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The effect of impurity on a spin-filter device based on graphene

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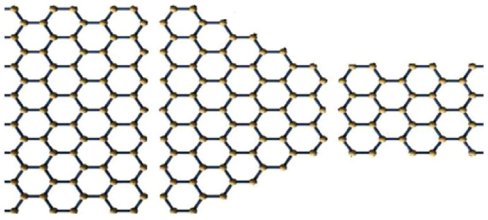
HIGHLIGHTS

- We report the spin-polarized transport in a system based fully on graphene.
- Our system consists of a zigzag edge nanoflake connected to two nanoribbons as electrodes.
- We consider the effect of impurity in this system in three different configurations.
- We demonstrate that the pure system shows high spin filtering properties.
- Our results show the presence of impurity atoms reduces the spin filtering properties.

GRAPHICAL ABSTRACT

We study the spin-filtering properties of an electronic device which is fully based on graphene, (AGNR/ZGF/AGNR). We investigate how the presence of the boron atoms can affect the conduction properties of this system.



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ABSTRACT

We report the coherent spin-polarized transport through a pure and doped zigzag-edge graphene flake (ZGF) connected from left and right to two armchair graphene nanoribbons, using the Hubbard model in the nearest neighbor approximation within the framework of the Green function's technique and Landauer formalism. We consider the effect of boron impurity atoms in three different spatial configurations in the central part of the system (ZGF). We found that the pure system shows considerable spin filtering properties, which is due to the interaction of the spin of the carriers with the local zigzag-edge magnetism. However, our results show that the presence of the impurity atoms reduces the spin filtering property which could be due to the decrease in the effective spin interaction.

1. Introduction

The last two decades were marked with the discoveries of new allotropic modifications of carbon and related nanostructures. Graphene, currently under intense experimental and theoretical investigations, is the starting point for many carbon nanomaterials [1] and consists of a single layer of carbon atoms arranged in a honeycomb lattice made of two interpenetrating, σ-bonded triangular sublattices, A and B [2]. It was only isolated 440 years after its invention [3] by Andre Geim and Kostya Novoselov. They started with three-dimensional graphite and extracted a single sheet (a monolayer of atoms) using a technique called micromechanical cleavage [4]. The properties of the graphene-based materials are renowned and clearly indicate that planar graphene must be a very remarkable material for nanotechnological applications. It is expected to be stable at temperatures up to 3000 °C and should be extremely flexible, but at the same time as hard to tear apart as diamond, similar in fact to carbon nanotubes.

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The electronic properties of planar graphene are extraordinary too [3–6] with room-temperature mobilities reaching 15,000 [7]. In addition, remarkably, the spin relaxation length is measured to be as long as ~1.5 μm in low-mobility devices, which makes graphene very interesting candidate for spintronic applications [2].

Considering the novel electronic properties of graphene, there has been enormous number of research on the development of the nanoscale technology of graphene, and its different variations such as nanoribbon and nanoflakes, and a number of nanodevices have also been proposed to explore the spin-dependent transport phenomena, especially in graphene nanoribbons [8]. Graphene nanoribbons (GNR) are infinite in length and finite in width about < 1 μm–1 nm. They have attracted extensive interest recently because they are recognized as a new class of materials and building blocks for nanoelectronics and spintronics [9]. The electronic structure of ideal GNR is theoretically well established and it is very sensitive to the ribbon geometry, i.e., orientation relative to the crystal axes and their exact width and also geometry of edges [10]. There are two types of graphene edge nanoribons: armchair and zigzag edges. These two edges have a 30° difference in their orientation within the graphene sheet [11].

Several intriguing transport properties have been theoretically predicted especially for zigzag graphene nanoribbons (ZGNRs) [12]. It has been shown that ribbons with zigzag edges (zigzag ribbons) possess localized edge states with energies close to the Fermi level [11].The unique properties in the electronic transport properties of ZGNRs can be attributed to the characteristic band structures of ZGNR and the symmetry of wave functions near the Fermi level [13]. For instance, it is shown that ZGNRs can be utilized for generation of a spin polarized current [12]. It has also found a possibility of spontaneous magnetic ordering peculiar to nanometer-scale zigzag edge graphene [14]. The ground state of ZGNRs has an antiferromagnetic spin configuration where the total spin (S) is zero. However, when the system has different number of A- and B-sublattice sites, the total spin of the ground state is $2S=N_A-N_B$ and by appropriate designing, one can form a ferromagnetic spin configuration at the zigzag edges [12]. This would enable the ribbon to have different conductance channels for spin up and spin down electrons, and thus show spin filtering property. The presence of impurities, however, would result in the scattering of the electrons and therefore could affect the spin filtering property of the system. In the case of boron impurity atoms, due to the anisotropic spin interaction, we shall have different transmittance channels for up and down spins [15]. It is therefore, interesting to study how the presence of such impurity atoms affects the spin filtering in the electronic devices based on zigzag-edge graphene.

