon nanotubes (CNTs) were first discovered in 1991 by Sumio Iijima (Iijima, 1991), and they have been a rapid and successful target of development by many researchers (Baughman et al., 2002). Especially with the end of Moore's law in sight (Wind et al., 2002), CNTs are being considered as possible candidates substituting silicon in the fabrication and design of analog and digital integrated circuits (ICs) (Guo et al., 2002; Wong, 2002).

Carbon nanotubes are basically two dimensional graphene sheets rolled into a one dimensional tubular structure (Martel et al., 1998). Their properties are determined by the chiral vector represented by the indices (n,m) (Tanaka et al., 1999; Wallace, 1947; Wildoer et al., 1998). Depending on the number of layers rolled, carbon nanotubes can be either single walled (one layer), or multi walled (two or more layers) (Dresselhaus et al., 2001). Single walled carbon nanotubes (SWNTs) are used in the fabrication of carbon nanotube field effect transistors (CNT-FETs), the first CNT-FETs were implemented in 1998 (Martel et al., 1998; Tans et al., 1998). The structure of a CNT-FET is similar to the structure of a typical MOSFET where the CNT forms the channel between two electrodes that work as the source and the drain of the transistor. The structure is build on top of an insulating layer and a substrate wafer that works as the back gate, (Nihey et al., 2003) (Wind et al., 2002). The basic structure of a CNT-FET based on a SWNT is shown in Fig. 1. Among the CNT-FETs reported (Martel et al., 1998; Wind et al., 2002), a 40 nm gate length transistor (Lin et al., 2005), a multistage complementary logic (Javey et al., 2002), oscillators (Chen et al., 2006), and an 80 GHz operating field effect transistor (Nougaret et al., 2009) have been achieved.

In addition, carbon nanotubes are one-dimensional conductors (1D), which confines the electrons to only back-scattering effects. This property provides a large electron mean free path in metallic carbon nanotubes of usually a few micrometers (White & Todorov, 1998). Carbon nanotubes also exhibit large current capabilities of $\sim 10^{-9}$ *A/cm*^{2}, (Wei et al., 2001; Yao et al., 2000) and it has also been reported that doping can be avoided in the CNT fabrication process, yet still achieving complementary CNT-FETs (Zhang et al., 2007). With carbon nanotubes interconnects being also a major target of research (Koo et al., 2007; Xu et al., 2008) and a completely carbon nanotube based integrated circuit (IC) already reported

(Liang et al., 2009), fabrication of fully integrated carbon nanotubes in custom designed ICs and systems on a chip is no longer a future circuit design promise but an attainable grasp.

