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Effect of temperature, electric and magnetic field on spin relaxation in single layer graphene: A Monte Carlo simulation study

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ABSTRACT

In this article, we employ the semiclassical Monte Carlo approach to study the spin polarized electron transport in single layer graphene channel. The Monte Carlo method can treat non-equilibrium carrier transport and effects of external electric and magnetic fields on carrier transport can be incorporated in the formalism. Graphene is the ideal material for spintronics application due to very low Spin Orbit Interaction. Spin relaxation in graphene is caused by D'yakonov-Perel (DP) relaxation and Elliott-Yafet (EY) relaxation. We study effect of electron electron scattering, temperature, magnetic field and driving electric field on spin relaxation length in single layer graphene. We have considered injection polarization along *z*-direction which is perpendicular to the plane of graphene and the magnitude of ensemble averaged spin variation is studied along the *x*-direction which is the transport direction. This theoretical investigation is particularly important in order to identify the factors responsible for experimentally observed spin relaxation length in graphene.

1. Introduction

As the device dimensions shrink the leakage power becomes significant portion of total power dissipation while there is no significant improvement in switching speed. The demonstrated potential of spintronics namely non volatility, low power dissipation and higher switching speeds, have motivated the research community to experiment on spin based devices. Hence there is steady increase in exploring the spin degree of freedom [1] of an electron. Graphene is a prospective candidate for spintronics applications. In 2011 edition of ITRS it was claimed that Graphene exhibits spin transport characteristics that surpass those of any other semiconductor material studied to date. Graphene has drawn plenty of attention since its discovery due to its excellent properties, such as high electron mobility, long spin relaxation length and gate-tunable spin transport as demonstrated by Tombros et al. [2]. Significant amount of experimental and theoretical work have been done on graphene [3–10]. In the work of Novoselov et al. [11], graphene was isolated for the first time and its long mean free path was demonstrated experimentally. In the work of McCann et al. [12], the possibility of opening the bandgap in bilayer graphene by an external electric field was demonstrated. In the work of Wallace [13], the existence of Dirac like Fermionic states in a single layer graphene (SLG) was derived theoretically. In the work of Guimaraes et al. [14] long spin relaxation length in suspended intrinsic graphene layer was demonstrated experimentally. In the work of Y. Gao et al. [15] authors demonstrated long spin relaxation length in few layer graphene flakes at room temperature. In the work of Zomer et al. [16] long spin relaxation length in monolayer graphene on hexagonal boron nitride substrate was demonstrated experimentally. In the work of Zhang Xiao-Wei et al. [17] the authors numerically studied spin transport in arm chair GNRs when charge and spin biases coexist. Long spin relaxation length observed in a SLG is due to the fact that the low atomic masses of carbon cause low spin-orbit interaction [2,18,19] and most of the isotopes of carbon have weak hyperfine interaction between the nuclear and the electronic spins. A single layer graphene is exactly one atomic layer thick with bond length of 1.42 Å.

In this work, we use a semiclassical Monte Carlo approach to model the spin relaxation and study the effects of external magnetic and electric fields in single layer graphene. Monte Carlo simulations have been extensively used to model the charge transport and recently the spin transport [20–24] in devices. Monte Carlo approach is best suited for studies on the spin dephasing since the spin evolution occurs continuously along with the evolution of momentum which is taken care of easily by a Monte Carlo simulation.

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The paper is organized as follows. In Section 2 we present the SLG model used in our simulations and discuss different spin orbit interactions. Section 3 deals with the result and discussion. Section 4 concludes this paper.

2. Model

Single layer graphene basically is a hexagonal monolayer of carbon atoms with linear dispersion, close to the Dirac point, and zero bandgap. Monolayer graphene sheet shows ambipolar characteristic where electrons and holes coexist symmetrically across the Fermi level (Dirac Point). The basis of the simulation model is the dispersion relation of SLG [18],

$$\varepsilon(k) = \hbar v_F k, \tag{1}$$

where ε is the energy of a carrier, k is the magnitude of the momentum wave vector and v_F is the Fermi velocity.

The Monte Carlo method has been discussed earlier in detail [20,25–27].We shall restrict our discussion only to the essential features of the model. The scattering mechanisms incorporated in our simulations include the electron electron scattering, acoustic phonon and optical phonon scatterings and the spin flip scattering.

