Spin-dependent transport in armchair graphene nanoribbon structures with edge roughness effects

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Abstract. We analyze the spin-dependent transport in single ferromagnetic gate structures based on armchair graphene nanoribbon (GNR) using the non-equilibrium Green’s function method in a tight binding model. It is shown that the spin polarized current oscillates as a function of the gate-induced barrier height. For perfect GNRs, the larger the energy band gap, the stronger the oscillation of the spin polarization. However, though the edge roughness of the ribbons tends to enlarge the band gap, it also strongly reduces the conductance which finally degrades the spin polarized current.

Key words: Graphene nanoribbon, spin polarized transport, Green’s functions method

1. Introduction

Due to unique electronic properties [1], graphene materials may be a key to envision future applications in nano-electronics [2] and spintronics [3]. The charge carriers in 2D-graphene structures behave as relativistic particles and can be described by a Dirac’s equation [4]. This property originates to a lot of peculiar phenomena such as the finite conductivity at zero density [5], the unusual integer quantum Hall effect [6], and the Klein tunnelling [7]. In addition, due to very weak spin orbit interaction which leads to a long spin flip length (≈ 1 µm) [8], graphene also offers a good candidate for spintronics applications. Many spin-dependent properties such as the spin field effect transistor [9], the spin Hall effect [10], the spin valve effect [3,11], and the electrical control of spin polarized current [12-14] have been explored in graphene-based structures. Especially, because of their finite energy gap [15-17], graphene nanoribbons (finite width graphene strips) are expected to be a basic material for designing high performance devices. However, their electronic properties have been demonstrated to be drastically affected by the disorder induced by defects [15,17], impurities [18], edge roughness [19], etc... For narrow graphene nanoribbons (GNR) the edge roughness effects are very important since they can govern the whole of transport phenomena of the structures [15,20,21].

In a recent work [14], we have investigated the spin-controllable possibilities of a structure based on armchair-edge ribbons without considering effects of the edge roughness. Our goal here is, therefore, to address this problem. The non-equilibrium Green’s functions (NEGf) formalism for an appropriate tight binding model is used as a calculation method. Section 2 is devoted to a brief
introduction of the considered structure and the model. Obtained results and discussions are then presented in Section 3. Finally, some conclusions are addressed in Section 4.

2. Model and calculation method

The structure under consideration is schematized in Fig. 1: it consists of a GNR sample with rough edges coupled to two semi-infinite perfect GNR leads. The ferromagnetic gate is deposited in the centre part to create a spin-dependent potential barrier which can control electrically the spin-polarized current through the structure. The system is described by a tight binding model with one π electron per atom and the calculation procedure is based on the NEGF technique described in Ref. [14].

![Figure 1](image)

**Figure 1:** (color online) Schematic illustration of the considered structure which is similar to that in Fig. 1(a) of Ref. [14] but the edge roughness is studied in the sample.

To model the rough edges, we assume that each pair of carbon atoms of edge rows has a probability $\Theta_d$ to be removed. Missing atoms are modelled by setting the corresponding hopping elements to zero in the lattice description. The perfect GNR leads have the same width as the central part which is characterized by the number $M$ of carbon atom chains between the two edges. It is worth noting that in the nearest neighbour tight-binding model the perfect GNR behaves as a semiconductor (finite band gap) for the armchair row $M \neq 3n + 2$ while is a metal for $M = 3n + 2$ (gapless).

3. Results and discussions

![Figure 2](image)

**Figure 2:** (color online) Spin polarization vs the barrier height in perfect structures: role of the band gap. In (a), the solid and dashed curves correspond to metallic ($M = 74$) and semiconducting ($M = 76$) GNRs, respectively. The curves in (b) are for semiconducting ribbons of different widths: $M = 76$ (dashed), 100 (dotted) and 124 (solid line).

