

Simulation of Self Gating Effect of a Liquid Gate Carbon Nanotube Field Effect Transistor

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Abstract—A simulation of the carbon nanotube network (CNN) based FET device is proposed. The device structure has two concentric electrodes used as source and drain, which are connected by a CNN as a semiconductor channel layer and merged into aqueous solution for sensor application. The simulation system is based on the transport equation in the CNN, the Poisson equation in the insulator, CNN, and aqueous solution with appropriate auxiliary equations for carrier statistics in the various regions. Current versus voltage relationships were obtained and compared with the measurements. The new phenomenon, hereafter called the self gating effect, has been observed.

I. INTRODUCTION

There have been many efforts to fabricate carbon nanotube (CNT) based devices such as field effect transistors (FETs) [2], [3] or sensors [4] making use of CNTs' semiconducting properties and high sensitivity to their environment. The gate of CNT based FETs is often made of liquid material such as distilled water, buffer solution or electrolyte [6] especially when they are utilized as molecular sensors. Most of such types of devices require an external gate electrode to control the voltage of the liquid gate in order to prevent it from being electrically floated. This additional external electrode, which is usually made hang over the channel, makes the fabrication and integration of the device difficult and makes the device vulnerable to external mechanical stresses. Our group has recently developed [1] a new structure of device with a liquid gate which does not require an external gate electrode but only has two concentric electrodes where the relatively smaller electrode is fully enclosed by the larger electrode (cf. Figure 1a). The electrodes are not passivated but exposed directly to the liquid to be capacitively coupled to the liquid by the electric double layer.

Due to H^+ and OH^- ions (or other types of ions depending on the application) in the liquid, an electric double layer (EDL) is formed between each of the electrode and the liquid. The EDL capacitively couples the voltages of the electrodes and the liquid. Consequently, the voltage of the liquid follows that of the enclosing electrode because the enclosing electrode has wider area, which means larger capacitance. Thus, the enclosing electrode is expected to stabilize the voltage of the liquid by the self gating effect, which removes the need of an external gate electrode. Besides, because the concentric electrode structure prevents interferences from adjacent devices, it helps to increase the degree of device integration. In this

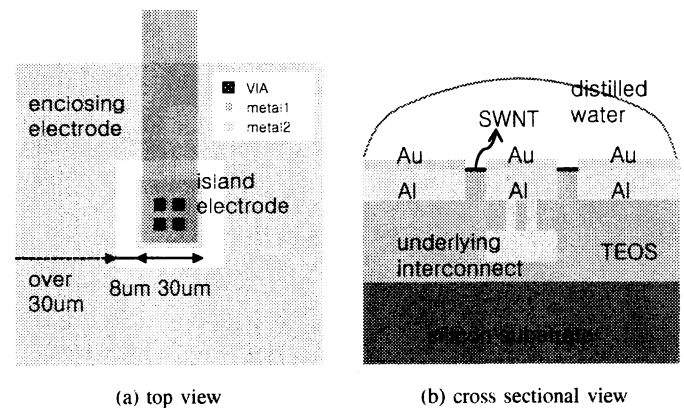


Fig. 1. Top and cross sectional views of the CNN FET structure immersed in the aqueous solution.

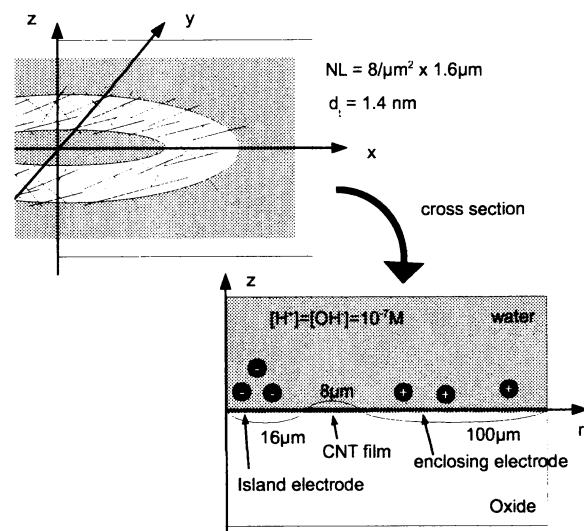


Fig. 2. Schematic of the simulation domain. The cylindrical coordinates are chosen to take advantage of the concentric feature of the electrodes.

paper, the simulation for the device structure described above is explained and compared with the measurements.

