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Giant magnetoresistance in bilayer graphene nanoflakes

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ABSTRACT

Coherent spin transport through bilayer graphene (BLG) nanoflakes sandwiched between two electrodes made of single-layer zigzag graphene nanoribbon was investigated by means of Landauer-Buttiker formalism. Application of a magnetic field only on BLG structure as a channel produces a perfect spin polarization in a large energy region. Moreover, the conductance could be strongly modulated by magnetization of the zigzag edge of AB-stacked BLG, and the junction, entirely made of carbon, produces a giant magnetoresistance (GMR) up to 100%. Intestinally, GMR and spin polarization could be tuned by varying BLG width and length. Generally, MR in a AB-stacked BLG strongly increases (decreases) with length (width).

1. Introduction

Graphene systems, which are composed of one or a few carbon monoatomic layers, have attracted much attention due to their unusual electronic properties even at room temperature, such as a high carrier mobility, thermal and structural stabilities, low spin orbit, hyperfine interactions, long spin relaxation length, and gate-tunable spin transport, and their potential for applications in nanoelectronic and spintronic devices [1–5]. Currently, there is a continuous interest in BLG properties, both theoretically and experimentally. A bilayer graphene consists of two single graphene layers and has two different stacking arrangements: AB (Bernal) and AA. Energy band gap in BLG nanoribbon and nanoflake could be controlled by substrate properties and the applied vertical electric field, so these structures could be used as a channel material in carbon-based transistors [6–12].

Moreover, several studies have been performed, both theoretically and experimentally, on transport properties in BLG structure [6–9,12–17]. Interestingly, BLG field-effect-transistors with high on/off current ratios at room temperature have been reported [9]. In BLG nanoribbons with zigzag edges, electronic transport is dominated by edge-states similar to those of single-layer graphene [18–23].

These states are expected to be spin-polarized and make zigzag-edge BLG nanoribbons' junctions attractive for spin-polarized transport [20–23]. On the other hand, long spin relaxation length in bilayer graphene nanoribbons and few-layer graphene flakes was observed at room temperature [24]. Moreover, spin-filtering and spin-dependent transport properties of BLG with ferromagnetic electrode and gate, external magnetic field, and exchange field have been investigated theoretically and experimentally [2,3,9,10,25–27]. Another important feature of graphene in spintronic devices is its magnetoresistance. Giant magnetoresistance (GMR) in graphene junction with ferromagnetic electrodes [28–31] and magnetic states of zigzag edges have been extensively investigated [32–35]. But there has been a little attention to the magnetoresistance effects in BLG junction [3].

In this paper, we studied the coherent magnetic transport properties of a BLG nanoflake connected to two single-layer zigzag graphene nanoribbon (ZGNR) electrodes. The results showed that the application of a magnetic field only on BLG as a channel changes the spin configuration and conductivity of the BLG zigzag edge and induces a perfect spin-polarized conductance in the AB-stacked BLG structures. Moreover, we studied the magnetic transport properties by changing BLG width and length connected between ZGNR electrodes. Finally, we found a GMR up to 100% and suggested that the GMR could be tuned by varying BLG width and length.

2. Model and method

We simulated the system depicted in Fig. 1a using a π-orbital tight-binding model and Hubbard repulsion treated in the mean-field approximation. This formalism that includes $e-e$ interaction

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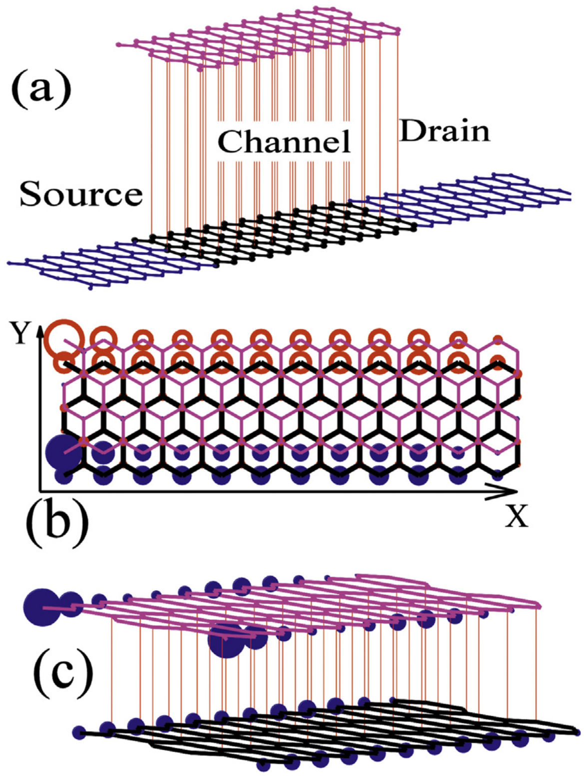

Fig. 1. (Color online) (a) Schematic view of BLG nonoflake with the width N_y=4 and length N_x=12 attached between semi-infinite ZGNR electrodes, (b) (top view) and (c) AB-stacked BLG as a channel with AFM and FM spin configurations on zigzag edges, respectively. Open (red in online version) and filled (blue in online version) circles represent spin-down and spin-up densities, respectively. The magnetic moments are within $[-0.25{:}0.25]\ \mu_B$ and $[-0.05{:}0.25]\ \mu_B$ in cases b and c , respectively.

