Carbon Nanotubes as Schottky Barrier Transistors

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We show that carbon nanotube transistors operate as unconventional ''Schottky barrier transistors,'' in which transistor action occurs primarily by varying the contact resistance rather than the channel conductance. Transistor characteristics are calculated for both idealized and realistic geometries, and scaling behavior is demonstrated. Our results explain a variety of experimental observations, including the quite different effects of doping and adsorbed gases. The electrode geometry is shown to be crucial for good device performance.

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Carbon nanotubes show great promise for nanoscale field-effect transistors (FETs) [1,2]. However, despite considerable progress in device fabrication [3–5], the theoretical understanding remains incomplete. Initially, it was naturally assumed that the gate voltage modified the nanotube (NT) conductance, in analogy with the channel of an ordinary FET. However, there has been increasing evidence that Schottky barriers at the contacts may play a central role [4–7]. In fact, ordinary FETs require Ohmic contacts for effective switching, while reasonable work function estimates suggest significant Schottky barriers at NT-metal contacts [8,9].

Here we show that, whenever there is a substantial Schottky barrier (SB) at the contact, NT-FETs operate as unconventional *Schottky barrier transistors*, in which switching occurs primarily by modulation of the contact resistance rather than the channel conductance. SB-FETs have already been considered as a possible future silicon technology [10], because of their potential to operate at extremely small dimensions. We calculate the characteristics of such NT devices, and show that they explain a number of key experimental observations, including the effect of dopants, and the nonideal switching behavior. In particular, we find that the effect of adsorbed gases can be explained simply by their effect on work functions, without any doping, as has been generally assumed. The geometry of the contact electrode plays a central role, primarily by scaling the required gate voltage. We predict that the device characteristics can be *radically improved* by tailoring the contact geometry.

We begin by calculating the characteristics of the device shown in Fig. 1(a), consisting of a NT embedded in a dielectric between a top gate and a ground plane, with two metal electrodes as source and drain. Such devices have recently been reported [11]. We solve numerically for the self-consistent electrostatic potential as in Ref. [12], with the source, drain, and gate voltages as boundary conditions. For simplicity, the calculations in Fig. 1 use a local approximation to the electrostatic kernel for charge on the NT [13]. This is justified below by comparisons with a more complete calculation.

The current is then given by the Landauer formula,

$$I(V) = \frac{4e}{h} \int [F(E) - F(E + eV_D)] P(E) dE. \qquad (1)$$

Here V_D is the drain voltage (with the source taken as ground), and F is the Fermi function. We calculate the energy dependent transmission probability $P(E)$ within the WKB approximation for a semiconducting NT of band gap 0.6 eV. (WKB is relatively accurate when the tunneling resistance is high, so it describes the overall ''turn-on'' well. However, it neglects the reflection that would occur even in the absence of a barrier, so the conductance of the actual device may be somewhat lower than the WKB estimate.)

Figure 1(b) shows the conductance for different SB heights. When the metal Fermi level falls in the middle of the NT band gap (as determined by the respective work functions [14]), the conductance at zero drain voltage shows a symmetric dependence on the gate voltage. There is significant conductance at gate voltages of 5–10 V, but the ''turn-on'' is very far from ideal, with a conductance well below its maximum value of $4e^2/h \approx 1.5 \times 10^{-4}$ S even at 20 V.

The underlying mechanism for the transistor action is illustrated in Fig. 1(c). Already at 4 V there is substantial carrier density in the channel, but current is blocked by the SB. Increasing the voltage difference between source and gate electrodes leads to a large electric field at the contact, reducing the width of the Schottky barrier and allowing thermally assisted tunneling.

If the metal Fermi level does not fall in the center of the NT band gap, the SB height is different for electrons and holes, resulting in an asymmetric conductance curve (dashed and dotted curve in Fig. 1(b)). Whenever the SB is large enough to effectively block current, the device operates as a SB-FET. For very small SBs, however, the device operates as a normal (channel-limited) FET.

