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Switching behavior of semiconducting carbon nanotubes under an external electric field

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We investigate theoretically the switching characteristics of semiconducting carbon nanotubes connected to gold electrodes under an external (gate) electric field. We find that the external introduction of holes is necessary to account for the experimental observations. We identify metal-induced gap states (MIGS) at the contacts and find that the MIGS of an undoped tube would not significantly affect the switching behavior, even for very short tube lengths. We also explore the miniaturization limits of nanotube transistors, and, on the basis of their switching ratio, we conclude that transistors with channels as short as 50 Å would have adequate switching characteristics. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1367295]

One of the most important findings of carbon nanotube (NT) research is that the current in semiconducting tubes can be switched by an external electric field which allows semiconducting tubes to be used as the channel of field-effect transistors (FETs). Several groups have demonstrated such functional FETs.[1–3] The current through the NT has been found to be maximized at a negative gate bias, indicating that the NTs behave as p-type semiconductors, despite the fact that the tubes have not been intentionally doped. The detailed shape of the source–drain current versus gate voltage curves varies somewhat from experiment to experiment, and switching occurs over a relatively broad voltage range due to complications arising from charged traps and ''mobile charges'' in the gate dielectric.[4] As for the origin of the p-type character, a number of interpretations have been proposed, including interaction with the metal electrodes,[1] impurities and defects introduced during synthesis or processing,[2] or interaction with atmospheric oxygen.[5]

So far, the NT segments used in the FET experiments have been relatively long, in the order of several hundred nm to a micron. However, the process of device miniaturization aims primarily at reducing the channel length. The question then arises if short nanotube devices can preserve the operational characteristics of long devices.

Here, we use Green's function techniques to theoretically model nanotube FETs and address some of these issues. Specifically, we examine the switching characteristics of both intrinsic and p- and n-doped nanotubes of different lengths. The interaction of the nanotubes with the metal (gold) electrodes that generates metal-induced gap states (MIGS) is studied, along with the role of these states in the switching process, and the extent of the resulting ''metallization'' of the short tubes. Finally, the issue of how short NT FETs can be made is addressed.

Our calculations are performed on segments of semiconducting (10,0) nanotubes. The tubes are bonded with their dangling-bond bearing ends to two gold electrodes.[6] Each electrode is modeled by a layer of 22 gold atoms in a (111) crystalline arrangement. We also performed calculations with the tubes lying parallel to the gold electrodes. The main difference between devices with side bonding from those with end bonding is a higher contact resistance (several MΩ as compared to a few kΩ).[6,7] The electrical transport properties of the devices were calculated within the Landauer–Büttiker formalism using a Green's function approach.[8,9] The Green's function $\mathcal{G}_{\mathrm{NT}}$ of the combined electrode–nanotube–electrode system is written in the form

$$\mathcal{G}_{\mathrm{NT}}=[E\mathcal{S}_{\mathrm{NT}}-\mathcal{H}_{\mathrm{NT}}-\Sigma_1-\Sigma_2]^{-1}, \tag{1}$$

where $\mathcal{S}_{\mathrm{NT}}$ and $\mathcal{H}_{\mathrm{NT}}$ are the overlap and the Hamiltonian matrices, respectively, and $\Sigma_{1,2}$ are self-energy terms that describe the effect of the electronic structure of the two leads. The Hamiltonian $\mathcal{H}_{\mathrm{NT}}$ and overlap matrices are determined using the extended Hückel model with s,p_x,p_y,p_z orbitals for each carbon atom and one s orbital for each gold atom [s orbitals dominate the density of states (DOS) of gold near E_F]. The field of the gate is approximated as a capacitor field normal to the NT axis. In this case, the Hamiltonian $\mathcal{H}_{\mathrm{NT}}$ can be written as

$$\mathcal{H}_{\mathrm{NT}}=\mathcal{H}^0_{\mathrm{NT}}+\mathcal{H}^1_{\mathrm{NT}}, \tag{2}$$

where $\mathcal{H}^0_{\mathrm{NT}}$ is the Hamiltonian of the unperturbed NT and $\mathcal{H}^1_{\mathrm{NT}}=e\mathbf{R}\boldsymbol{\varepsilon}$. Here, e is the electron charge, $\mathbf{R}$ is the position of the atoms, and $\boldsymbol{\varepsilon}(\mathbf{r})$ is the external field.[10] Only diagonal elements of the Hamiltonian $\mathcal{H}^1_{\mathrm{NT}}$ on the extended Hückel