II. SIMULATION

Figure 2 shows the simulation structure and simulation domain. Thanks to the concentric nature of the electrodes, it is convenient to choose to use the cylindrical coordinates. Since the azimuthal symmetry can be assumed the simulation reduces to a two-dimensional problem with only two coordinates r and z . $1 \times 10^{-7} \text{M}$ of H^+ and OH^- ions are considered as the charged carriers in the water to account for the electric double layer capacitance. The electrodes and SW(Single Wall) NT network are assumed to be thin film conductors and semiconductor, respectively.¹ The current density in the SWNT is proportional to the gradient of carriers' Fermi potential and their concentration. The CNN contains 30% of metallic SWNTs. Very thick oxide lies beneath the channel and the electrodes.

A. Governing equations

We use the following governing equations for the simulation of the device described. In the water, by the Guoy-Chapman model for electric double layers:

$$\nabla^2 \psi = -\frac{q}{\epsilon} n_0 \left(e^{-\frac{q(\psi - \Psi_0)}{k_B T}} - e^{\frac{q(\psi - \Psi_0)}{k_B T}} \right) \quad (1)$$

where n_0 is the concentration of the ions under zero bias condition and Ψ_0 is such that²

$$\int_{\text{water}} \left(e^{-\frac{q(\psi - \Psi_0)}{k_B T}} - e^{\frac{q(\psi - \Psi_0)}{k_B T}} \right) dv = 0 \quad (2)$$

which accounts for the electrical neutrality of the water drop. Note that $qn_0 e^{-\frac{q(\psi - \Psi_0)}{k_B T}}$ and $qn_0 e^{\frac{q(\psi - \Psi_0)}{k_B T}}$ are the charge densities of the positive and negative ions respectively obeying the Boltzmann statistics. Then Equation (1) can be understood to be the Poisson equation with the charge densities obeying the Boltzmann statistics. In the oxide:

$$\nabla^2 \psi = 0. \quad (3)$$

In the CNT film, the areal concentration of carriers(holes and electrons) is calculated by the following:

$$p, n = \frac{NL}{\pi} \int_{-\infty}^{\infty} \frac{1}{1 + e^{\frac{\mathcal{E}(k) \pm q(\phi_F - \psi)}{kT}}} dk \quad (+ \text{ for } p, - \text{ for } n) \quad (4)$$

where [7]

$$\mathcal{E}(k) = \sqrt{\left(\frac{3}{4} a_{C-C} t k \right)^2 + \left(\frac{\mathcal{E}_G}{2} \right)^2}. \quad (5)$$

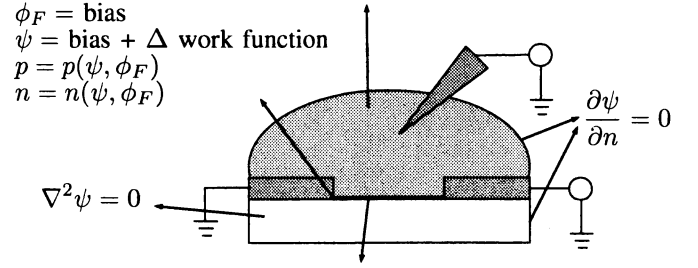
N is the number of SWNTs per unit area. L is the length of SWNTs. $-q\phi_F$ is the Fermi level of the carriers in SWNTs. It is taken to be -0.3eV relative to the intrinsic level at equilibrium. a_{C-C} is the distance between a pair of two adjacent atoms of SWNTs. t is the overlap integral parameter used in the tight binding calculation, for which 3eV is widely

¹so thin that the charges in the film are considered as interface(or surface) charges and the current in it as surface current. See Equation 7.