We now consider the crucial role of the device geometry. We focus on the case of midgap barrier, where the conductance is symmetric with respect to the gate voltage, so it

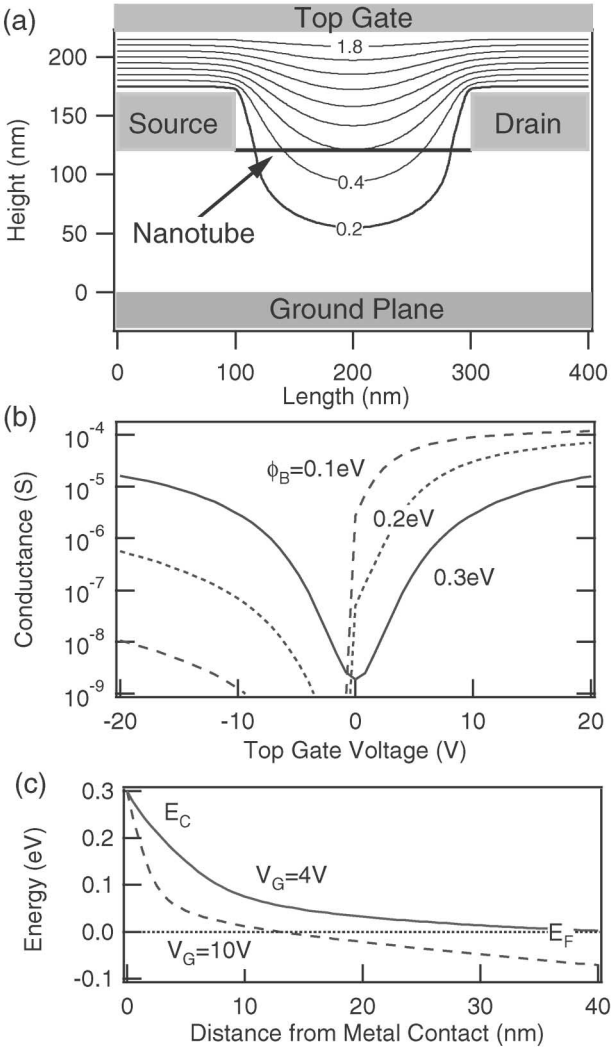

FIG. 1. Conductance for realistic FET geometries. (a) Device geometry, with metal contacts on the left and right, a ground plane, and a top gate. Contour lines show the electrostatic potential for a top gate voltage of 2 V. (b) Corresponding conductance versus gate voltage at room temperature, for different SBs. The SB height for electrons is indicated for each curve. (c) NT conduction-band energy near the contact, for gate voltages of 4 and 10 V.

is sufficient to consider positive gate voltages. (Our general conclusions apply equally to any case where the Fermi level at the interface falls deep in the gap, so the barriers for both electrons and holes are substantial.) Figure 2 displays the conductance as a function of gate voltage for a variety of device geometries. As expected, the turn-on is better for thinner oxides. However, even for the thinnest oxide (60 nm), the device requires a rather large gate voltage for full turn-on.

In standard FETs, the conductance is controlled by the electrostatic potential (and resulting carrier density) in the channel; so the key to improved performance is increased capacitance between channel and gate by reduction of the oxide thickness. In contrast to this, for a SB-FET the