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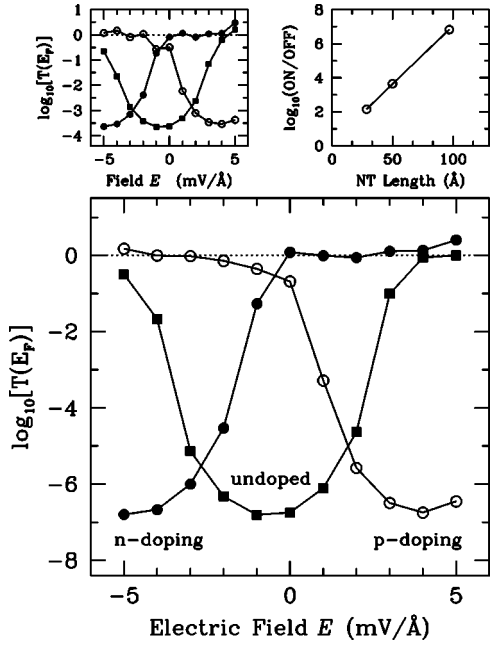

FIG. 1. Variation of the transmission of a 100-Å-long (main panel) and a 50-Å-long (upper-left panel). (10,0) semiconducting nanotube (NT) as a function of the applied field. Squares: undoped NT, open circles: p-doped, closed circles: n-doped NT. The on/off switching ratio is plotted as a function of the NT length in the upper-right panel.

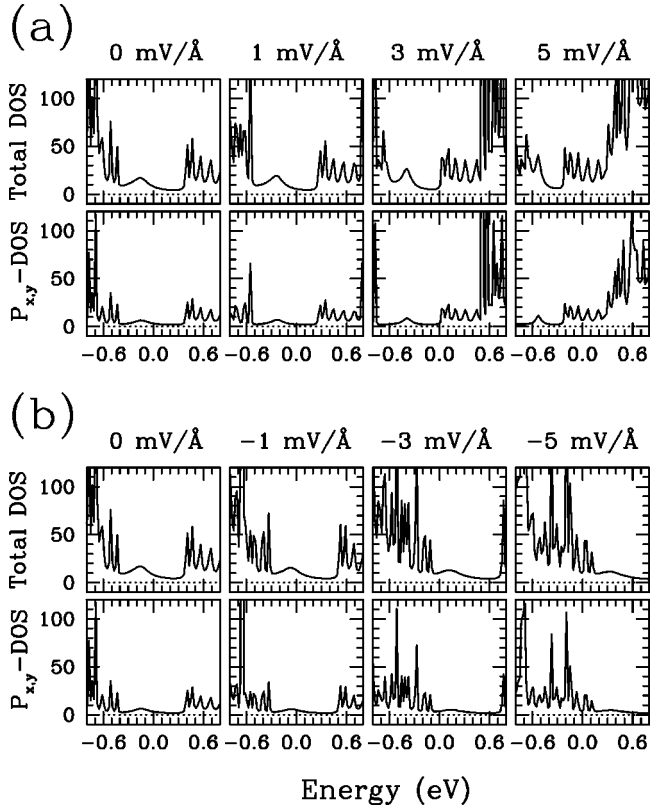

FIG. 2. Effect of (a) positive and (b) negative gate fields on the position of the valence and conduction bands of a 100 Å (10,0) NT. The total DOS and projected p_x and p_y DOS are plotted as a function of the magnitude of the electric field.

basis set are taken into account. This approximation assumes that all the charge of the carbon atoms is located at the center of the atoms.[11] This approximation has been proven to give quite accurate results for semiconductors,[11] and to reproduce the trends from first-principles transport calculations on molecular species.[12] Finally, the transmission function $T(E)$ is given by[8]

$$T(E)=T_{21}=\mathrm{Tr}[\Gamma_2\mathcal{G}_{\mathrm{NT}}\Gamma_1\mathcal{G}_{\mathrm{NT}}^{\dagger}], \tag{3}$$

where $\Gamma_{1,2}=i(\Sigma_{1,2}-\Sigma_{1,2}^{\dagger})$.

