Modeling a Schottky-barrier carbon nanotube field-effect transistor with ferromagnetic contacts

S Krompiewski

Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland

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Abstract

In this study, a model of a Schottky-barrier carbon nanotube field-effect transistor (CNT-FET), with ferromagnetic contacts, has been developed. The emphasis is put on analysis of current–voltage characteristics as well as shot (and thermal) noise. The method is based on the tight-binding model and the non-equilibrium Green’s function technique. The calculations show that, at room temperature, the shot noise of the CNT-FET is Poissonian in the sub-threshold region, whereas in elevated gate and drain/source voltage regions the Fano factor gets strongly reduced. Moreover, transport properties strongly depend on relative magnetization orientations in the source and drain contacts. In particular, one observes quite a large tunnel magnetoresistance, whose absolute value may exceed 50%.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In view of the well-known size reduction problems of conventional Si-based electronics, there have recently been intensive studies on new technologies based on nanostructured materials which are formed by organized growth and self-assembly methods [1]. A remarkable example of such self-organized structures are carbon nanotubes (CNTs), which due to their fascinating physical properties have been studied for more than 15 years and are believed to have commercial applications in the near future. In particular a nanotube-based transistor was first demonstrated in [2], and has since been studied extensively [3–5]. CNTs are also very promising for spintronic applications, they may act as magnetoresistive switches [6, 7], and can maintain spin coherence over long distances. The latter property is crucial for the tunnel (giant) magnetoresistance TMR (GMR) effect to be observable. In fact the TMR effect in CNTs was first reported in [8], where the spin diffusion length of electrons flowing through a carbon tube was estimated to be of the order of routinely used contact separations in electric transport measurements. Subsequent studies confirm that the TMR effect in CNTs can be quite large, ranging typically from a few up to several tens per cent [9–15]. Here it is shown that the situation is similar for the Schottky-barrier nanotube transistor.

Shot noise is another important phenomenon of current interest. It only appears in a non-equilibrium situation (finite source/drain voltage) and originates from the discreteness of the electron charge. In spite of there being a lot of papers on shot noise in nanostructures [16–19] (see [20] for a comprehensive review of recent advances), to the author’s knowledge there have hitherto been no attempts to investigate shot noise in ferromagnetically contacted Schottky-barrier nanotube transistors.

The paper is organized in the following way. In section 2 a short discussion of the adopted approach is presented, including the way the electrostatics has been dealt with, and basic equations concerning the non-equilibrium Green’s function method. Section 3 is devoted to the main results of the paper, i.e. current and shot noise dependences on the gate and drain/source voltages, as well as the impact of ferromagnetic electrodes on the above-mentioned transport characteristics. Finally, section 4 concludes the paper.

2. Methodology

A nanotransistor under consideration consists of a single wall CNT, described in terms of π-orbital electrons, end-contacted to s-type itinerant-electron slabs of fcc (111) crystallographic
structure. The latter may be either paramagnetic or ferromagnetic. The system considered here is end-contacted, in contrast to other widespread geometries, like those of side-contacted or embedded ones. The device has been relaxed in order to find energetically favorable positions of interface atoms represented by big and small spheres with diameters of $d_M = 2.51$ Å and $d_C = 1.421$ Å for metal and carbon, respectively [10, 11]. The studies are carried out within the framework of the tight-binding model and the non-equilibrium Green’s function technique. The basic idea of this study is to adopt the methodology known for one-dimensional transistor models [21–23] so as to make it useful for description of a Schottky-barrier nanotube transistor. This method bears much similarity to earlier methods [24–26], except that here the calculations are performed in real space for a CNT of finite length, and there is no need to use any ideal nanotube energy spectra (nor the Wentzel–Kramers–Brillouin, WKB, approximation). It should, however, be stated in this context that there are very few of theoretical studies on nanotube transistors (see e.g. [27–31]), which successfully avoid reducing the Poisson equation to the 1D problem, and thereby handle the electrostatics on a higher level than is done here. Nevertheless, the present approach, while benefiting enormously from the mathematical simplicity, still leads to qualitatively correct results. The one-dimensional Poisson equation and its solutions are regarded here as spin-dependent (however, spin indexes are skipped for brevity), and read [21]

$$\frac{\partial^2}{\partial x^2} V(x) + \frac{1}{\lambda^2} [V_G - V(x)] + \frac{1}{\epsilon_{CNT} A} \rho(x) = 0,$$  

