Possibility of a metallic field-effect transistor

Slava V. Rotkin and Karl Hess
Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana–Champaign, 405 N. Mathews, Urbana, Illinois 61801

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We develop theoretical arguments that demonstrate the possibility of metallic field-effect transistors in one-dimensional systems and particularly in armchair carbon nanotubes. A very inhomogeneous electric field, such as the field of a tunneling tip, can penetrate the relatively weakly screened nanotubes and open an energy gap. As a consequence, an energy barrier forms that impedes electron flow and thus permits transistor action. This type of metallic field effect is advantageous because of the high conductance of the metallic tubes in the ON state.

Field-effect transistors in current use are semiconductor devices. The scaling trend to nanometer dimensions calls for ever higher doping and channel conductance of these devices. Ultimately one desires a conductance close to that of a metal if one wants to scale devices to the smallest possible size. However, a metallic conductance also prevents the penetration of the electric field except for extremely short distances; ordinarily too short to achieve device function.

We propose here an approach to control electron transport in metallic one-dimensional (1D) systems by use of the inhomogeneous electric field of a low-dimensional highly localized "modulating" gate (MG) such as nanometer tips or metal nano-interconnects. Use of a highly localized gate results in a strong enhancement of the electric field in a narrow region. Thus any depletion of charge is easier to achieve since it occurs only in extremely small volumes. In addition, the weak screening of electric potentials in 1D channels further enhances possible field effects.

The purpose of this letter is to show that metallic carbon nanotubes may be suitable for use as metallic field-effect transistors (METFETs). Key to this metallic field effect is the opening of a band gap due to the breaking of the mirror symmetry by the MG. Note that a region of spatially nonuniform electric field also represents a barrier that reflects electrons, while the homogeneous field of an extended gate changes predominantly the carrier density. These qualitative factors are discussed in the following in a more quantitative way and their potential for device applications is illustrated.

Metallic field effect in armchair NTs. IBM researchers have enunciated the vision of combining metallic and semiconducting single-wall nanotubes (M-SWNTs and S-SWNTs) in circuits. The M-SWNTs would serve as interconnects and the S-SWNTs as active devices of the extremely small size (typically, the SWNT radius is \( \sim 0.7 \) nm). Here we discuss the possibility to also use metallic tubes as transistors or switching devices, which is appealing because of their virtually ballistic conductance.

The band structure of an armchair SWNT, as shown in Fig. 1, has two subbands A and B (shown as bold green and blue curves) crossing at the Fermi level. Absence of the gap is ultimately related to the SWNT mirror symmetry, which forbids any mixing of these subbands. We propose to break this mirror symmetry by applying very nonuniform electric fields by use of a MG. Two possible mechanisms for gap opening in armchair SWNTs are: (1) by a direct mixing of electron and hole states of the A and B subbands, which happens if the external potential has an atomic scale corrugation, and (2) by the indirect subband mixing in a higher order of the perturbation theory, which essentially can be realized for any nonuniform potential. Both mechanisms require (i) a relatively high electric field (order of \( 10^7 \) V/cm) and (ii) SWNT symmetry breaking.

Group theory proves that the direct matrix element is nonzero if the Fourier transform of the potential \( U_{q,\delta m} \) is a full scalar with respect to the rotations of the symmetry group of the nanotube. This is fulfilled for \( \delta m = sn \), where \( s = 2, 4, \ldots \) is a positive even integer and \( n \) is the integer appearing in the notation \( [n,n] \) for armchair SWNTs.

Then, the energy dispersion of two new subbands \( \{A \pm B\} \) in vicinity of the Fermi point reads as: \( E_u = \pm \sqrt{(E_A(q))^2 + U_{q,\delta m}^2} \). Here \( E_A(q) = -E_B(q) = E_B(-q) \) is the dispersion in A/B subband at zero gate voltage. At the Fermi point \( E_A(0) = 0 \) and, thus, a gap opens:

\[
E_{g}(\pm) = 2\left|U_{q,\delta m}\right|.
\]

This is a direct mixing of the subbands A and B. The band gap is linear in the applied gate potential (see the inset in Fig. 1). A full calculation presenting a self-consistent solution of joint Schrödinger and Poisson equations following the derivation of Refs. 11 and 12 will be published elsewhere. Except for a natural condition that the field must not cause an electric breakdown, there exists no upper limit for the magnitude of the gap that opens in this case and we estimate the possibility of a gap of several electron volts.