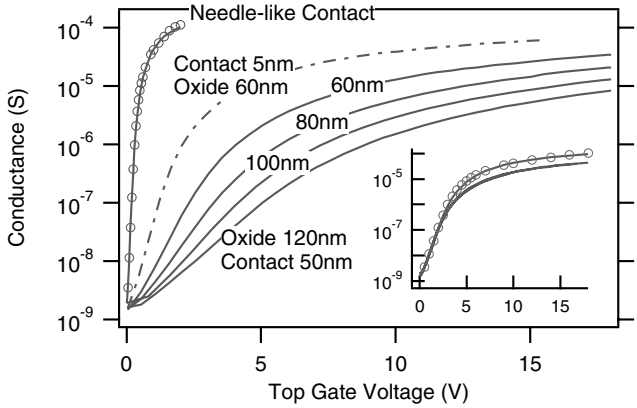

FIG. 2. Influence of the FET geometry on the device characteristics. The four right-most curves correspond to different thicknesses of the oxide above the NT, as labeled, with all other parameters as in Fig. 1. (The curve for 100 nm is the same as that in Fig. 1(b) for a SB height of 0.3 eV.) The dot-dashed curve shows the conductance when the contact thickness is reduced to 5 nm. The curve at the left corresponds to a needlelike metal electrode and cylindrical gate, see text. Open circles are calculated as for the other curves, solid curve uses the exact electrostatic kernel. All calculations are at room temperature. The inset shows the same curves, but for each curve the gate voltage is rescaled by the voltage at which the conductance is 10^{-8} S. (The five rightmost curves cannot be distinguished on this scale, forming a single line.)

performance is largely controlled by the *electric field at the contact*, as illustrated in Fig. 1(c). A sharper contact leads to field focusing, and hence a larger field at the contact. Thus, the device performance can be dramatically improved by varying the *geometry of the contacts*, in addition to the familiar dependence on gate distance. For example, if the thickness of the metal electrode is reduced from 50 to 5 nm, there is a striking improvement of the device performance, as shown in Fig. 2. The threshold voltage is lower, and the conductance approaches the maximum value at a lower gate voltages. This improvement would not occur for channel-limited conduction.

The relative position of contact and gate is also important. Most experiments reported to date have actually used a bottom gate underneath a thick oxide (100 to 1000 nm). From the field lines of Fig. 1(a), it is clear that the electric field at the metal-NT contact is larger when the gate is on the same side of the electrode as the NT. This suggests why, with a bottom gate, substantial modulation of the conductance was obtained even with thick oxides.

For good switching at a modest gate voltage, one wishes to maximize the electric field at the contact for a given gate voltage. Thus the ideal geometry would be a sharp needlelike contact, with a wraparound cylindrical gate. The electrode could be either a metal wire, or a metallic NT [15]. The conductance for such a device (with gate radius 50 nm and a SiO_2 dielectric) is included in Fig. 2. The huge gain in performance is quite striking.

This simple geometry also provides an opportunity to test our local approximation for the electrostatics of the charge on the NT. A solid line in Fig. 2 shows the results using the exact kernel for this geometry [9]. The difference is barely visible. This justifies the approximation used for the other geometries in Figs. 1 and 2.

The various device geometries lead to very different conductance curves in Fig. 2. However, the difference is primarily in the scale of gate voltage needed to modulate the conductance. In fact, we can scale the five realistic devices to a single "universal" conductance characteristic, as demonstrated in the inset of Fig. 2. Even the idealized needle-contact geometry is well approximated by the same scaling function. (The scaling is less closely obeyed at low temperature, where the detailed shape of the barrier becomes more important.) The scaling basically reflects the ratio of gate voltage to electric field at the contact. This scaling behavior is of great value in providing a broad perspective on the performance of NT SB-FETs.

One puzzling aspect of NT devices has been the dramatic effect of adsorbed gases on the behavior. It has been naturally assumed that this effect arises from doping of the NT [16,17]. However, recent work showed that the effect of adorbed oxygen was qualitatively different than that of alkali metals like potassium [7], which are also assumed to act as dopants.

For NTs, the Schottky barrier is sensitive to the metal work function [8]; and work functions are well known to be sensitive to adsorbed gases [18]. In most experiments, the metal contacts and NT have been directly exposed to O_2. Thus, one inevitable effect of gases will be to change the metal work function. (The NT work function may also be changed; but because of the weaker binding to these chemically inert structures, we focus on changes in the work function of the metal electrode.)