(1)

where $\lambda = (R/2) \sqrt{2(\epsilon_{CNT}/\epsilon_{SiO2}) \ln(1 + d_{ox}/R)} + T$ is the effective screening length [23], $\epsilon_{CNT}$ and $R$ stand for the dielectric constant and the radius of the CNT, whereas the subscript $ox$ refers to the coaxial gate oxide layer SiO$_2$ ($d_{ox}$ in thickness). The other symbols have the following meaning: $V_S$, $V_D$, $V_G$ are the source, drain and gate voltages; $L$ is the length of the CNT; $f_{Si}$ is the Fermi function at $V_S$ and $V_D$; and $A$ is the cross-sectional area of the CNT.

As regards the non-equilibrium Green’s function (GF) technique, a recursive method, similar to that of [32], was used, with obvious modifications which consisted of including the potential profile $V(x)$ (equation (2)) in the CNT Hamiltonian and the $V_S$ and $V_D$ voltages in the contacts. This procedure corresponds to the Hartree approximation, which is sufficient for the present room-temperature model, far beyond the Coulomb blockade and Kondo regimes. With this proviso one can write down equations for spin-projected current ($I$), zero-frequency noise power ($S$) and transmission matrix ($T$) as follows:

$$I = \frac{e}{h} \int dE (f_S - f_D) \text{Tr}(T(E)),$$

$$S = \frac{2e^2}{h} \int dE [(f_S(1 - f_S) + f_D(1 - f_D)) \text{Tr}(T(E))$$

$$+ (f_S - f_D)^2 \text{Tr}(T(E)(1 - T(E)))],$$

(5)

$$T = \Gamma_S G T \Gamma_D G^\dagger,$$

where trace (Tr) is taken over the orbital indexes, and $\Gamma_\alpha = i(\Sigma_\alpha' - \Sigma_\alpha)$ (with $\alpha = S, D$ for source and drain, respectively). The first term of the noise power $S$ is the thermal noise, it disappears at zero temperature, but dominates at finite temperatures and vanishing source/drain potentials. The Fano factor is defined here—assuming that both spin channels are independent (no spin relaxation processes)—in the usual way as $F = \langle S^2 \rangle / \langle 2e (S^2 + 1) \rangle$, so that it is 1 for the Schottky shot noise (Poissonian limit). Instead of a rather common wide-band type approximation, the present method uses energy-dependent self-energies ($\Sigma_\alpha(E)$) which have been expressed in terms of: (i) recursively computed surface Green functions ($g_\alpha(E)$) of infinite fcc-(111) contacts, and (ii) the CNT/contact coupling matrices ($u_i$), i.e $\Sigma_\alpha(E) = u_i g_\alpha(E) u_i^\dagger$. Here the retarded $G^+$ (advanced, $G^-$) GF is a matrix of rank equal to the number of atoms in the unit cell it refers to. The density matrix is defined as $\rho = -i/2\pi \int dE G^- G^+$ in terms of the lesser GF, which can be brought into the following form: $G_- = -f_0 G^+ G^0 + i(f_0 - f_D)G^0\Sigma G^+$. While integrating $G^+$, the contribution of its first term is found by integral over the contour in the complex energy plane, and of the second one by integrating along the real energy axis (using the Gaussian quadrature). The so-determined integral makes it possible to get an extra (excess or deficit) electric charge per CNT atom, with respect to the charge neutrality situation (no external potentials). The procedure is self-consistent because the potential $V$ enters the diagonal of the Hamiltonian, which in turn is present in the GF denominator. In order to make the recursive algorithm work effectively, and speed up the convergence, an additional assumption has been made, namely the potential profile is only dependent on the unit cell number and remains constant within the given unit cell.