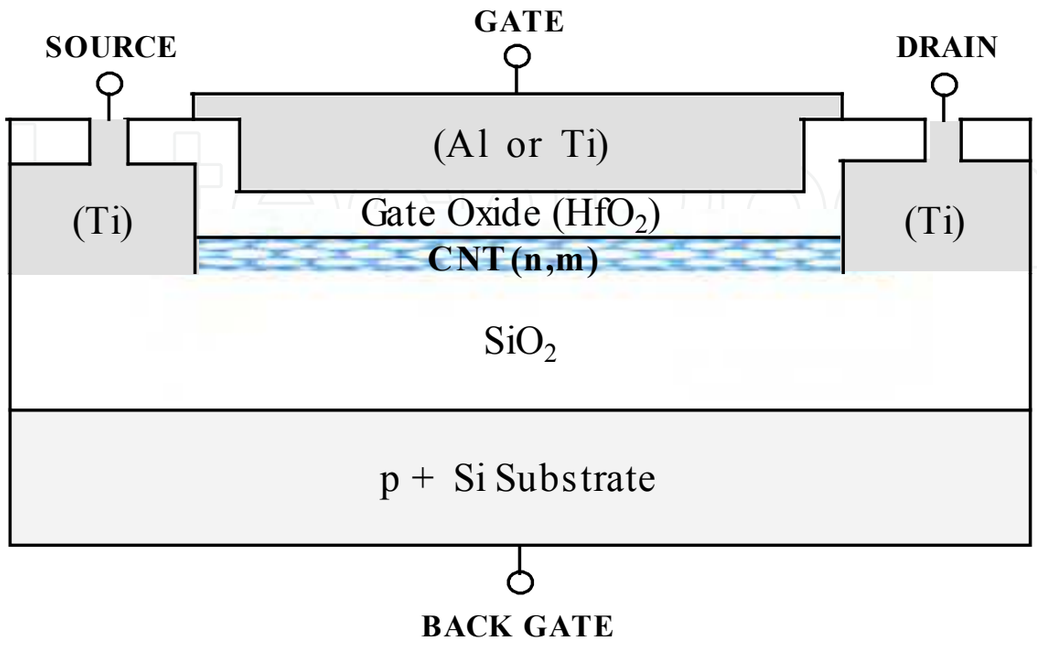

Fig. 1. Cross sectional view of a CNT-FET. Note: HfO_2 (Halfnium dioxide) is a high *k*-dielectric (~17-20) (Javey et al., 2004; Wang et al., 2003).

In this paper, we have used our modeling of the potential and charge balance of CNT-FETs (Marulanda, 2009; Marulanda et al., 2008; Srivastava et al., 2009) to develop a numerical model of the current-voltage relation for a CNT-FET of n-type behaviour. This model uses numerical approximation methods to solve this current and voltage equations and present the I-V characteristics of different CNT-FETs.

2. Current Equation

The current per band in a semiconductor (Datta, 1999; Xia et al., 2004) can be expressed as:

$$I_{ds_i} = \frac{q}{\pi\hbar}\int_{E_{c_i}}^{E_{max}} T_i(E)\left[f_s(E) - f_d(E)\right]dE, \tag{1}$$

where E_{ci} and $T_i(E)$ are respectively the conduction band energy minimum and transmission coefficient for the i_{th} band, h is Planck's constant divided by 2π, and $f_s(E)$ and $f_d(E)$ are the Fermi distributions at the source and drain, respectively.

Although the total I_{ds} will be the sum of all I_{dsi} over all bands, the summation in Eq. (1) can be dropped, as only the first band is sufficient. The reason is because the remaining energy bands will have negligible contribution to the current due to the vanishing exponential behaviour of the Fermi distribution for high-energy conduction band values.

By letting the limit of E_{max} go to infinity and the transmission coefficient be a constant equal to unity for the energy range of integration, Eq. (1) becomes (Marulanda et al., 2008):

$$I_{ds} = \frac{qKT}{\pi\hbar}\left[\ln\left(1+e^{\frac{E_{Fs}-E_c}{KT}}\right)-\ln\left(1+e^{\frac{E_{Fd}-E_c}{KT}}\right)\right], \tag{2}$$

where E_{Fs} and E_{Fd} are the Fermi level energies at the source and drain, respectively. This equation for the current can be used in the linear and saturation regions.

3. Gate and Carbon Nanotube Potential Relation

Figure 2(a) shows the basic cross section of a CNT-FET including the charge distributions, Fig. 2(b) shows the corresponding potential distributions between the gate and substrate. In Fig. 2(a), charge distributions are explained as follows: the charge on the gate is Q_g, charges in oxide layers are Q_{01} and Q_{02}, charge inside the CNT is Q_{cnt} and the charge in the substrate is Q_{subs}. In Fig. 2(b), six different potential distributions are shown, which are also described as follows. The voltage between the gate and the substrate (back gate) is V_{gb}, the potential drop across the oxides ψ_{ox1} and ψ_{ox2}, the surface potential in the substrate with respect to the back gate is ψ_{subs}, the potential across the CNT is ψ_{cnt}, and the work function difference between the gate and the substrate materials is ϕ_{ms}. The work function, ϕ_{ms} can be divided in two parts and is expressed as follows,

