2011 International Conference on Nanotechnology and Biosensors
IPCBEE vol.25(2011) © (2011) IACSIT Press, Singapore

Carbon Nanotube Field Effect Transistor-Based Gas Sensor for NH_3 Detection

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Abstract. In this paper, we propose the effect of reaction between NH_3 molecules and the surface of the Single Wall Carbon nanotube (SWCNT) channel in a Carbon Nanotube Field Effect Transistor (CNTFET) device as a sensor. Reaction between NH_3 molecules and SWCNT changes the surface charge and potential of the CNT channel, which in its turn, causes the corresponded variations in device characteristics. Here, the reaction between NH_3 and SWCNT is simulated in Virtual Nanolab (VNL) software which leads to the changes in i-v curve of CNTFET through the affecting in gate control parameter and drain control parameter. We insert this parameters in FETToy area (a code developed under MATLAB) to extract the i-v curve, and compare i-v curves. This comparison clearly shows that the NH_3 molecule will affect the performance of CNTFET as its sensor.

Keywords: Carbon Nanotube, Sensor, CNTFET, NH_3, FETToy

1. Introduction

After the discovery of fullerene, carbon nanotubes (CNTs) have been re-discovered in 1991 by Iijima [1]. The conductance of the semiconducting CNT changes when biomolecules are adsorbed on the walls, causing changes in local electrostatic environment [2]. The unique electrical properties of single-wall carbon nano-tubes (SWNTs) have generated a huge amount of research on nano-electronic devices and nano-sensors. In 1998, Tans et al. demonstrated the possibility of using an individual semi-conducting SWNT as a field-effect transistor. Based on this transistor layout, several research groups started to construct SWNT nano-sensors, where the solid-state gate is replaced by nearby molecules that modulate the tube conductance. Because semi-conducting SWNTs have a very high mobility and all their atoms are located at the surface, they are the ideal material for ultra-small sensors.

The proposed device is a nano-electronic sensor that relies on electronic readout from a single-walled nanotube field effect transistor. Since this sensor is a molecular device, it will be able to detect NH_3 at lower levels than current detection methods. Here, we demonstrate that SWNT transistors can indeed be developed into such sensors [3]. Immobilization of NH_3 onto the sidewall of a semi-conducting SWNT is found to change the gate and drain control parameters of the CNTFET. This work consists of three major steps: in the first step, it immobilizes NH_3 on the sidewall of carbon nanotube channel of the device via linking them in virtual nanolab program, the modeling and simulation interaction between NH_3 and sidewall of SWCNT in CNTFET. The second step includes calculating drain and gate control parameters; and as the third step, the resulted parameters are applied to the FETToy model to extract the i-v curves, which represents the effect of NH_3 on the device.

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2. Modeling and Methodology

The theoretical basis of CNTFETToy is a model developed by Natori for ballistic FETs which was expanded upon by Rahman and is a simple analytical model for determining the device current vs. voltage curves. This FETToy model focuses on the height of the energy barrier in the channel. The main concept emphasize that the charge in the channel is controlled by the height of the barrier. However, basing the model on the height of the barrier allows a more concise analytical model.

Ignoring mobile charge in the channel, the Laplace potential at the top of the barrier is then:

$$U_L = - q\,(\alpha_G V_G + \alpha_D V_D + \alpha_S V_S) \tag{1}$$

The three α's in equation (1) describe the gate, drain and source's control over the Laplace solution and depend on the two-dimensional structure of the device [4,5].

$$\frac{1}{\alpha_G} = 1 + \frac{C_{Q'}}{C_{ins}}\ ,\ \alpha_D = \frac{1-\alpha_G}{2} \tag{2}$$

where (as introduced in Fig. 1) [6]

$$C_{Q'} = \frac{2C_D.C_Q}{C_Q + 2C_D}\ ,\ C_Q = \frac{\Delta Q_{CNT}}{\Delta V_{CNT}}\ ,\ C_{ins} = \frac{\Delta Q_{CNT}}{\Delta V_{ins}} = \frac{\Delta Q_{CNT}}{V_G - \Delta V_{CNT}}$$

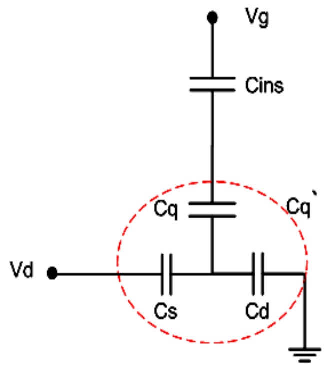


Fig. 1: Capacitive circuital model for the coaxially gated CNTFET [6].