3. Results and discussion

Detailed computations have been carried out for a zigzag semiconducting CNT with a chiral vector $(n, 0)$ and the energy gap $\Delta = 2\pi t/(\sqrt{3}a)$, where $a = 0.249$ nm is the graphene lattice constant and $t = 2.7$ eV is the $\pi$-orbital hopping integral. Additionally, we have set: $\epsilon_{CNT} = 1, \epsilon_{ox} = 4$ and $d_{ox} = 2.5$ nm. The CNT is $l$ unit cells long ($L = la\sqrt{3}$), and the calculations are performed for $l = 100$ (as well as for the ultra-short length $l = 15$). It is well known that the Schottky barrier at a semiconductor/metal interface depends mainly on the relative work functions (WF) of materials which form the junction [30, 31, 33]. Here it is assumed that the metal WF is greater than that of the CNT, as e.g. for Pt, Au, Ni, Fe (as opposed to Ti), and locate the Fermi energies below the mid-gap. To be specific, the metal Fermi energy has been fixed at one-quarter of the band gap.
clearly shows that, depending on the boundary conditions characteristics differ considerably from each other. Notably, versus antiparallel alignment (AP), the current–gate voltage imposed by the magnetic contacts (parallel alignment (P) versus the presence of the inner uncontacted shell in a double-walled CNT, leading essentially to similar results for current–voltage characteristics (in the non-magnetic case). Figure 2.

Figure 1. Spin-split surface densities of states (DOS) of a contact (thin line). In the antiparallel configuration the second contact has got interchanged ↑, ↓ sub-bands (no interchange in the parallel case). The thick curve is for the CNT DOS. Inset: band bending at the interface for $V_G > 0$ (short-dash line) and $V_G < 0$ (solid line).

Figure 2.

The current versus gate-voltage characteristics for the parallel alignment of the contact magnetizations (solid line) and the antiparallel alignment (dashed line). The drain/source voltage is equal to 0.2 V, length $L = 100$ unit cells and temperature $T = 300$ K.