Figure 3(a) shows the calculated conductance vs gate voltage, for varying work functions of the metal source electrode. (The gate work function is assumed to be unaffected, since the bottom gate used in experiments is protected by the oxide. A different gate work function would simply shift the zero of gate voltage.) Figure 3(b) shows the same for varying doping of the NT. For doping, the charge on the tube plays a central role, so we use the idealized cylindrical geometry and exact electrostatic kernel for these calculations. We have already seen that the behavior for this model is almost identical to that for realistic geometries, aside from a scaling of the gate voltage; so the results apply rather generally.

The characteristics show a qualitatively different behavior for doping vs work function changes. The work function difference leads to a lowering of the conductance for one sign of gate voltage and an increase for the opposite sign. There is little change in the range of gate voltage at which the FET is "off," with conductance nearly zero. For doping, in contrast, the curves shift—to negative gate voltages for n-type doping, and to positive gate voltages

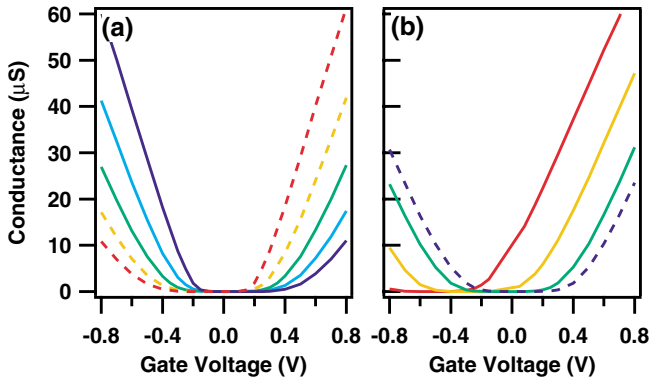

FIG. 3 (color online). Calculated conductance vs gate voltage at room temperature, varying (a) the work function of the metal electrode, and (b) doping of the NT. In (a) the work function of the metal electrode is changed by -0.2 eV (red dashed), -0.1 eV (orange dashed), 0 eV (green), $+0.1$ eV (light blue), and $+0.2$ eV (blue), from left to right, respectively. In (b) the doping atomic fraction is n-type 10^{-3} (red), 5×10^{-4} (orange), and 10^{-4} (green), and p-type 10^{-4} (blue dashed), from left to right, respectively.

for p-type doping. At a sufficiently high level of doping, a finite conductance is observed even at zero gate voltage.

This general behavior of the conductance is in striking qualitative agreement with the experimental measurements shown in Fig. 4. (Details of the experiment are given elsewhere [7].) We therefore conclude that the principle effect of oxygen exposure in the experiment is not to dope the NT, but rather to change the work function of the exposed portion of the metal electrode.

The distinctive dependence on gate voltage for the two cases can be understood from the respective band

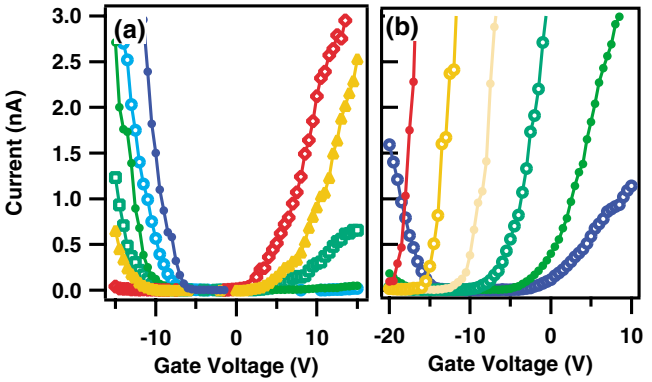

FIG. 4 (color online). The experimentally measured effect of (a) oxygen adsorption and (b) potassium doping on NT-FETs. In (a) the annealed (n-type) FET has been exposed to oxygen for 2 min at $P = 0$ Torr (red), $P = 10^{-4}$ Torr (orange), $P = 5 \times 10^{-4}$ Torr (light green), $P = 5 \times 10^{-3}$ Torr (dark green), $P = 10^{-1}$ Torr (light blue), and in ambient (blue), from left to right respectively. Details are given in Ref. [7]. In (b) the curves from right to left (blue, dark and light green, light and dark orange, red) correspond to increasing deposited amounts of potassium.