²One can think of Ψ_0 as the chemical potential of the ions. It is decided so that it satisfies the charge neutrality of the water drop.

$$\nabla^2 \phi = -\frac{q}{\epsilon} n_0 \left(e^{-\frac{q(\psi - \Phi)}{k_B T}} - e^{\frac{q(\psi - \Phi)}{k_B T}} \right)$$

$$\int_{\text{water}} \left(e^{-\frac{q(\psi - \Psi_0)}{k_B T}} - e^{\frac{q(\psi - \Psi_0)}{k_B T}} \right) dv = 0$$



$$q \nabla \cdot ((\mu_n n + \mu_p p) \nabla \phi_F) = 0$$

$$n, p = \frac{NL}{\pi} \int_{-\infty}^{\infty} \frac{1}{1 + e^{\frac{\sqrt{(\frac{3}{4} a_{C-C} t k)^2 + (\frac{\mathcal{E}_G}{2})^2} \pm q(\phi_F - \psi)}{kT}}} dk$$

$$\hat{n} \cdot (\epsilon_{\text{water}} \mathbf{E}_{\text{water}} - \epsilon_{\text{ox}} \mathbf{E}_{\text{ox}}) = q(p - n)$$

Fig. 3. The governing equations and the boundary conditions

accepted. \mathcal{E}_G is the band gap of the SWNTs, which has an asymptotic relationship with the diameter d_t of SWNTs as $\mathcal{E}_G = 0.8(\text{eV} \cdot \text{nm})/d_t$.³ For metallic CNTs, \mathcal{E}_G is taken to be 0.

Finally, the continuity equation for the current on the channel is:

$$q \nabla \cdot (\mu_p p \nabla \phi_F + \mu_n n \nabla \phi_F) = 0 \quad (6)$$

where μ_p and μ_n are the mobility of the holes and electrons in the CNN channel.⁴ These values are to be decided to fit the simulation results to the measurements.

B. Boundary conditions

Between the water and the oxide is one of the important interfaces for there is the CNT film. The charged carriers in the CNT film are regarded as interface charges in considering the boundary condition. Thus the boundary condition for the water-oxide interface containing the CNT film is:

$$\hat{n} \cdot (\epsilon_{\text{water}} \mathbf{E}_{\text{water}} - \epsilon_{\text{ox}} \mathbf{E}_{\text{ox}}) = q(p - n) \quad (7)$$

where \hat{n} is the normal vector to the interface directing the z direction. ϵ_{water} and ϵ_{ox} are the permittivities of water and

³The diameter of the SWNTs in the simulation is 1.4nm , thus the band gap is 0.57eV . Then the Fermi level (-0.3eV) is located below the valence band edge (-0.285eV). This seems implausible because it would mean the SWNTs are highly doped (although it is not doped.) There are $1.58 \times 10^9/\text{cm}$ carbon atoms in a SWNT of diameter of 1.4nm and $1.84 \times 10^6/\text{cm}$ holes in it if it has the Fermi level of -0.3eV . Thus if only 0.1% of carbon atoms acted as acceptors the Fermi level could lie well below the valence band edge. When the high surface-volume ratio of SWNTs and the very chemically active environment different from that of the vacuum are considered one could justify that this is not so impossible.

⁴Local equilibria are assumed to be maintained at every point in the channel. It means there is no separation between the hole quasi Fermi potential and the electron quasi Fermi potential.