On- and off-states of the FET are illustrated in the inset to figure 1, where the lower curves correspond to the maximum of the valence band and the upper curves correspond to the minimum of the conduction band. Accordingly, the present model device represents a case of ‘$E_F$ close to valence band maximum’ (cf [4]). It is seen that, depending on the gate voltage, the CNT-FET is either in the on-state (solid lines) or the off-state (short-dash lines). The former is due to the hole tunneling through the Schottky barrier, whereas the latter results from the fact that the transport energy-window falls within the energy gap. The location of $E_F$ beyond the mid-gap of the isolated CNT introduces the electron–hole asymmetry; as shown recently [34] a similar effect may be caused by the presence of the inner uncontacted shell in a double-walled CNT, leading essentially to similar results for current–voltage characteristics (in the non-magnetic case). Figure 2 clearly shows that, depending on the boundary conditions imposed by the magnetic contacts (parallel alignment (P) versus antiparallel alignment (AP)), the current–gate voltage characteristics differ considerably from each other. Notably, the ON/OFF current ratio is also different for both the alignments. This is because the sub-threshold region reveals a conventional (Julliere type [35]) behavior with $I_P$ clearly greater than $I_{AP}$, whereas beyond this region both the currents differ far less from each other. Within the ‘non-Julliere’ region the negative TMR apparently appears as a result of the shift of threshold $V_G$ for electron conduction between P and AP configurations. Figure 3 presents the corresponding Fano factors. The shot noise of the CNT-FET is Poissonian ($F = 1$) in the sub-threshold region, and gets substantially reduced for elevated $V_G$ and $V_{DS}$. A still stronger reduction would be possible if, for example, the transport regime was either ballistic or of the electron billiard type (with a short dwell time) [16, 36]. As expected, magnetic conditions of the contacts, which strongly influence the current, also have a considerable effect on the noise. It is readily seen from figure 3 that the Fano factor corresponding to the P alignment, when compared to that of the AP alignment, is predominantly suppressed. The suppression takes place in a large region of the gate voltage, where current in the P configuration is greater than in the AP configuration (cf figure 2), in agreement with the fact that $F \sim 1/I$. It should be stressed that the transport regime considered here is phase coherent, although with noticeably reduced transmission due to the presence of Schottky barriers. That is why the length effects, as shown in the inset to figure 3, are quite moderate, in contrast to what could be expected in the diffusive transport regime. Spin-dependent electron wave interferences are responsible for non-monotonic behavior of presented plots and accompanying sharp features. Similar features have been reported both in conductance and TMR [9, 13, 37] as well as in the differential Fano factor [19]. The TMR is defined here in a ‘pessimistic’ way as $TMR = (I_P - I_{AP})/I_P$, where $I_P$ ($I_{AP}$) is the current flowing through the system in the P (AP) magnetic configuration. The calculations are performed for spin polarizations in the ferromagnetic contacts equal to $(n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow) = 0.5$ ($n_\sigma$ is the number of $\sigma$-spin electrons per atom). The results for TMR against $V_G$ and $V_{DS}$ are presented in figures 3 and 4, respectively. The corresponding insets clearly show that the TMR absolute value may be quite

Figure 3. As in figure 2 but for the Fano factor. Note that reversal of the magnetic configuration from AP to P, for $V_G < 0$, may result in a considerable suppression of $F$. Inset: TMR for two different CNT lengths and $V_{DS} = 0.2$ V.
findings are relevant to prospective applications of nanotubes in spintronics.

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4. Conclusions

An approach has been developed to describe nanotube transistors, which combines a simplified (analytical) treatment of the electrostatics and a state-of-the-art non-equilibrium GF technique. Unprecedented studies of electric transport through a Schottky-barrier CNT transistor with ferromagnetic electrodes have been carried out. It has been shown that the tunneling ability of particles depends strongly on the alignment of contact magnetizations. Remarkably, the tunnel magnetoresistance can exceed 50%, whereas the Fano factor is usually subjected to some extra suppression when the magnetization alignment gets reoriented from antiparallel to parallel, thereby improving the noise-to-signal ratio. These two

Figure 4. Drain/source voltage dependence of \( I, \) TMR and \( F \) (main, left and right panels) for \( V_D = 0.3 \, V, \) \( T = 300 \, K \) and \( L = 15. \) In the interval \( \pm 2k_B T \) around \( V_D = 0 \) thermal noise dominates and \( I \rightarrow 0, \) so \( F \) is ill-defined.

substantial and exceed several tens per cent both in the sub-threshold region and at elevated voltages. Interestingly enough, TMR can assume large negative values (inverse TMR) and is strongly sensitive to both the gate- and \( V_D \) voltages. Another important observation is a striking asymmetry of the Fano factor and the GMR effect with respect to the sign of the voltage (p-channel versus n-channel). These features are due to the aforementioned location of \( E_F \) with respect to the mid-gap, which makes the Schottky barrier for electrons higher than that for holes, and consequently the hole current (for negative voltages) is higher than the electron current (for positive voltages). It is noteworthy, that the oscillations present in figures 2-4 are due to the size-dependent quantization of the CNT energy levels, so the local maxima (minima) therein depend on to what extent the voltage-driven active channels and the transport energy window fit together. This mechanism is also responsible for the occurrence of the inverse GMR; in fact it is similar to the mechanism based on resonant tunneling suggested in [12].