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First-principles study of transport of V doped boron nitride nanotube

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ABSTRACT

We perform first-principles calculations of spin-dependent quantum transport in V doped boron nitride nanotube: the junction of pristine (6, 0) boron nitride nanotube in contact with V doped (6, 0) boron nitride nanotube electrodes. Large tunnel magnetoresistance and perfect spin filtration effect are obtained. The zero bias tunnel magnetoresistance is found to be several thousand percent, it reduces monotonically to zero with a voltage scale of about 0.65 V, and eventually goes to negative values after the bias of 0.65 V. The ratio of spin injection is above 95% till the bias of 0.85 V and is even as large as 99% for the bias from 0.25 eV to 0.55 eV when the magnetic configurations of two electrodes are parallel. The understanding of the spin-dependent nonequilibrium transport is presented by investigating microscopic details of the transmission coefficients.

1. Introduction

Because of important applications in magnetoresistive random-access memory [1], programmable logic elements [2] and magnetic sensors, the giant magnetoresistance (GMR) and tunnel magnetoresistance (TMR) effects in systems with spin-polarized transport are at the heart of spintronics [3] and attract many theoretical and experimental investigations. A basic magnetic tunnel junction (MTJ) device consists of tunnel barrier separating two ferromagnetic (FM) layers which play the role of device leads. During a tunneling process, the spin-up and spin-down electrons from the metal layers traverse the nonmagnetic tunnel barrier with different Fermi wave function due to electronic structure of the ferromagnetic material. The electrical resistance of MTJ is therefore sensitive to the relative orientation of the magnetic configuration of the electrodes, resulting to a TMR [4]. When the magnetic configuration of the electrodes is antiparallel, the tunnel conductance tends to be smallest. Hence, the MTJs behave as spin valves [4–8]. It is possible to control the orientation of magnetic moments by imposing an external magnetic field in experiments [9,10]. It is worthy mentioned that, MgO-based MTJ has progressed at a rapid pace in recent years and produced the highest measured TMR at room temperature.

When the electrodes and the tunnel barrier are all one-dimensional (1D) materials such as nanowires or nanotubes, it is experimentally feasible to achieve MTJ at the 1D scale. It is worthy mentioned that Wang et al. [12] construct a 1D TMJ using Fe-doped carbon nanotubes and theoretically investigate its spin-dependent transport properties. What is a pity that, the zero bias magnetoresistance ratio is only $\sim 40\%$, which may restrict the spintronics applications in nanodevices where the large magnetoresistance ratio is desired. Here, we theoretically investigate the spin-polarized transport of a 1D MTJ constructed by V atoms doped single-walled (6, 0) boron nitride nanotube (BNNT). BNNTs, another prevailing tubular nanomaterials which was successfully synthesized shortly after the discovery of carbon nanotubes, are known to be wide-gap semiconductors whose band gaps (~ 5.5 eV) are almost independent of the tube diameter, helicity, and the number of walls. The pristine BNNTs with large energy gap can be used as ideal tunnel barrier for 1D or molecular-scaled MTJ. The BNNTs with transition metal (TM) adsorption or encapsulating attract much experimental and theoretical study interesting [13–19]. As representation, the V doped zigzag (6, 0) BNNT is chose in this work. The tunnel barrier is pristine single-wall (6, 0) BNNT while the two electrodes are semi-infinite single-wall (6, 0) BNNT with V atoms adsorption. Large TMR and perfect spin filtration

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effect are obtained according to the first-principles calculations of spin-polarized quantum transport by adopting nonequilibrium Green's function method combined with density-functional theory. TMR has already led to the construction of the present generation of magnetic data storage devices. However, in order to reach storage densities of the order of Terabit/inch^2, a substantial downscaling of the read/write devices is extensively expected. Such 1D MTJ and spin filter with diameter less than 1 nm may realize the storage densities of the order of Terabit/inch^2 and hold promise for extensive spintronics applications of nanodevices.

2. Computational details and simulation model

Our investigation is based on a recently developed self-consistent first-principles technique which combines the Keldysh nonequilibrium Green's-function formalism (NEGF) with a self-consistent density-functional theory (DFT). The package we use is the Atomistix Toolkit [20], which incorporates the NEGF technique into the well tested SIESTA method [21] to realize the simulation of electrical or spin-polarized quantum transport in the molecular conductors under nonequilibrium situations. In the calculation, the local density approximation (LDA) in the form of the Perdew and Zunger [22] exchange-correlation functional is used. Only valence electrons are self-consistently calculated, and the atomic cores are described by standard norm conserving pseudopotential [23]. The valence wave functions are expanded by the localized numerical (pseudo) atom orbitals [24]. The k-points sampling is 1, 1, and 200 in the x, y, and z direction, which has been proven to be enough to give the converged results. The convergence criterion for the Hamiltonian, charge density, and band-structure energy is 10^{-5} via the mixture of the Hamiltonian. The positions of V atoms in the surface of BN nanotube are relaxed until the force tolerance 0.05 eV/Å is achieved. The spin-current (spin-polarized charge current) is calculated [25] as

$$I_{\uparrow(\downarrow)} = \frac{e}{h} \int_{-\infty}^{+\infty} T_{\uparrow(\downarrow)}(E, V_b)\left[f_l(E-\mu_L) - f_r(E-\mu_R)\right] dE, \tag{1}$$

where f is the Fermi–Dirac distribution, $\mu_{L,R}$ are the chemical potentials of left-electrode (L) and right-electrode (R). $T_{\uparrow(\downarrow)}(E, V_b)$ is the transmission coefficient for spin channel ($\uparrow, \downarrow$) at the energy E and bias voltage V_b.