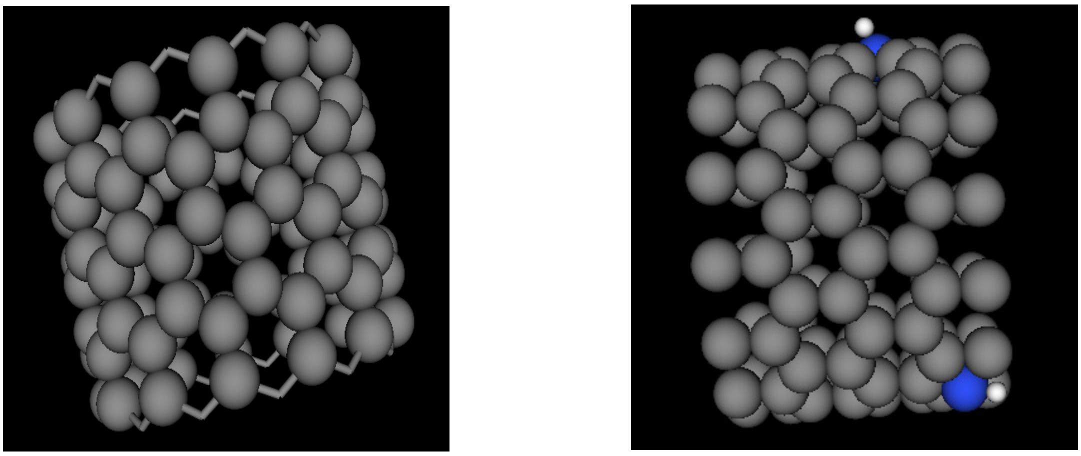
3. Simulation Results

We employ a (13,0) semiconductor nanotube with the following table as a channel of CNTFET in our simulation work.

Table 1: Nanotube parameters and properties

n: 13	m: 0
C-C Bond length: 0.1422 nm	Type: Zigzag
Radius: 0.5096 nm	Period: 0.4266 nm
Band gap: 0.663 eV (Semiconducting)	Chiral angle: 0.0 °

At first, we simulate the simple nanotube channel in Virtual Nanolab (VNL) program. We define the geometry of SWCNTFET channel (two-probe systems) in Atomic Manipulator tool of VNL program. Then define theoretical (and numerical) method that will be used to find the self-consistent electron density in NanoLanguage Scripter tool. In configuration tab we choose Quasi Newton Optimized Atomic Geometry and in the method tab we specify the single zeta basis set and other parameters that are needed to define and set up the DFT calculation. Then we run the Created NanoLanguage scripts in Job Manager to find out raw data. With calculations on raw data, we find out the amounts described in the tables according to the model used in Fig. 1 and equations 1 and 2 to find α_G, α_D.



(a) (b)

Fig. 2: (a) (13,0) simple SWCNT as a CNTFET channel, (b) (13,0) SWCNT channel of CNTFET with attachment NH_3 on sidewalls.

Secondly, we attach NH_3 molecules to the sidewall of the nanotube channel of CNTFET and repeat the above steps to obtain corresponded α_G and α_D.

Table 2: The equivalent circuit values for two-stage simulation

Simple SWCNT	NH_3 attachment SWCNT sidewall
C_D = 6.63E-22	C_D = 6.63E-22
C_Q = 4.545E-20	C_Q =7.0297E-22
C_{ins} = 1.0929E-21	C_{ins} = 1.0929E-21
$C_{Q'}$ = 1.29E-21	$C_{Q'}$ = 4.594E-22
α_G = 0.459	α_G = 0.704
α_D = 0.2705	α_D = 0.148

To plot the i-v curves in MATLAB program we use of FETTOY tool that to this work we need to some parameters, such as gate insulator thickness, gate insulator dielectric constant and temperature that we assume these values according to Table 3. Also we use the Nanotube Grower tool in Virtual NanoLab that design for creating and previewing single-wall carbon nanotubes to compute the nanotube diameter. Source Fermi level find out by the simulation source electrode in VNL software same method of SWCNT calculations.

Table 3: Device specifications in FETTOY

Gate insulator thickness (m)	t = 20E-9
Gate insulator dielectric Const.	2.47
Nanotube diameter (m)	D = 1.0192E-9
Temperature (K)	T = 300

Source Fermi level (eV)	$E_f = -0.32$

After plot the i-v curves we compare curves of two stages. Output characteristics for SWCNT channel of CNTFET in two steps are plotted in Fig. 3. The comparing between two output characteristics shows that the saturation current in CNTFET with simple SWCNT channel (Fig. 3-a) is lower than CNTFET with NH_3 molecules attached to the sidewall of SWCNT channel (Fig. 3-b). This trend will be reversed when V_D increases.

Also Fig. 4 shows the input characteristics for two steps. In this figure it is clear that the drain current and its changes for CNTFET with simple SWCNT channel (Fig. 4-a) is more than CNTFET with NH_3 molecules attached to the sidewall of SWCNT channel (Fig. 4-b).

This comparison obviously shows that the NH_3 molecule will affect the performance of CNTFET as a sensor.