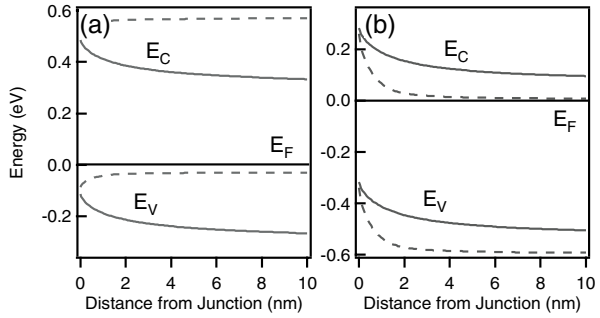

FIG. 5. Bending of NT valence and conduction bands at room temperature in the case of (a) metal electrode work function increased by 0.2 eV and (b) *n*-type doping of the NT at atomic fraction 5×10^{-4}. The solid lines correspond to zero gate voltage. The dashed lines are for -500 mV in (a) and $+500$ mV in (b). All energies are with respect to the Fermi energy.

diagrams. Figure 5 shows the band diagrams, for the case where the Fermi level originally falls at midgap. In Fig. 5(a), the work function of the electrode has been increased (e.g., by adsorbates) relative to the NT and gate. For zero gate voltage there is no channel conductance, and this is unaffected by the work function change. For one sign of gate voltage, shown in Fig. 5(a), when the channel turns on, the Schottky barrier is already reduced by the work function change; so the effect of the work function change is to enhance the turn-on. For the opposite gate voltage, when the channel turns on, the Schottky barrier at the contact is increased by the work function change, suppressing turn-on. This gives the characteristic asymmetric turn-on, without a shift in the voltage range where the channel conductance is suppressed.

Doping, in contrast, shifts the bands in the channel, and hence shifts the voltage range in which the channel is nonconducting. This accounts for the most dramatic difference between the two cases. Figure 5(b) shows the behavior for *n*-type doping. The width of the depletion barrier can be reduced by applying a positive gate voltage, allowing electron tunneling through the thin barrier. For negative gate voltage, however, it is extremely difficult to turn on the FET conductance—the gate voltage must be large enough both to achieve inversion in the doped channel and to narrow the Schottky barrier enough to permit tunneling. Thus in the experiment of Fig. 4(b), turn-on at negative gate voltages is seen only for the lowest doping levels studied.

In conclusion, the transistor action observed in carbon nanotube FETs can be understood on the basis of transport across a Schottky barrier at the metal-NT contact. The gate induces an electric field at the contact, which controls the width of the barrier and hence the current. A sharper contact leads to focusing of the electrical field, allowing operation at lower gate voltages. Changes in work function, e.g., by adsorbed gases, affect the Schottky barrier and hence the device characteristics. By comparing calculations with experimental data for FETs exposed to oxygen or doped with potassium, we suggest that the main effect of oxygen exposure is to change the work function of the metal contact rather than to dope the NT.

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[14] In general there may be "pinning" of the lineup at the metal-NT interface; but here we neglect such pinning, because it is much less important for NT Schottky barriers than for planar interfaces [8].
[15] The latter would be a particularly elegant approach, and such a junction was considered by Odintsov [9]. Here we focus on the case of a metallic wire having the same radius as the NT; but we find little difference in performance between the two cases.
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