$$\phi_{ms} = \phi_{mc} + \phi_{cs}, \tag{3}$$

where ϕ_{mc} and ϕ_{cs} are the work function differences between the metal gate and carbon nanotube materials and the carbon nanotube and substrate materials, respectively. We can also combine potentials ψ_{cnt}, ψ_{ox2}, ϕ_{cs}, and ψ_{subs} into a single potential, $\psi_{cnt,s}$, which describes the potential at the interface of the gate oxide and carbon nanotube with respect to the back gate, we can call $\psi_{cnt,s}$ the carbon nanotube surface potential.
Using Kirchoff's voltage law, the potential balance, and the charge neutrality condition, we can write for Fig. 2,

$$V_{gb} = \phi_{ms} + \psi_{ox1} + \psi_{cnt,s}, \tag{4}$$

$$Q'_g + Q'_{01} + Q'_{cnt} + Q'_{02} + Q'_{subs} = 0. \tag{5}$$

The prime in Eq. (4) denotes the charge per unit area. From basic laws of electrostatics (Cheston, 1964; Langmuir, 1961; Shen & Kong, 1995; Thomas, 1972), we can utilize Eqs. (4) and (5) and the charge modeling described in (Marulanda, 2009; Marulanda et al., 2008; Srivastava et al., 2009), to express the gate voltage in a CNT-FET as,

$$V_{gb} = \psi_{cnt,s} - \frac{Q_{cnt}}{C_{ox1}} + V_{fb}, \tag{6}$$

where V_{fb} is the flat band voltage, which is the voltage needed at the gate with respect to the

back gate to compensate for the band bending at the gate oxide and carbon nanotube interface and it is given by,

$$V_{fb} = \phi_{mc} - \frac{Q_{01}}{C_{ox1}}. \tag{7}$$

In addition, C_{ox1} and C_{ox2} are the oxide capacitances for the respective oxide regions, T_{ox1} and T_{ox2} and are described for a carbon nanotube of length, L and radius, r as follows (Cheston, 1964; Thomas, 1972),

$$C_{ox} = \frac{2\pi\varepsilon_{ox}L}{\ln\left(\frac{T_{ox}+r+\sqrt{T_{ox}^2+2T_{ox}r}}{r}\right)}. \tag{8}$$

In Eqs. (6), (7), and (8), Q_{cnt}, Q_{01} and C_{ox1} are the total charges and capacitance, respectively, which are obtained by multiplying Q'_{01}, Q'_{cnt}, and C'_{ox} with their respective areas.