The unit cell of V atoms doped $(6,0)$ single-wall BNNT is constructed as follow: A tetragonal unit cell is used; whose size is $20 \times 20 \times 4.26$ Å^3. The doped unit cell contains 12 B and 12 N atoms as well as three V atoms which are individually placed on the outer surface of BNNT. Fig. 1(a) shows the V atoms doped $(6,0)$ single-wall BNNT after geometrical optimization. The 1D MTJ is schematically shown in Fig. 1(b), where a pristine $(6,0)$ single-wall BNNT is connected with two electrodes of V doped $(6,0)$ BNNT. The whole system is divided into three parts from left to right in practical theoretical simulations: the left electrode, the central scattering region, and the right electrode. The left electrode is same to right electrode which is constructed by four doped unit cells. The scattering region is constructed by two pristine unit cells and two doped unit cells. The electrode and scattering region contain 108 atoms (48 B, 48 N and 12 V atoms) and 102 atoms (48 B, 48 N and 6 V atoms), respectively. 20 Å is chosen in the x and y direction so that the device has no interaction with its mirror images due to the large vacuum.

3. Results and discussions

Fig. 2(a) and (b) plot the current–voltage (I–V) characteristics for the parallel magnetization configuration (PC) and the antiparallel magnetization configuration (APC) of the two electrodes, respectively. In the case of PC, the spin-down current ($I_\downarrow$) are always much larger than the spin-up current ($I_\uparrow$). The $I_\downarrow$ increases linearly while the $I_\uparrow$ is almost absolutely inhibited below the bias of 0.65 V. The total equilibrium conductance of $0.37G_0$ is found at zero bias, where G_0 is the conductance quanta, $G_0 = 2e^2/h$. After 0.75 V, the $I_\downarrow$ stop increasing and the $I_\uparrow$ "turns on". In the case of APC, the $I_\downarrow$ is not equal to $I_\uparrow$ due to asymmetry of geometry. Because the spin direction of scattering region is same to left electrode, the $I_\downarrow$ is always larger than $I_\uparrow$. The total equilibrium conductance of $0.051G_0$ is found at zero bias. The $I_\downarrow$ and $I_\uparrow$ all linearly increase.

From the I–V curves, we infer a TMR ratio using the common definition: $R_{\text{TMR}} = (I_{\text{PC}} - I_{\text{APC}})/I_{\text{APC}}$, where $I_{\text{PC,APC}}$ are the total currents in PC and APC, respectively. At $V_b = 0$ when all currents vanish, we calculate R_{TMR} using equilibrium conductance. Fig. 2(c) shows the R_{TMR}, where the $R_{\text{TMR}} \sim 631\%$ at zero bias is obtained, which indicate in the perfect tunneling magnetoresistance effect. It's dramatic that the R_{TMR} increases from 631% to 789% at the bias of 0.05 V. After that, the R_{TMR} decay to zero and change sign at the bias of 0.65 V, then eventually to negative values when bias is increased. The origin of the quenching and negative values of TMR is due to a very fast rise in the I_{APC} relative to the I_{PC} as a function of bias. The negative R_{TMR} (i.e., the APC current exceed PC current after the bias of 0.65 V) is a dramatic phenomena, which is found in Ref. [12] but is not found in Ref. [11]. The resonant transmission mediated by V(3d)–B(3p), V(3d)–N(3p) hybridized states resulted from V, B, N atoms interaction maybe responsible for the negative R_{TMR} after the bias of 0.65 V. We expect such behavior of R_{TMR} to tune the sign as well as the magnitude of spin currents in situ by adjusting bias voltage is a generic feature of nanodevices or molecule spintronics. The 1D TMJ studied here has large TMR as MgO-based MTJ and presents an excellent opportunity for spintronics of nanodevices.

The spin-injection factor η which is defined by spin currents: $\eta = (I_\downarrow - I_\uparrow)/(I_\downarrow + I_\uparrow)$ are plotted in Fig. 2(d). In the bias of 0.0 V, the current is 0 A. We use the equilibrium conductance represent the current. For the case of PC, η is not below 95% until the bias of 0.85 V. This value is as large as 99% at the bias between 0.15 V and 0.55 V, which indicate in the perfect spin filtration effect. After the bias of 0.85 V, the $I_\uparrow$ increase significantly while the $I_\downarrow$ stop increase, the η decreases significantly. For the case of APC, the η is as high as 92% at the zero bias. It rapidly decreases to 59% when the bias increases to 0.05 V. After that, the η oscillate with the bias and the maximum is 63% at the bias of 0.15 V. The source of this behavior maybe originates from the quantum size effect which results in the quantized subbands in the cross section of 1D electrode. Detailed analysis is in the below. Spin injection into semiconductors has been measured experimentally using the optical techniques [26,27]. Such 1D TMJ controlled spin injection into semiconductors should occur in devices that are smaller than a spin relaxation length in extent and have resistance that is limited by the insulating BNNT.

The voltage dependent of spin current, TMR ratio and spin-injection factor can be understood from the behavior of the transmission coefficients $[T(E, V_b)]$, since the current is essentially given by the energy integral of the $T(E, V_b)$ over the bias window [see Eq. (1)]. The $T(E, V_b)$ for several bias are shown in Fig. 3, where the (a) and (b) are spin-up and spin-down channel of PC setup respectively and the (c) and (d) are spin-up and spin-down channel of APC setup respectively. For both PC and APC setup, these bias-depended $T(E, V_b)$ have several sharp peaks especially after the bias of 0.35 V, due to quantized subbands in the cross section of the 1D electrodes, already mentioned above. The spin-up channel contribute to the $T(E, V_b)$ above the Fermi level and spin-down channel contribute both above and below the Fermi