As discussed in Refs. [12,13], the conductance and the spin polarization in the 2D-graphene structures have an oscillatory behaviour with respect to the barrier height controlled by the gate voltage $U_G$. This feature has been also observed in the GNRs [14], i.e., as illustrated in Fig. 2. Here, the GNRs have been assumed to be perfect, the Fermi energy $E_F = 75 \text{meV}$, the gate length $L_G = 42.6 \text{nm}$ and the exchange energy $h = 10 \text{meV}$. Actually, it has been shown that the transmission oscillation is stronger when the band gap is larger [14]. Therefore, the transport quantities such as the conductance and the spin polarization oscillate more strongly in semiconducting GNRs than in metallic ones, e.g., as presented in Fig. 2(a) for the cases of $M = 74$ (metallic, solid line) and $M = 76$ (semiconducting,
Moreover, it is also found that the amplitude of spin polarization in the semiconducting GNRs is significantly higher than in 2D-graphene, i.e., it is about 67% for $M=76$ in Fig. 2(a) while its maximum value is only about 30% in the 2D-graphene [12,13]. However, in semiconducting GNRs, as a result of band gap reduction [15], the oscillation of transport quantities gradually weakens when increasing the ribbon’s width (see in Fig. 2(b)). For instance, the amplitude of spin polarization reduces from 67% for $M=76$ (dashed line) to 38.5% for $M=100$ (dotted line) and 26% for $M=124$ (solid line). It is worth mentioning that the band gap in graphene can be induced by the interaction of the sample with the substrate [22,23] besides by the effect of finite width. The gap has been predicted to be about 0.26 eV and decreases as the number of graphene layers increases [22].

In Fig. 3, we display the edge roughness effects on the transport quantities. For $W=9.1\text{nm}$, $\Theta_d=50\%$ and $L_D=85.2\text{nm}$, Fig. 3(a) shows that: (i) with rough edges the GNRs are always semiconducting, i.e., they exhibit a finite conduction gap $E_g$ (as a consequence of energy band gap) and (ii) the edge disorder also makes the conductance smaller than in the case of perfect GNRs. The width-dependence of the conduction gap ($E_g-I/W$) and of the conductance plotted in Figs. 3(b) and 3(c), respectively, are in good agreement with experimental data of Ref. [15]. In Figs. 3(d) and 3(e), we also show the dependence of conduction gap and conductance on the intensity of edge disorder which is characterized by the probability $\Theta_d$. Obviously, the conduction gap (conductance) is enlarged (reduced) when increasing $\Theta_d$. The GNR’s metallic behavior disappears as soon as a small amount of edge disorder is considered. Here, the conductance is calculated at $E_F=0.5\text{eV}$.

![Figure 3](color online) (a) comparison between the conductance in perfect (dashed) and rough (solid) GNRs; (b) conduction gap and (c) conductance vs the ribbon’s width $W$; (d) conduction gap and (e) conductance depending on the disorder probability $\Theta_d$.

Definitely, the edge roughness affects strongly the possibilities of gate controlled spin polarized current. In Figs. 4(a) and 4(b), we plot the spin polarization versus the barrier height obtained when taking into account the edge roughness, with the leads considered to be perfectly metallic and semiconducting GNRs, respectively. On the one hand, due to the enhancement of conduction gap, the spin polarization in the structures with metallic GNR leads is enhanced when increasing the intensity of edge disorder $\Theta_d$. On the other hand, because of the roughness-induced decrease of transport quantities as the conductance, the spin polarized current in the structures with semiconducting leads is reduced when increasing $\Theta_d$. Moreover, the edge disorder makes the gate controllability of spin polarized current blurred. It can be obviously concluded that nearly-perfect semiconducting GNRs with limited edge disorder are desirable to provide the tunability of spin polarized current suitable for designing efficient spintronics devices.
4. Conclusions

Using NEGF method, we have considered the spin-dependent transport in armchair GNRs. It is shown that a highly tunable spin current can be achieved in semiconducting structures. The edge roughness tends to enlarge the conduction gap and to reduce the conductance. These two effects influence differently the spin polarization. Finally, the results suggest that GNRs with nearly perfect edges and large energy band gap should be appropriate for designing efficient spintronics devices.

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