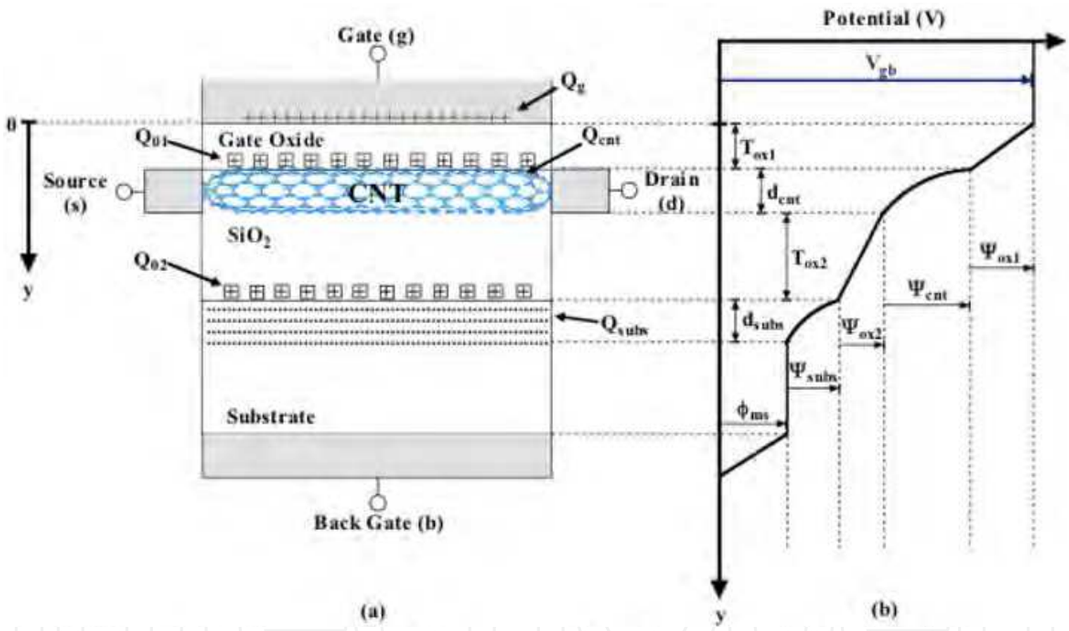

Fig. 2. (a) Plot of the charges from the gate to the substrate and (b) plot of the potential distribution from the gate to the substrate in a CNT-FET.

Using the carrier concentration modeling in (Marulanda & Srivastava, 2008) and charge modeling described in (Marulanda, 2009; Marulanda et al., 2008; Srivastava et al., 2009), we can express Eq. (6) as:

$$V_{gb} = \psi_{cnt,s} + \delta f\left(\psi_{cnt,s}, V_{cb}\right) + V_{fb}, \tag{9}$$

where

$$f\left(\psi_{cnt,s},V_{cb}\right)=\begin{cases} Ie^{\frac{\Delta E_F+q\left(\psi_{cnt,s}-V_{cb}-\phi_0\right)-E_c}{kT}}; & for\ \ \psi_{cnt,s}\le V_{cb}+\phi_0-\frac{\Delta E_F}{q}+\frac{E_c}{q}-\frac{kT}{q} \\ \frac{\sqrt{\left(\Delta E_F+q\psi_{cnt,s}-qV_{cb}-q\phi_0\right)^2-E_c^2}}{kT}; & for\ \ \psi_{cnt,s}\ge V_{cb}+\phi_0-\frac{\Delta E_F}{q}+\frac{E_c}{q}+\frac{kT}{q} \end{cases} \tag{10}$$

and

$$\delta=\frac{qLN_c}{C_{ox1}}. \tag{11}$$

In Eq. (9), V_{cb} is the induced potential between the carbon nanotube and the substrate due to the drain and source terminal voltages. The potential, V_{cb} varies from V_{sb} (source to back gate potential) to V_{db} (drain to back gate potential). Furthermore, in Eq. (10), k is Boltzmann constant, T is temperature, ϕ_0 is the carbon nanotube surface potential, $q\psi_{cnt,s}$ when $V_{gb} = V_{fb}$ and $\psi_{cnt} = 0$, ΔE_F is the shift in the Fermi level of the carbon nanotube depending upon doping, , ϕ_0 and ΔE_F are given by,

$$\phi_0=\psi_{ox2}+\psi_{subs}+\phi_{cs}, \tag{12}$$

$$\Delta E_F=\pm kT\ln\left(1+\frac{N}{n_{cnt,i}}\right), \tag{13}$$

where $n_{cnt,i}$ is the intrinsic concentration of a CNT (n,m) and N is the impurity doping concentration. ΔE_F is positive for an n-type carbon nanotube (donors impurity concentration, $N = N_D$) and negative for a p-type carbon nanotubes (acceptors impurity concentration, $N = N_A$).

