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FERROMAGNETICALLY CONTACTED METALLIC CARBON NANOTUBES WITH SPIN-SELECTIVE INTERFACES

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Abstract. Spin-dependent transport through single-wall armchair carbon nanotubes (SWCNT) is studied theoretically within the single-band tight-binding model, by means of the Green's function partitioning technique. The emphasis is put on the effect of an extra magnetic monolayer at the electrodes on electrical conductance and giant magnetoresistance (GMR). In order to meet the charge neutrality requirement – the so-called extended molecule concept has been used. It has been shown that in the case when the monolayers have got enhanced magnetic moments and are antiferromagnetically exchange-coupled to the electrodes, the GMR value can approach 100%, i.e. both the spin-dependent conductance channels may become blocked in the anti-aligned electrodes configuration. A remarkable feature of the conductance spectra is that they reveal to a large degree the "finger prints" of the SWCNTs. In particular, the conductance spectra peaks" are separated from one another roughly as in isolated nanotubes.

1. INTRODUCTION

A particularly challenging class of materials for the future electronics are carbon nanotubes, i.e. graphite sheets rolled up in such a manner that they form very long and thin (in atomic scale) cylinders. Their length can be of the order of several micrometers whereas a typical cross-section of single wall carbon nanotubes (SWCNT) is a few tens Å in diameter. The SWCNT have been attracting attention of many researchers since they were discovered [1] in view of their exceptional mechanical and electrical properties. In the present paper we study the latter, motivated by a series of significant experiments devoted to the giant magnetoresistance of ferromagnetically contacted nanotubes [2-5]. It turns out that carbon nanotubes, although magnetically inert, can lead to a quite considerable GMR effect (see also theoretical papers [6-8]). The experimental results seem however to be rather discordant with one another. Reported GMR results very often differ not only in magnitude but in sign as well. Moreover there are reports on SWCNT-mediated GMR approaching 100% [4]. There is no doubt that discrepancies of that type are mainly due to carbon nanotube/electrode interface conditions. This is a well-known problem always encountered when a molecule is to be connected to macroscopic electrodes. For a recent review of the state-of-the-art in molecular electronics refer to Ref. [9].

2. FORMALISM

We use a standard single-band tight-binding Hamiltonian to describe π- and s-electrons in the SWCNTs and ferromagnetic metal atoms, respectively. Following [10, 11] we make use of the so-called extended molecule concept, by incorporating to the central part of the system not only the entire molecule (SWCNT) but also two closest magnetic atomic planes from the left- and righthand side. Within the partitioning method, the following relations for the Green's function are used:

$$\begin{pmatrix} E-H_L & V_{LC} & 0 \\ V_{LC}^{\dagger} & E-H_C & V_{CR} \\ 0 & V_{CR}^{\dagger} & E-H_R \end{pmatrix} \hat{G} = \hat{1}\,, \tag{1}$$

$$G_C = (\hat{1}\,E - H_C - \Sigma_L - \Sigma_R)^{-1}\,, \tag{2}$$

whereas the number of electrons, the conductance (per spin) and GMR are given by:

$$n = \frac{1}{2\pi}\int dE\,[G_C f_L \Gamma_L + f_R \Gamma_R G_C^{\dagger}]\,, \tag{3}$$

$$\mathcal{G} = \frac{e^2}{h}\,Tr\,[\Gamma_L G_C \Gamma_R G_C^{\dagger}]\,, \tag{4}$$

$$GMR = 100(\mathcal{G}_{\uparrow,\uparrow} - \mathcal{G}_{\uparrow,\downarrow})/\mathcal{G}_{\uparrow,\uparrow}\,, \tag{5}$$

where L, R, C refer to the left, right electrodes and the extended molecule, respectively, and the submatices $V_{L(R),C}$ describe the coupling between $H_{L(R)}$ (electrode Hamiltonian) and H_C (extended molecule Hamiltonian). Moreover $\alpha = L, R$, $\Gamma_\alpha = i(\Sigma_\alpha - \Sigma_\alpha^{\dagger})$, $\Sigma\alpha = V_{C,\alpha}\, g_\alpha\, V_{C,\alpha}^{\dagger}$ and f_α is the Fermi-Dirac distribution function. The g_α is the α-th electrode surface Green's function. The latter has been calculated as in [12], but summed over the 2-dimensional Brillouin zone (while Fourier transforming back to the real space) by the special-k-points method [13]. The arrows in the definition of GMR indicate the relative magnetization alignments of the left and right external electrodes.