The dynamics of the carriers are described by the relationship between the momentum wave vector k and velocity v and is obtained as shown below [18],

$$v = v_F \frac{k}{|k|}, \tag{2}$$

The magnitude of the velocities of the carriers in SLG is constant and change of momentum results in a change in direction. Thus, the force experienced by a carrier changes the magnitude of its momentum without changing the magnitude of its velocity and the classical equation $p = mv$ does not hold as mass for SLG carriers is meaningless.

We consider the effects of DP spin relaxation mechanism as mentioned in [28].

$$\frac{ds}{dt} = \frac{2\lambda}{\hbar}(n \times s), \tag{3}$$

where S denotes the spin vector and n is the unit vector in the plane of the SLG and,

$$\lambda = \zeta \cdot E, \tag{4}$$

where ζ is the Rashba parameter and E the vertical electric field perpendicular to the graphene plane.

The analytical relation between momentum relaxation time τ_p and spin relaxation time τ_s for DP relaxation is given by [29],

$$\frac{1}{\tau_s^{DP}} = \left(\frac{4\Delta}{\hbar}\right)^2 \tau_p, \tag{5}$$

here Δ is the spin orbit splitting.

The effects of electron electron scattering is incorporated along the lines of [30–32]. In [30] Goodnick and Lugli have discussed the transport phenomenon in 3D systems. In this work, we have used their model as reference and modified the results for 2D systems, such as, single layer graphene. We calculate the maximum e-e scattering rate and use it to calculate the frequency of electron-electron scattering and the actual value is calculated only if e-e scattering event is selected [30]. The maximum value of e-e scattering rate in single layer graphene is given by

$$\Gamma_{max} = \frac{2\pi^2 e^4 N_s |k| I}{\hbar^2 (\varepsilon_r \varepsilon_0)^2 v_F} \frac{1}{q_0^2}, \tag{6}$$

where N_s represents the total sheet density of electrons, ε_r is the dielectric constant for graphene, k denotes the net momentum of electron, v_F denotes the Fermi velocity in graphene and q_0 is the inverse screening length in two dimensions [31,32].

The EY spin relaxation mechanism also been considered along the lines of [33].

$$\frac{1}{\tau_s^{EY}} = A\left(\frac{k_B T}{E_g}\right)^2 \eta^2 \left(\frac{1-\eta/2}{1-\eta/3}\right)^2 \frac{1}{\tau_p}, \tag{7}$$

τ_s^{EY} here represents the spin relaxation time due to spin flip scattering, τ_p represents the total momentum relaxation time, E_g is the bandgap and η is given by the following expression

$$\eta = \frac{\Delta}{E_g + \Delta}, \tag{8}$$

here Δ is the spin orbit splitting. In the above expression, $1/\tau_p$ is obtained by summing all the scattering rates considered.

For the scattering mechanisms considered, the scattering events change the wave-vector of a particle from k to k'. The scattering due to phonons is assumed to be isotropic.

3. Simulation results and discussion

For the simulation purpose a SLG channel of length 5 μm is considered. Simulations were performed with a time step of 0.05 fs and the electrons were evolved for 10^6 steps to achieve the steady state. For time averaging the data were recorded for the last 10^5 iterations. 100% spin injection was considered. The drain voltage considered is 4 V.

$$|\langle S\rangle(x,T)| = \sqrt{\langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2}. \tag{9}$$

The spin relaxation length is defined to be the distance from the point of injection to the point where the magnitude of the average spin vector drops to $1/e$ times its initial value at injection. In our simulations, electrons are injected with initial polarization of 100% in z direction.

3.1. Spin dephasing along single layer graphene channel

Fig. 1 shows the magnitude of ensemble averaged spin along a single layer graphene channel with length 5 μm at 300 K and drain voltage 4 V. The electrons are injected polarized along z direction. We have considered 100% spin polarization. The value of the Rashba parameter is taken to be $\eta = 0.005$ m eV (V/nm). We have compared spin relaxation length without electron electron (e–e) scattering and with electron electron scattering as shown in Fig. 1. In the first case, spin relaxation length is found to be 1.2 μm while in the latter case it becomes 0.8 μm. Hence e-e scattering causes a decrease of 33.3% in spin relaxation length which shows the significant influence of e-e scattering on spin transport in single layer graphene.

3.2. Temperature dependent spin transport in single layer graphene

Fig. 2 shows the profile of the magnitude of ensemble averaged spin at different temperatures for a SLG at a driving voltage of 4 V. The spin relaxation length is about 1.4 um at 4 K and 0.8 μm at 300 K.