In Eq. (10), I is an indefinite integral involved in finding the carrier concentration of a carbon nanotube, we have found an analytical solution in (Marulanda, 2009; Marulanda & Srivastava, 2008); however, the general form of the integral, I is given by,

$$I=\frac{1}{\sqrt{kT}}\int_0^{\frac{6E_c}{kT}}\frac{\left(kTx+E_c\right)}{x^{1/2}\left(kTx+2E_c\right)^{1/2}}e^{-x}dx. \tag{14}$$

The term N_c introduced by Eq. (11) is found from our carrier concentration model for carbon nanotubes (Marulanda & Srivastava, 2007; Marulanda & Srivastava, 2008) and is given by,

$$N_c=\frac{8kT}{\pi V_{pp\pi}a\sqrt{3}}, \tag{11}$$

where $V_{pp\pi}$ is the carbon-carbon (C-C) tight binding overlap energy, a is the lattice constant with a value of $\sqrt{3}\,a_{c\text{-}c}$, and $a_{c\text{-}c}$ is the nearest neighbor distance between C-C bonds (0.144 nm) (Dresselhaus et al.).

4. I-V Characteristic Simulation

Equation (9) cannot be solved explicitly for the carbon nanotube surface potential, $\psi_{cnt,s}$ in terms of the terminal voltages, hence, a numerical solution technique must be taken in order to find the exact channel potential given a gate voltage input.

In a CNT-FET, when the terminal voltages V_{db}, V_{sb}, and V_{gb} are applied, the two terms $(E_{Fs} - E_c)$ and $(E_{Fd} - E_c)$, referred in Eq. (2) can be replaced by $\Delta E_F + q\left(\psi_{cnt,s} - V_{sb} - \phi_0\right) - E_c$ and $\Delta E_F + q\left(\psi_{cnt,s} - V_{db} - \phi_0\right) - E_c$, respectively (Marulanda, 2009; Raychowdhury et al., 2004; Srivastava et al., 2009; Tsividis, 1999). V_{sb} and V_{db} are the source to bulk and drain to bulk voltages, respectively; furthermore, $\psi_{cnt,s}$ is calculated using Eq. (9) employing a numerical solution approach. Thus, our Eq. (2) becomes:

$$I_{ds} = \frac{qkT}{\pi\,\mathrm{h}}\left[\ln\left(1+e^{\frac{\Delta E_F + q\left(\psi_{cnt,s}(0) - V_{sb} - \phi_0\right) - E_c}{kT}}\right) - \ln\left(1+e^{\frac{\Delta E_F + q\left(\psi_{cnt,s}(L) - V_{db} - \phi_0\right) - E_c}{kT}}\right)\right]. \tag{15}$$

The complete process to find the current I_{ds} is as follows:

1. Define the voltages V_{db}, V_{sb}, and V_{gb}.
2. Use a numerical method to find $\psi_{cnt,s}$ from Eq. (9).
3. Compute the current, I_{ds}, using Eq. (15).
4. Repeat steps 1 – 3 for each of the input voltages, V_{db}, V_{sb}, and V_{gb} combination.

Figure 4 shows the I-V characteristics for a CNT-FET with a carbon nanotube of chiral vector (5,3) and diameter of 0.2759 nm, under different overdrive gate voltages. These plots were derived following the four steps just mentioned.