Since, in the experiments, the potential difference between the source and drain electrodes is usually very small (typically, less than 100 meV), we evaluate the conductance at the Fermi energy, $G(E_F)=[2e^2T(E_F)]/h$.

The main panel in Fig. 1 shows the variation of the conductance of a 100-Å-long (10,0) NT as a function of the applied gate field. Figures 2(a) and 2(b) show the corresponding total density of states and the DOS projected on the p_x and p_y components, for positive and negative gate fields, respectively. The gap of the NT at zero gate field is about 0.8 eV as defined by the two peaks at about -0.4 eV (valence-band edge) and $+0.4$ eV (conduction-band edge). The n (p) doping in Fig. 1 corresponds to the conductance calculated with the Fermi level located a few meV above (below) the conduction- (valence-)band edge. In the undoped case the Fermi level is placed in the middle of the gap. The ballistic limit for a semiconducting tube [$T(E_F)=1$] is also indicated by the horizontal dot line. By increasing the gate field in the mV/Å range, the C(p_x) and C(p_y) derived orbitals are shifted by the field to higher (lower) energy for negative (positive) fields (see Fig. 2). Therefore, the Fermi level crosses states with higher (lower) DOS for the n- (p-) doped NT, with corresponding increase (decrease) in the conductance. The conductance saturates when it approaches the ballistic regime.[13] The modulation of the current (on/off ratio) achieved with this NT is more than six orders of magnitude. Experimentally, FETs with side-bonding configurations have shown on/off ratios of 10^5.[1,2] Recent experiments with end-bonded low-contact-resistance tubes have yielded a ratio of 10^6.[14]

In undoped nanotubes, the DOS is quite symmetric around the Fermi level and this should lead to a symmetric conductance versus gate field curve. However, Fig. 1 shows a small asymmetry for small fields. This asymmetry is due to the metal-induced gap states produced by the interaction of the tube with the metal electrodes. This interaction produces weak DOS features at about -0.15 eV which extend up to about 8 Å away from the contacts. The computed MIGS features correlate very well with gap features observed in the scanning tunneling spectroscopy (STS) of semiconducting NTs on a gold substrate,[15] whose origin was not previously clarified.

It is important to explore the possible role of the above gap states in the current modulation process. In an undoped NT, the Fermi level (E_F) will be pinned close to the energy position of these states. Furthermore, it has been shown experimentally[16] that the band gap of semiconducting tubes does not change significantly down to at least 50 Å segments. Figure 3 shows the electronic DOS near E_F of 30-, 50-, and 100-Å-long NTs connected to gold electrodes. Carbon atoms bonded to gold (C–Au) and gold atoms (Au) provide the main contributions to the gap states. Assuming that small variations can occur in the filling of the MIGS, we have calculated the conductance by varying the Fermi level

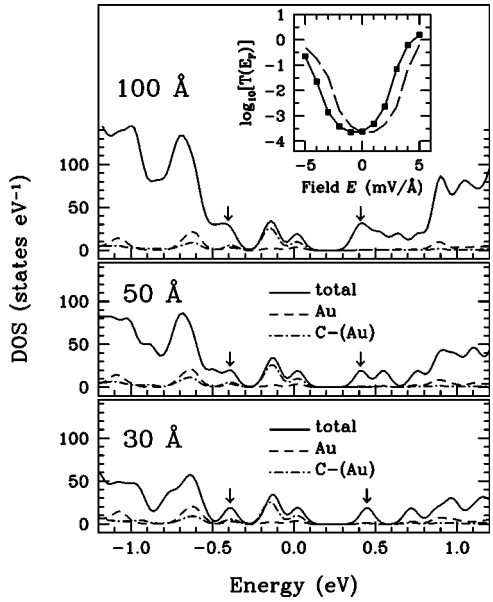

FIG. 3. Energy, composition, and relative intensity of the metal-induced gap states (MIGS) in the vicinity of Fermi energy for a 30-Å-long (lower panel), 50-Å-long (middle panel), and a 100-Å-long (upper panel) (10,0) NT (the valence- and conduction-band edges are indicated by the down arrows). The inset shows the effect of displacing the Fermi level (full line) to the energy of the MIGS (dashed line) on the conductance of the 50 Å NT.