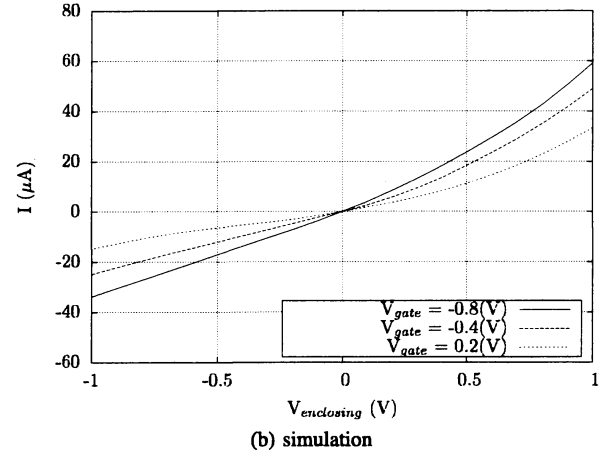
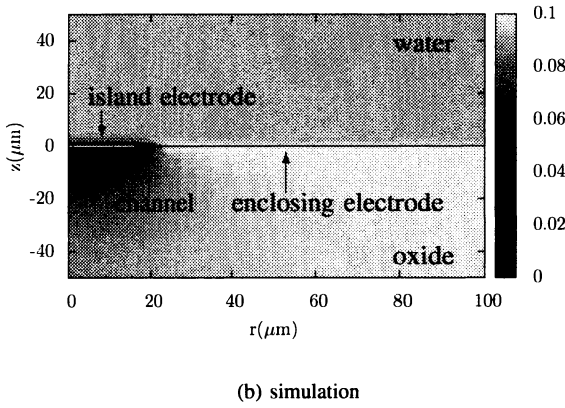
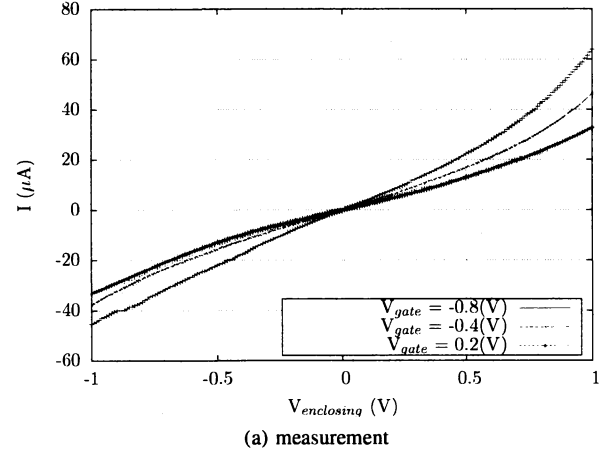
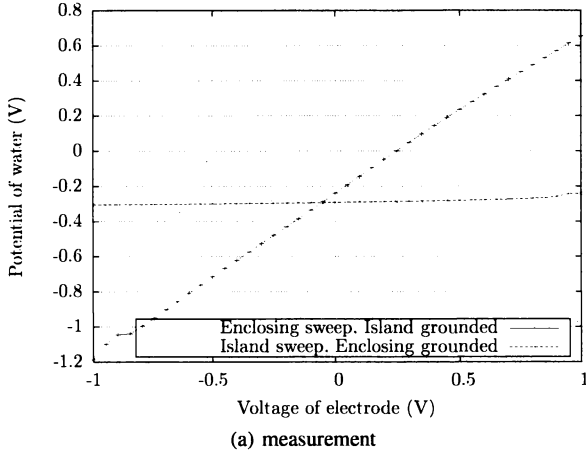


Fig. 4. (a) Measured water voltages versus the enclosing and island electrode voltages. (b) Potential profile in the simulation domain. 0.1V is applied to the enclosing electrode while the island is grounded. $N = 8/\mu\text{m}^2$, $L = 1.6\mu\text{m}$ and $d_t = 1.4\text{nm}$ are used.

Fig. 5. (a) Measured I-V curves between the enclosing and island electrodes at different external gate voltages. (b) Simulated results of Figure 5a. The mobility of CNN film was chosen to be $20\text{cm}^2/\text{V}\cdot\text{s}$ to fit the magnitudes of the simulated curves to the measurement data.

oxide respectively. $\mathbf{E}_{\text{water}}$ and \mathbf{E}_{ox} are the electric field on the water side and oxide side of the interface, respectively. p and q are the areal densities of the holes and electrons in the CNT film(cf. Equation 4).

The contacts between the CNT film and the electrodes are assumed ohmic:

$$\begin{aligned} \phi_F &= \text{bias} \\ \psi &= \text{bias} + \Delta \text{work function} \\ n &= n(\phi_F, \psi) \\ p &= p(\phi_F, \psi) \end{aligned} \quad (8)$$

The work function difference(Δ work function) is set to zero in this simulation for simplicity. Equation 4 is used for the evaluation of the last two equations of Equations 8.