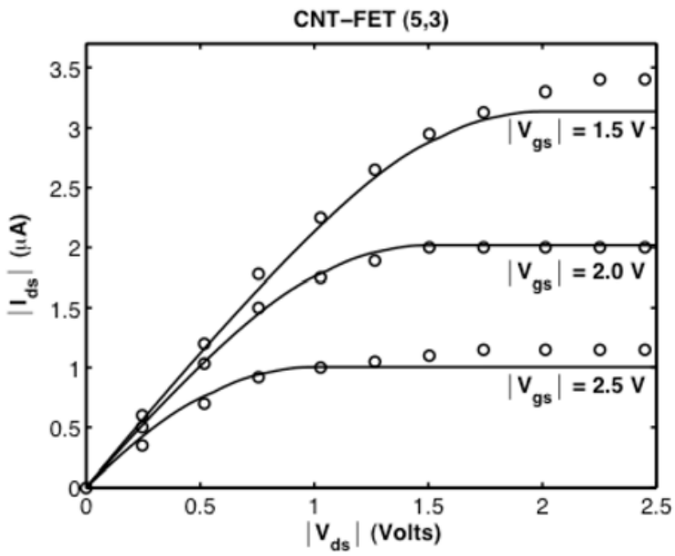

Fig. 3. I–V characteristics for a CNT-FET (5,3) with $V_{fb} = 0$, $\phi_0 = 0$, $\Delta E_F = 0$, and device dimensions of $L = 3\ \mu m$, $T_{ox1} = 500\ nm$, and $T_{ox2} = 1\ \mu m$.