Thus direct mixing of the crossing subbands allows one to open a large gap. It does require, however, a very high multipole moment of the potential in order to break the symmetry (we must at least have \( \delta m = 2n \)) and this is difficult to achieve because the amplitude of any high multipole component will be typically much smaller than the gate voltage, \( U_{q,2n} \ll V_g \). Nevertheless, it may be possible to create such a
potential by applying the gate voltage to a chemically modified surface of the SWNT. This approach is technologically complex.

Fortunately, there exists a more straightforward possibility to open a band gap by virtually any kind of inhomogeneous electric field that breaks the mirror symmetry. A band gap opens also by indirect mixing of the subbands. This band gap opening is smaller because it arises from higher order perturbation terms (similar to a nonlinear Stark effect) and thus has consequences for the conductance only at low temperatures. In particular, any potential that contains both a uniform field and a higher order (quadrupole) component will lead to a gap which scales with the third power of the gate voltage. In what follows we consider an example of two metal tips at opposite sidewalls of the SWNT at the tunneling distance of 0.5 nm from the tube: one at $+2V_g$ and the other at $-V_g$ bias. Note that the potential of a metal tip together with its image charge in the insulator substrate, e.g., SiO$_2$, is equivalent to the potential of two tips at $+1.69V_g$ and $-V_g$. Therefore, the METFET setup illustrated in Fig. 2 should have a valid geometry to generate a band gap and METFET effect. We only have shown two tips for the current example because the METFET effect is somewhat bigger and the simulation is more clear cut. In both cases the gap $E_g$ has qualitatively the same dependence on $V_g$ as shown for [5,5] and [10,10] armchair SWNTs in the inset of Fig. 3. The $E_g$ first increases with $V_g$ and decreases beyond $\pi \gamma/(en)$ where $\gamma=3$ eV is a hopping integral. Perturbation theory\textsuperscript{10,11,13} predicts a maximum gap that depends only on the size of the tube and scales in a universal way for nanotubes of arbitrary chirality: 

$$E_{g}^{(c)} \sim \frac{\hbar v_F b}{2R^2} \gamma \frac{\gamma}{n^2}. \tag{2}$$

This was confirmed by numerical calculations in Refs. 11 and 13. Here $v_F = 3\gamma b/2\hbar$ is the Fermi velocity for a M-SWNT, and $b=0.14$ nm is the bond length. This gap may be possible to achieve experimentally by use of the inhomogeneous electric field of a tunneling tip. Also, ultranarrow leads,\textsuperscript{14} fabricated closely to the nanotube channel, special (electro-)chemical function groups at the tube sidewalls or inside the tube\textsuperscript{15} may be used as a MG. We notice that use of a dual gate (both local and backgate) may be beneficial for 1D METFETs because the uniform backgate controls the Fermi level (charge density) while the MG controls the conductivity of the channel.

Field-effect modulation of metallic conductance. Any opening of the gate induced semiconductor gap along the armchair metallic tube will create a potential barrier for the electrons and therefore modulate conduction. (Note that this modulation may be enhanced by Coulomb blockade).\textsuperscript{10} In-
clusion of tunneling is important for the calculation of the current because the effective mass of the electrons in SWNTs is very small (~0.06m_e, similar to the in-plane effective mass of graphite\textsuperscript{18}). At nonzero temperature thermionic emission must be taken into account as well. Although the rate of tunneling through the classically forbidden (gated) region is high, a significant metallic field effect can be achieved by increasing the width of the gated region, or by operating the device at low source–drain voltage, V_d, and low temperature, T. (The ON/OFF current ratio is controlled by the parameter E_g/V_d). Because the transport in the armchair SWNT METFET is ballistic, its conductance in the ON state is limited only by reflections at the contact. We will use in what follows (mainly for normalization purposes) a maximum conductance of 4G_0 = 2e^2/h\textsuperscript{19}.