With this motivation, in the present work, we consider the effect of boron atoms in a system which consists of a zigzag-edge graphene nanoflake connected to two armchair-edge graphene nanoribbons (AGNRs) as the left and right electrodes (AGNR/ZGF/AGNR). To investigate the effect of the interaction of the spin of boron atom with those of the edges of flake (ZGF) we consider the impurity atoms in the nanoflake in three different configurations. We employ the Hubbard model, the Green function's technique and the Landauer formalism to study the spin filter effect on this system for these configurations. We demonstrate that the spin-filtering property is very sensitive to the presence and location of boron atoms and generally would result in decreasing spin filtering.

2. Model and formalism

The system under study consists of a zigzag-edge graphene nanoflake which is connected to two armchair-edge graphene nanoribbons as the left and right electrodes. In this junction, the left electrode has a ribbon index $n=15$, while the right GNR electrode has a ribbon index $n=7$. Furthermore, the central region (nanoflake) with a trapezoidal shape consists of $N_C=70$ carbon atoms and produces a ferromagnetic spin configuration at its edges.

We examine the effect of the electron–electron interaction using the Hubbard model within the mean field approximation. The Hamiltonian is, therefore, written as

$$\widehat{H_C} = \sum_{i,j,\sigma} -t_{ij} C_{i\sigma}^{\dagger} C_{j\sigma} + \overline{U} \sum_{i,\sigma} \widehat{n_{i,-\sigma}} \left[n_{i,\sigma} - \frac{1}{2} n_{i,\sigma} \right] \quad (1)$$

Where $C^{\dagger}_{i\sigma}$ and $C_{j\sigma}$ are the electron creation and annihilation operators, respectively, and $n_{i\sigma}=C^{\dagger}_{i\sigma}C_{i\sigma}$ is the number operator for an electron with spin σ at site i. $t=2.66$ eV is the transfer integral between all the nearest neighbor sites and $U=1/06t$ is the on-site Coulomb interaction [12]. The Fermi energy was also set to zero, i.e. $E_f=0$.

We solve the mean-field Hamiltonian selfconsistently by the iteration method. Therefore, the Green's function and the spin density on each atom of the channel should be calculated iteratively until a convergence of the spin density is reached. The Green's function of the nanoflake is expressed as

$$\widehat{G_C}(\omega) = [(\omega + i\eta)\widehat{I} - \widehat{H_C} - \Sigma_L - \widehat{\Sigma_R}]^{-1} \quad (2)$$

Where η is a positive infinitesimal and $\Sigma_{R,L}$ are the selfenergy matrices due to the connection of left and right GNR electrodes to the channel. The effect of semi-infinite electrodes on the Hamiltonian of system is described using the self-energy terms. The selfenergies are then calculated iteratively, too [16]. The spin-dependent density of states and the expectation value for the number operator of electron on each site of the channel (ZGF) are given as

$$g_{i\sigma}(\omega) = -\frac{1}{\pi} \mathrm{Im} \ \langle i\sigma \left| \widehat{G_C}(\omega) \right| i\sigma \rangle \quad (3)$$

$$\langle \widehat{n_{i,\sigma}} \rangle = \int_{-\infty}^{E_F} g_{i\sigma}(\omega) d_{\omega} \quad (4)$$

Our Hamiltonian is in fact within the mean-field approximation, and it does not contain spin–flip scattering interactions. Therefore, the spin-polarized transport through such a junction can be considered within the coherent regime. In the coherent transport, the spin-dependent conductance at low temperature can be written as

$$G_{\sigma} = \frac{e^2}{h} \mathrm{Tr} \left[\Gamma_L G_c \Gamma_R G_c^{\dagger} \right] \quad (5)$$

Where $\Gamma_{L,R}$, the coupling matrices can be expressed as $\Gamma_{L,R} = -2\mathrm{Im}(\Sigma_{L,R})$ [12].

For doping the system, some carbon atoms are replaced by born atoms in the central part i.e. the ZGF. It has been well-known that the electronic scattering process is spin-anisotropic in presence of boron atoms, namely the transmittance channels are separated for up and down spin differently [15].

The boron atoms are distributed in the system with three different spatial configurations. For each configuration, 10% of carbon atoms in the central part (ZGF) is replaced by boron atoms. Fig. 1 shows the pure system and also the three different impurity configurations in the doped systems under study.

The Hamiltonian of the doped systems is now modified as follows. Here for doped systems, we improve the Hamiltonian (Eq. (1)). First, we introduce onsite energies on boron atomic sites and then modify a value of the hopping integral between boron and carbon atoms (−2 eV).i.e. we substitute 2 eV instead of 2.66 eV for boron atoms hopping [16]. After that, other calculations are followed without any change.