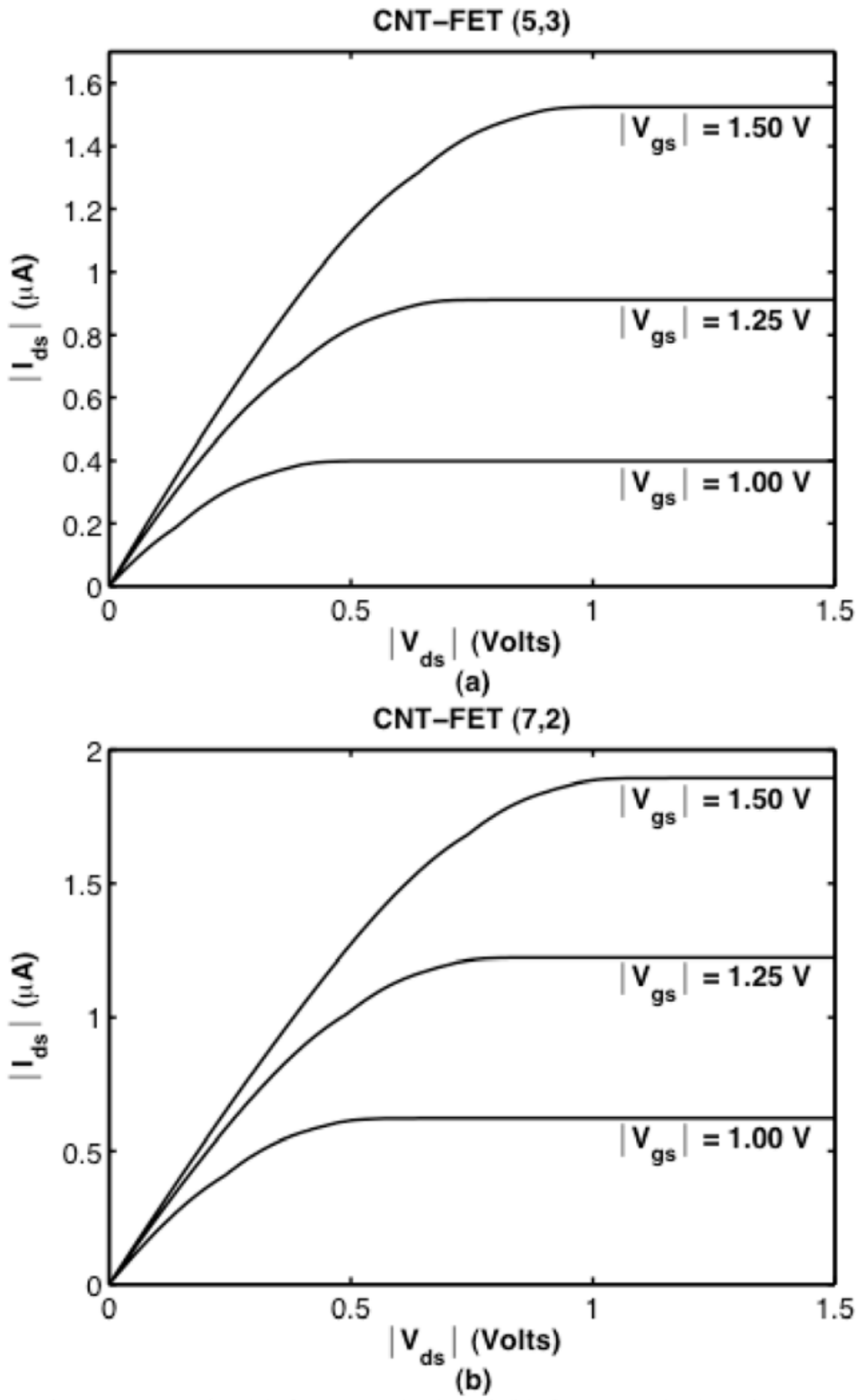

Fig. 4. I–V characteristics for (a) CNT-FET (5,3) and (b) CNT-FET (7,2) with $V_{fb} = 0$, $\phi_0 = 0$, $\Delta E_F = 0$, and device dimensions of $L = 25\ nm$, $T_{ox1} = 40\ nm$, and $T_{ox2} = 400\ nm$.