3. RESULTS

The surface density of states (DOS) for the *fcc* (111) structure considered here is depicted in Fig. 1. The central dotted vertical line indicates the Fermi energy corresponding to the paramag-

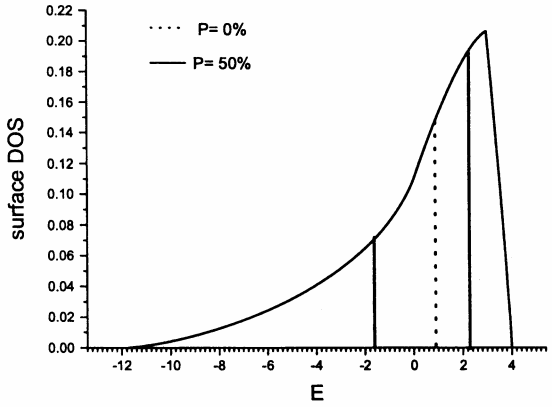

Fig. 1. Surface density of states of the *fcc*(111) electrodes. For just one electron per atom, the dotted line and the solid lines indicate the paramagnetic (E_F) and ferromagnetic ($E_{F\uparrow}$, $E_{F\downarrow}$) Fermi energies, respectively

netic case with the number of electrons per site equal to $n = 1$, whereas the solid lines correspond to the ferromagnetic case with the spin polarization $P = 50\%$ ($n_\uparrow = 0.75$, $n_\downarrow = 0.25$). In order to equalize these Fermi energies with the nominal one of the SWCNT ($E_F = 0$), atomic potentials in the electrodes have been accordingly displaced. The structural model under consideration consists of the armchair (6.6) SWCNT sandwiched between the infinite electrodes with the spin magnetization $P = 50\%$. It is assumed that on top of each interface there is another magnetic monolayer which can be either ferromagnetically or antiferromagnetically exchange-coupled to the electrode. In what follows we let the monolayer have an enhanced magnetization (nominally 75%) and reduced interface hopping integral. This is how we mimic the presence of a transition metal-oxide layer on real transition metal electrodes. As mentioned above, the charge neutrality requirement is met by adding to the central part the two closest magnetic layers at each end of

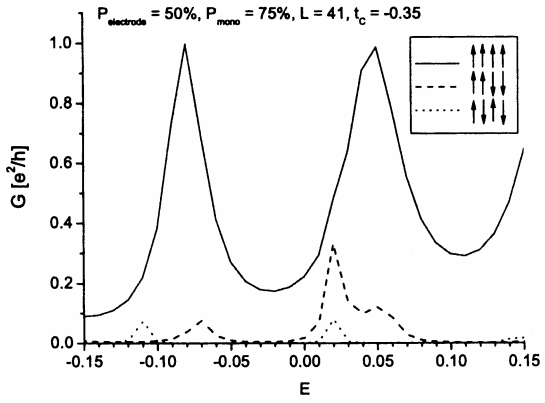

Fig. 2. Conductance of the device composed of: (i) the left electrode capped with (ii) the extra "oxide" monolayer, with (iii) the SWCNT in the middle, (iv) another interface monolayer, and (v) the right electrode. The arrows indicate the magnetization direction in the regions (i), (ii), (iv) and (v), respectively. The parameters are: $P_{\text{electrode}} = 50\%$, $P_{\text{mono}} = 75\%$, and the hopping integral between the regions (i)-(ii) and (iv)-(v) is $t = t_c = -0.35$ (otherwise $t = -1$)

the system, i.e. apart from the extra "oxide" monolayer also the last (first) finite atomic layer of the left (right) electrode. The so-defined extended molecule has been made neutral by shifting all its on-site potentials by the same value. Figure 2 shows the conductance spectrum for 3 different spin configurations. The solid curve corresponds to the saturated case (at high magnetic fields),

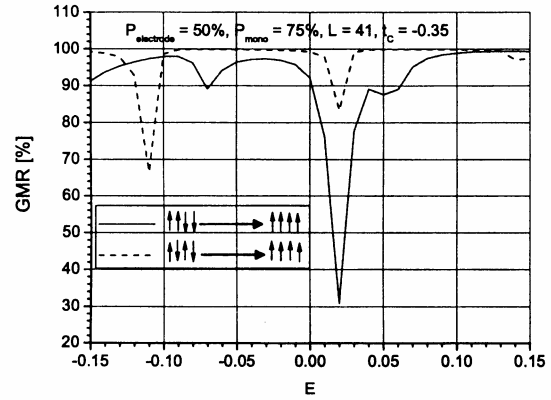

Fig. 3. Giant magnetoresistance corresponding to the conductances of Fig. 2. If the extra monolayers are antiferromagnetically exchange coupled to the electrodes the GMR effect approaches 100%

the dashed and doted curves correspond to the hypothetical spin configurations at zero magnetic field. It is readily seen that the most resistive configuration is when the magnetizations of electrodes and adjacent "oxide" monolayers are antiparallel. The corresponding GMR curves presented in Fig. 3 show that in the latter case the effect reaches almost 100%. It results also from this figure that the GMR curve in the vicinity of the Fermi energy is quite steep, so the GMR effect can be effectively controlled with the gate voltage.

4. CONCLUSIONS

It has been shown that additional magnetic monolayers adjacent to the magnetic electrodes critically influence the giant magnetoresistance. In the case when the monolayers have enhanced magnetic moments which are anti-parallel oriented with respect to the electrode magnetization the GMR value can approach 100%. We ascribe this behavior to the formation of spin-selective interfaces. It is noteworthy that there are "finger prints" in the conductance spectra of the device under study. They are visible in inter peak separations which are pretty close to those of perfect infinite SWCNTs. This observation gives the possibility to control the GMR by means of the gate voltage applied to the nanotube.

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