For the OFF state, we estimate a semiclassical Wentzel–Kramers–Brillouin transmission coefficient, T(E), by assuming a uniform gap of width W in the gated region. In order to extend the validity of our results to nonzero temperatures we calculate the total transmission of the channel by integrating the partial current, \sim T(E), multiplied by the difference of the Fermi distribution functions of the left and right electrodes.

Figure 3 shows typical I–V curves (I–V–C) for a METFET using a [5,5] armchair M-SWNT of the diameter 0.7 nm at T = 4 K, W = 50 nm. The upper (red) I–V–C corresponds to a zero gate voltage (no gap). The channel is fully open and the ON current is determined by injection from a contact and thus by the quantum conductance 4G_0.\textsuperscript{19} With increasing gate voltage one observes a substantial decrease of the current due to the opening of the gap and a depletion of electrons in this region (blue curve). In the right inset of Fig. 4, the METFET current is plotted versus the V_g for the dipole–quadrupole potential (two tip geometry) as described earlier. At low drain bias (blue curve) the METFET is switched OFF at V_g \sim 3 V.

The total transmission coefficient of the METFET, T(E) = G(E)/G_0, assuming transparent contacts, is plotted in the left inset of Fig. 4. Several families of curves are given for different temperatures. In the upper family of curves (room temperature) the suppression of transmission through the gated region is clearly seen as a function of an increased gap: from 0 to 0.12 eV (from green to red, top to bottom). At lower temperatures T = 77 and 4 K this effect is naturally sharper.

The current is an exponential function of the gap (and, hence, of the gate voltage). Results are shown in Fig. 4: by opening a gap of about 0.5 eV (which would certainly require sophisticated technology) one can decrease the current by five orders of magnitude.

In conclusion, we have proposed a novel type of electronic switching device based on carbon nanotubes: a one-dimensional metallic field-effect transistor (1D METFET). We have described armchair SWNTs in detail because of their special symmetry that also gives rise to virtually ballistic transport. Our calculations demonstrate, at least principle, the possibility to open a band gap by application of inhomogeneous electric fields that are created by special gates (modulation gates) that in the simplest case resemble a tunneling tip to break the SWNT symmetry. Assuming ballistic transport, we have calculated I–V curves for the METFETs with gate widths of the order of 15–50 nm and found significant modulation as well as reasonably large ON/OFF current ratios. We finally note that one can expect excellent scaling properties of the SWNT METFET because of the metallic conductivity enhanced by ballistic transport.

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\textsuperscript{16}At the points of metal–semiconductor junction (MSJ) a charge accumulation may happen. This MSJ boundary becomes a side of a 1D capacitor with a capacitance \sim W/2ln(W/R). Neglecting the logarithmic term, a classical charging energy of this capacitor is e^2/2W, which is large for a narrow gate. However, in this work we did not consider a Coulomb blockade because an effective gap is exponentially renormalized at a high conductance of the tunnel junction (Ref. 17). Large coupling between sides of the MSJ and quantum fluctuations of the charge wash out the correlation and destroy the Coulomb blockade.
\textsuperscript{18}The effective mass near the band edge m^* = h^2/2E_i(k^2)^{-1} = 2\hbar^2/9bR\gamma is about 0.06 of the free electron mass for the SWNT of the radius R \sim 0.7 nm.
\textsuperscript{19}For a circuit with macroscopic leads to the M-SWNT channel the total conductance will be about 4G_0 = 2e^2/h, 4 times of the conductance quantum (for two spin and two space channels). This gives a minimum resistance of the SWNT device \sim 6.5 k\Omega. The lower resistance can be expected in the case of entirely nanotube circuit (Ref. 2). The quantum contact resistance will not limit anymore the ON current in this case. That device can fully exploit all advantages of the METFET.