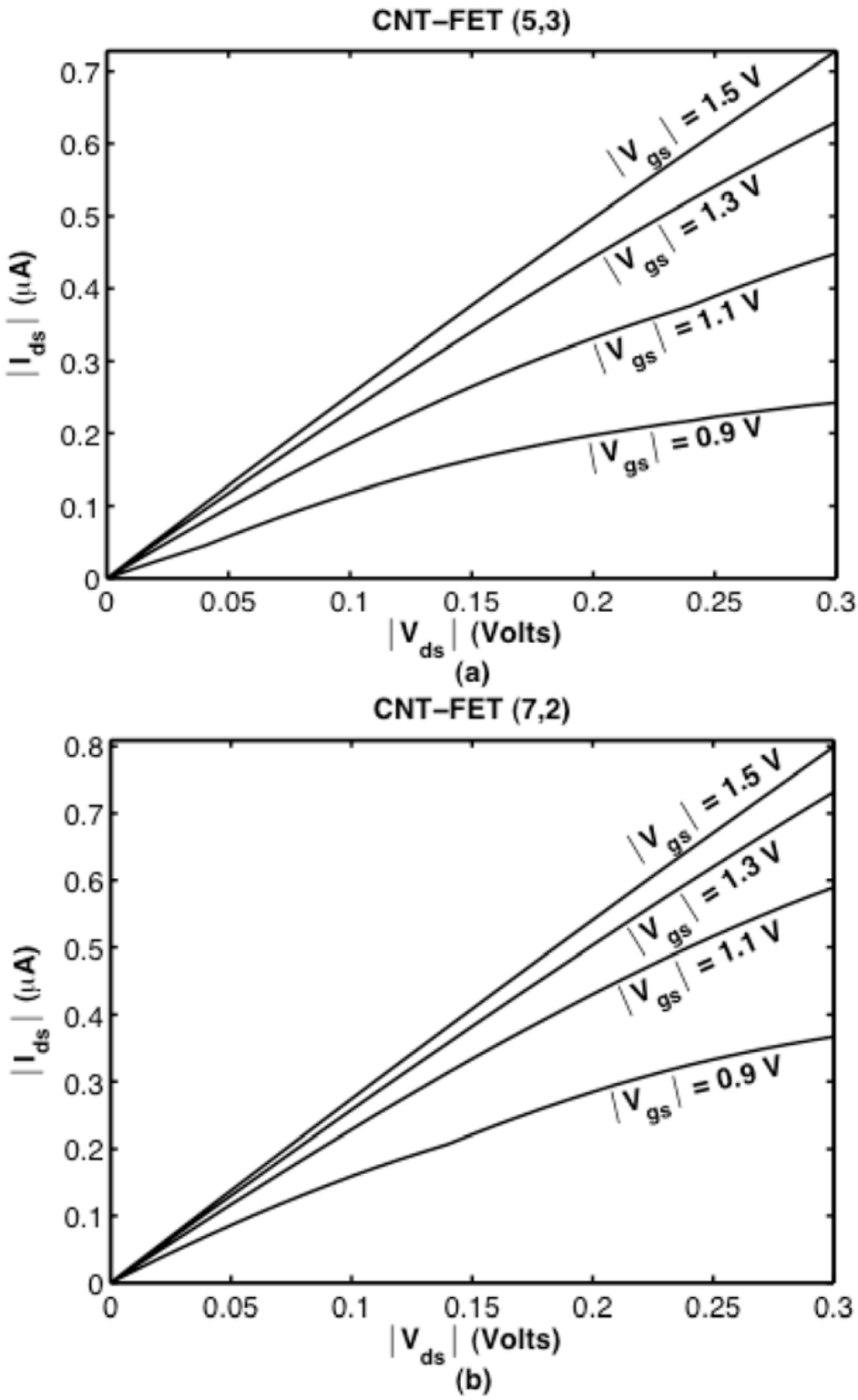

Fig. 5. I–V characteristics under low V_{ds} for (a) CNT-FET (5,3) and (b) CNT-FET (7,2) with $V_{fb} = 0$, $\phi_0 = 0$, $\Delta E_F = 0$, and device dimensions of $L = 25\ nm$, $T_{ox1} = 40\ nm$, and $T_{ox2} = 400\ nm$.

We have included in Fig. 3 experimentally measured data (Zhou et al., 2000) to validate the accuracy of our model. As we can see from Fig. 3, the model equation (Eq. 15) follows closely the experimentally measured data for the linear region. However, as the transistor enters the saturation region (in this region the current I_{ds} begins to saturate and becomes almost independent of V_{ds}), experimental values deviate from the model equation since our model equation does not include a correction term for the saturation region similar to the channel length modulation parameter in a MOSFET (Antognetti & Massobrio, 1988; Tsividis, 1999).

Using our numerical model approach we have also simulated the I-V characteristics for two more CNT-FETs. Figure 4 shows the I-V characteristics for two CNT-FETs with chiral vectors (5,3) and (7,2) and diameters 0.2759 nm and 0.3227 nm, respectively.

Using the same procedure described for Figs. 3 and 4, it is also possible to compute the I-V characteristics for small V_{ds}. Figure 5 shows the simulated I-V characteristics for small V_{ds} for the CNT-FET (5,3) and CNT-FET (7,2). As we can see in Fig. 5, for small V_{ds} the current shows approximately a linearly proportional relationship to the voltage of the drain with respect to the source, V_{ds}.

5. Conclusion

Previous works in carbon nanotubes describing a relationship between the gate voltage and the carbon nanotube potential have made possible the implementation of a current equation, which can be solved numerically using any mathematical software, in order to find the current voltage characteristic for any given CNT-FET. The results presented provide designers with useful mathematical relations describing the properties of conductivity of carbon nanotubes and their response in circuit applications. Even though the charge transport in the carbon nanotube is not yet fully understood, and the solutions for the equations presented are strictly based in numerical methods, the results presented in this work set a starting point for device modeling simulation of carbon nanotube field effect transistors (CNT-FETs) and their applications on integrated circuits, including a SPICE compatible model.

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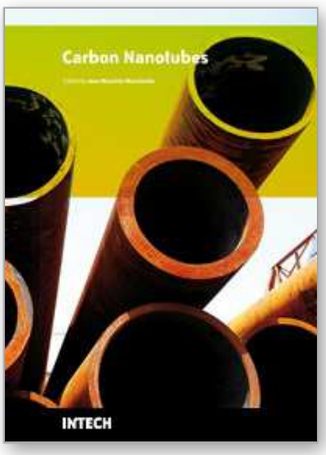

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This book has been outlined as follows: A review on the literature and increasing research interests in the field of carbon nanotubes. Fabrication techniques followed by an analysis on the physical properties of carbon nanotubes. The device physics 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.

How to reference

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