in BLG induces localized magnetic moments in zigzag-edge atoms. We wrote the mean-field Hamiltonian in the AB-stacked BLG as follows [5]:

$$H_C = t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_{i,\sigma}\hat{n}_{i,\sigma}\langle\hat{n}_{i,-\sigma}\rangle \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) stands for the creation (annihilation) operator of an electron with spin σ located on site. The tight-binding parameters t were fixed to their bulk values equal to $t = -2.66$ eV for the in-plane nearest neighbors of i and j and $t = -0.35$ eV for the interlayer hopping parameter [36], and U=2.82 eV is the on-site coulomb interaction. The Green's function of the junction is expressed as

$$\hat{G}_{C,\sigma}(\varepsilon) = [\varepsilon\hat{I} - \hat{H}_{C,\sigma} - \hat{\Sigma}_S(\varepsilon) - \hat{\Sigma}_D(\varepsilon)]^{-1}. \tag{2}$$

where $\hat{\Sigma}_S(\varepsilon)$, $\hat{\Sigma}_D(\varepsilon)$ are the self-energy matrices due to the connection of right and left ZGNR electrodes to the channel, respectively. The spin-dependent density of states (DOS) of the BLG in the presence of electrodes is given by

$$D_\sigma(\varepsilon) = (-1/\pi)Im\ \langle\sigma|G_{C,\sigma}(\varepsilon)|\sigma\rangle. \tag{3}$$

Accordingly, the magnetic moment at each atomic site can be expressed as $m_i = \mu_B(\langle\hat{n}_{i,\sigma}\rangle - \langle\hat{n}_{i,-\sigma}\rangle)$ According to the Landauer-Buttiker formalism [37,31] the spin-dependent conductance and currents can be written as

$$G^{\sigma}(\varepsilon) = (e^2/h)Tr[\hat{\Gamma}_S\hat{G}_{C,\sigma}\hat{\Gamma}_D\hat{G}^{\dagger}_{C,\sigma}]. \tag{4}$$

Using $\hat{\Sigma}_{(\varepsilon)}$, the coupling matrices $\hat{\Gamma}_\alpha$ can be expressed as $\hat{\Gamma}_\alpha = -2\,Im[\hat{\Sigma}_{(\varepsilon,\alpha)}]$. Also, the spin-dependent currents can be written as

$$I_\sigma = (1/e)\int_{-\infty}^{\infty} G_\sigma(\varepsilon)(f_S(\varepsilon-\mu_L) - f_D(\varepsilon-\mu_R))d\varepsilon. \tag{5}$$

where f is the Fermi–Dirac distribution function and consider the effect of temperature. We calculate the magnetoresistance of each device as

$$MR = (I_{FM} - I_{AFM})/(I_{AFM} + I_{AFM}) \times 100. \tag{6}$$

We solved equations (1)–(3) self-consistently by an iteration method. Moreover, the effect of single-layer graphene nanoribbon as an electrode on BLG was added via self-energies, and the Green function of BLG was subsequently calculated. Finally, the new expectation values of number operators were replaced in the Hamiltonian, and this process was repeated until convergence was achieved [38]. Note that in the bilayer graphene nanoflake, the upper single-layer graphene was only connected to the lower one through single-band tight binding model in the first nearest neighbors' approximation. The effect of electrodes on the upper monoatomic sheet was indirectly added through the hopping parameter between two monoatomic sheets in BLG nanoflake. Therefore, due to the effect of self-energy on the bottom layer the spin density in bottom and top layers is different. Also, the BLG has asymmetry in x-axis direction and hence the spin density shows asymmetry in this direction (see Fig. 1(b) and (c)). Modulation of hopping parameter between electrodes and BLG could broaden electron energy level and consequently lead to the decrease of edge magnetism in BLG nanoflakes [39].

3. Results and discussion

We considered AB-stacked BLG as a channel connected between two semi-infinite single-layer ZGNR electrodes. A similar junction (monolayer-bilayer junction) was proposed in previous works and its electronic and transport properties were investigated even under applied biases [40,36,41–44]. The number of armchair rows along x direction, N_x, defines a BLG length and the number of zigzag rows along y direction, N_y, defines a BLG width. Thus, BLG length and width are $L = N_x a$ and $W = (\sqrt{3}/2)N_y a$, respectively, with a=2.42 Å(Fig. 1b).

Anti-ferromagnetic (AFM) spin configuration of AB-stacked BLG (each layer has anti-ferromagnetic spin configuration and ferromagnetically coupled to other one, see Fig. 1b) is more stable than other spin configurations. However, in the presence of an external magnetic field, the edge spin orientations become parallel and BLG structure would have ferromagnetic (FM) spin configuration along all zigzag edges, similar to monolayer graphene nanoribbons and flakes [19,22,23] (see Fig. 1c). In our iterative solution, the effect of magnetic field was only considered as initial conditions for Eq. (1). By choosing anti-ferromagnetic (AFM) and ferromagnetic (FM) spin configurations as initial conditions in BLG nanofake, different spin configurations of AFM and FM were achieved, respectively. Also, rectangular BLGs with AFM spin configuration along zigzag edge have a zero net magnetic moment according to the Lieb's theorem [45]. Due to external magnetic field applied perpendicular to BLG, it has a FM spin configuration and a net magnetic moment in the channel. Consequently, the degeneracy between up- and down-spin electrons breaks. According to the prediction of density functional theory, the spin-correlation length limits long-range magnetic order to 1 nm at room temperature [46], therefore in our calculation the semi-infinite ZGNRs do not include edge magnetism and all spin-dependent scatterings are induced by the localized magnetic moments in BLG. In other words, the effect of edge magnetic moments on the zigzag-shaped edges in