across the MIGS energy position. We found that neither the switching behavior of the NT, nor the conductance at zero gate field are strongly affected by the movement of E_F (see the inset of Fig. 3). However, a small asymmetry is induced in the switching curve where a negatively biased gate becomes less effective in switching. This is because, in this case, E_F is scanned through the MIGS which are localized in the vicinity of the contacts, giving a lower transmission probability. The ''metallization'' of a NT segment decreases with its increasing length: the ratio of the DOS of MIGS to the DOS of the band edges (van Hove singularities) of the tube is reduced by a factor of 2/3 upon doubling the tube length (see Fig. 3). This trend should be valid for other quantum wires, and is in agreement with recent first-principles calculations on Si nanowires.[17] We thus conclude that MIGS do not play a significant role in the operation of NT field-effect transistors.

Next, we consider the miniaturization limit of nanotube FETs. Our calculations and STS measurements[16] indicate that there are no observable finite-size (length) effects on the band gap of semiconducting NTs down to at least 50 Å. Furthermore, the shift of the energy states of the NTs due to the gate field is independent of the length of the tube because the gate field is perpendicular to the NT axis. As a result, the conductance of the NTs at high gate fields should saturate at approximately the same value, irrespective of the tube's length. Thus, the tube length dependence of the on/off current ratio is determined by the off current. Using this ratio as a measure of how well the FET functions, taking MIGS into account and assuming that a ratio of 10^4 is the lowest acceptable for practical applications, then we can see from Fig. 1(c) that tubes as short as 50 Å can be used as channels of a FET. On this scale transport inside the tube is ballistic, there is no energy dissipation except at the contacts, and THz operation may be possible. These conclusions are not affected by temperature, since, for small source–drain voltages ($\leqslant 0.1$ V) the off current is proportional to the conductance via a factor eV/4 kT, which, at room temperature, is of order 1.

In conclusion, we have calculated the switching behavior of intrinsic and *n*- and *p*-doped semiconducting nanotubes. We have identified the metal-induced gap states and examined their role in the field-induced switching of the tubes. On the basis of the calculated current modulation, we conclude that NT segments as small as 50 Å can produce functional transistors.

[1] S. J. Tans, A. R. M. Verschueren, and C. Dekker, Nature (London) **393**, 49 (1998).
[2] R. Martel, T. Schmidt, H. R. Shea, T. Hertel, and Ph. Avouris, Appl. Phys. Lett. **73**, 2447 (1998).
[3] C. Zhou, J. Kong, and H. Dai, Appl. Phys. Lett. **76**, 1597 (1999).
[4] S. M. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981).
[5] P. G. Collins, K. Bradley, M. Ishigami, and A. Zettl, Science **287**, 1801 (2000).
[6] A. Rochefort, Ph. Avouris, F. Lesage, and D. R. Salahub, Phys. Rev. B **60**, 13824 (1999).
[7] A. Hansson, M. Paulsson, and S. Stafström, Phys. Rev. B **62**, 7639 (2000).
[8] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University, Cambridge, U.K., 1995).
[9] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, New York, 1983).
[10] The field is assumed to be noncentrosymmetric with respect to the tube axis, as in the experiments.
[11] M. Di Ventra and P. Fernandez, Phys. Rev. B **56**, R12698 (1997); in the present case, modification of off-diagonal terms in the Hamiltonian due to the external gate field has a small effect on the transmission probability.
[12] M. Di Ventra, S. T. Pantelides, and N. D. Lang, Appl. Phys. Lett. **76**, 3448 (2000).
[13] If an extra non-Ohmic contact resistance is added to the resistance calculated with the present coherent approach, the total resistance would saturate to this extra resistance.
[14] R. Martel and Ph. Avouris (unpublished).
[15] J. W. G. Wildöer, L. C. Venema, A. G. Rinzler, R. E. Smalley, and C. Dekker, Nature (London) **391**, 59 (1998).
[16] T. W. Odom, J.-L. Huang, P. Kim, and C. M. Lieber, J. Phys. Chem. B **104**, 2794 (2000).
[17] U. Landman, R. N. Barnett, A. G. Scherbakov, and Ph. Avouris, Phys. Rev. Lett. **85**, 1958 (2000).