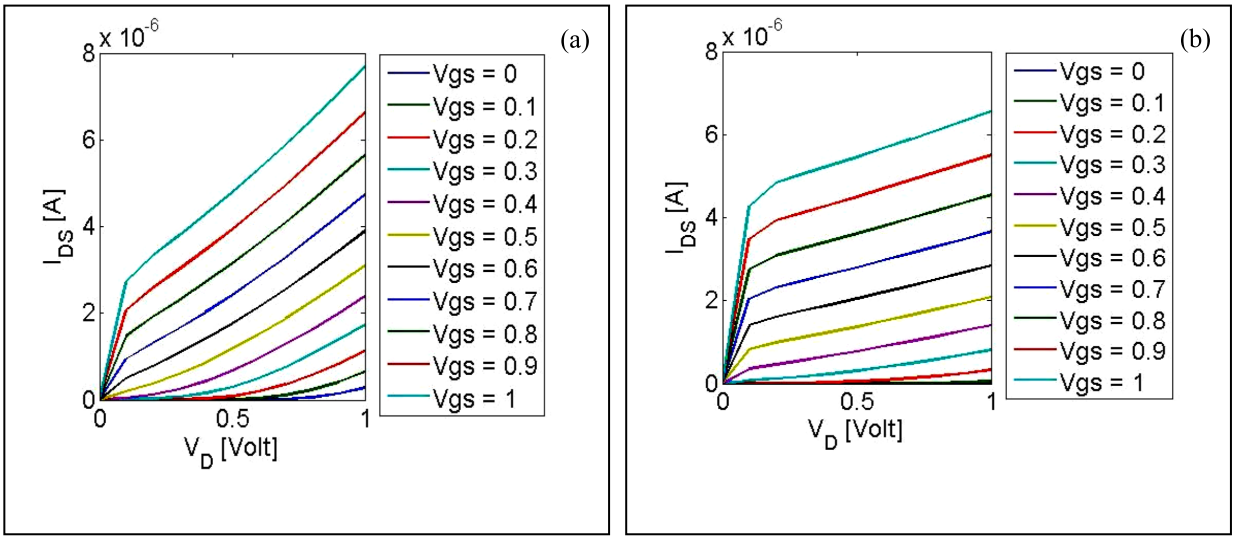


Fig. 3: i_{DS}-v_D Curves (output characteristic) of CNTFET with (a) simple SWCNT channel and (b) NH_3 molecules attached to the sidewall of SWCNT channel.

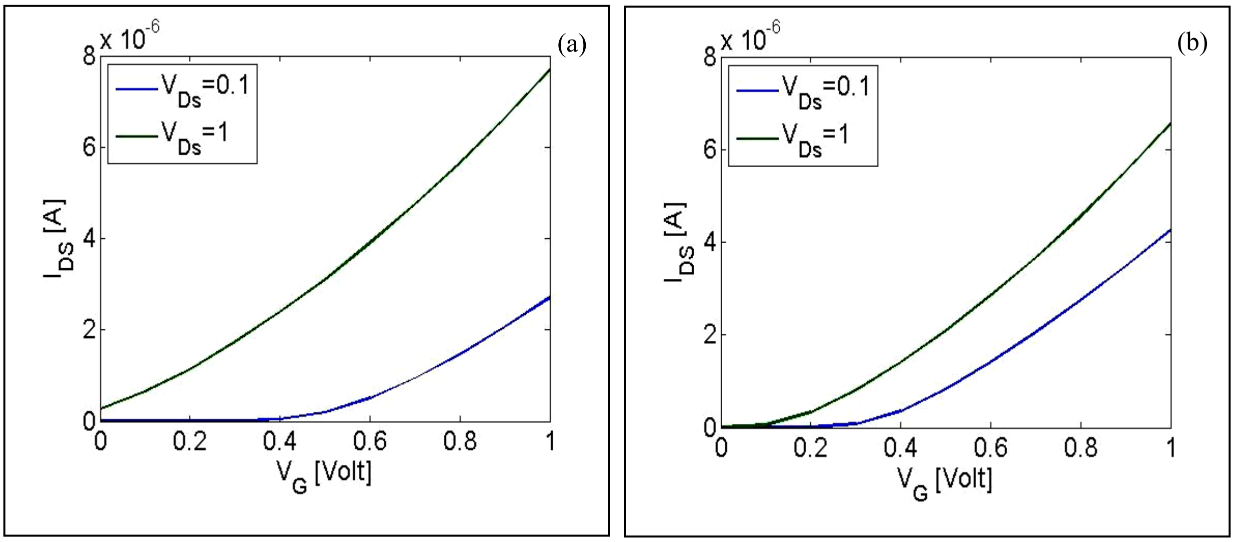


Fig. 4: i_{DS}-v_G Curves (input characteristic) of CNTFET with (a) simple SWCNT channel and (b) NH_3 molecules attached to the sidewall of SWCNT channel.

4. Conclusions

This paper has presented a CNTFET sensor by new modeling for detection of NH_3. Simulation results show that attachment of NH_3 to the sidewall of CNT reduces the capacitor channel (C_Q) and drain control parameter of CNTFET that it exchanges the i-v curves of CNTFET. The curves comparison clearly shows that the NH_3 molecule will affect the performance of CNTFET as its sensor.

5. References

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