And we give the Neumann boundary condition for the boundaries of the simulation domain:

$$\frac{\partial \psi}{\partial n} = 0 \quad (9)$$

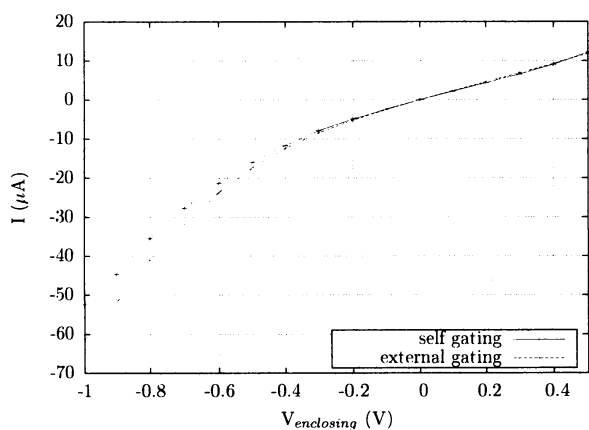
Figure 3 summarizes the governing equations and the boundary conditions.

ψ , Ψ_0 , p , n and ϕ_F are numerically solved using Equations (1) (or (3) in the oxide region), (2), (4) and (6) coupled together. Figure 4b shows the potential profile obtained when 0.1V is applied to the enclosing electrode. It is seen that the potential in the water follows that of the enclosing electrode as expected and thus that the enclosing electrode controls the potential of the channel reliably.

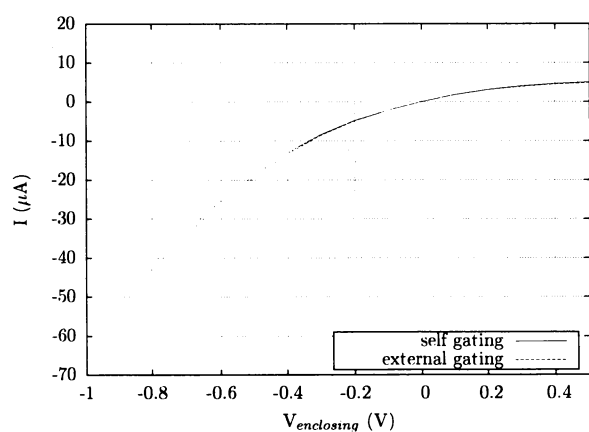
III. COMPARISON WITH THE MEASUREMENTS

In order to directly observe the self gating effect, a temporary external gate electrode was injected into the water to measure the voltage of the water or to apply voltages to the water. Figure 4a shows the voltages of the water which were measured while sweeping the voltage of the enclosing or island electrode with the other one grounded. From the figure it can be seen that the voltage of the water follows that of the enclosing electrode. It is consistent with the simulation result (Figure 4b).

Figure 5 shows the (a) measured and (b) simulated currents plotted versus the voltage of the enclosing electrode at various external gate voltages with the island grounded. The fact that



(a) measurement



(b) simulation

Fig. 6. (a) Measured I-V curves with the self gating and externally applied voltage. (b) Simulated self gating effect.

the more negative gate voltage increases the conductance of the channel leads us to that the CNTs are p-type.

Figure 6 compares, by both the (a) measurement and (b) simulation, the self gating effect with the results obtained by applying to the external gate electrode the same voltage as that

of the enclosing electrode while sweeping the voltage of the enclosing electrode. It shows that without the external gate electrode the voltage of the water can be stably fixed as if there were an external gate electrode. Each simulation result explains the corresponding measurement data qualitatively quite well.

IV. CONCLUSION

A simulator has been successfully developed to account for the self gating effect in the CNN FET structure immersed in the aqueous solution. The simulation considers the electric double layer taking place between the electrodes and the water. From the simulations and measurements, we learn that we can take advantage of the ions in the liquid and the associated electric double layer to stabilize the potential of the liquid.

ACKNOWLEDGMENT

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