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Monte Carlo simulation studies of spin transport in graphene armchair nanoribbons

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ABSTRACT

The research in the area of spintronics is gaining momentum due to the promise spintronics based devices have shown. Since spin degree of freedom of an electron is used to store and process information, spintronics can provide numerous advantages over conventional electronics by providing new functionalities. In this article, we study spin relaxation in graphene nanoribbons (GNR) of armchair type by employing semiclassical Monte Carlo approach. D'yakonov-Perel' relaxation due to structural inversion asymmetry (Rashba spin–orbit coupling) and Elliott–Yafet (EY) relaxation cause spin dephasing in armchair graphene nanoribbons. We investigate spin relaxation in α-,β- and γ-armchair GNR with varying width and temperature.

1. Introduction

Due to demonstrated potential, namely low power dissipation and higher switching speeds, spintronics has drawn a lot of attention in the electronic industry. Hence there is a gradual increase in exploring the spin degree of freedom [1] of an electron. Graphene has drawn plenty of attention for spintronic applications due to its excellent properties, such as long spin relaxation length and gate-tunable spin transport as demonstrated by Tombros et al. [2]. Significant amount of experimental and theoretical work has been done on graphene [3–10]. In Ref. [11], Novoselov et al. isolated graphene for the first time and its long mean free path was demonstrated experimentally. In Ref. [12], McCann et al. showed the possibility of opening the bandgap gap in bilayer graphene (BLG) by an external electric field. In Ref. [13] Wallace derived theoretically, the existence of Dirac like Fermionic states in single layer graphene (SLG). Long spin relaxation length observed in single layer graphene (SLG) is due to the fact that the low atomic masses of carbon cause low spin–orbit interaction and most of the isotopes of carbon have weak hyperfine interaction between the nuclear and the electronic spins. A lot of spin transport study, both experimental and theoretical, has focused on infinite graphene sheet and very little work has been done on spin transport in graphene nanoribbons (GNRs) [14,15].

Single layer graphene is a two dimensional hexagonal monolayer of carbon atoms with linear dispersion around the Dirac point and zero bandgap. Because of its semi-metallic behavior SLG is of little use in electronic industry. Spin transport in semiconductors is very attractive since one can exploit both charge and spin properties of an electron to transport the information. It can combine the capabilities of semiconductors with the capabilities of magnetic materials. Constraining one dimension of graphene sheet results in nanoribbons of armchair (ac) or zigzag (zg) type which is semiconducting [16–17]. The bandgap of these graphene nanoribbons (GNR) depends on the edge property, width and chirality. In this work, we study spin transport in ac GNR. Due to one dimensional quantization, acGNRs have velocities less than that in unconstrained graphene. Besides, the band structure has a parabolic nature around the band edge.

We use a semiclassical Monte Carlo approach to model spin relaxation in ac GNR. Monte Carlo simulations have been extensively used to model charge transport and recently spin transport [18–22] in SLG and BLG devices. Monte Carlo approach is best suited for studies on 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.

The paper is organized as follows. In Section 2, we present the armchair graphene nanoribbon model used in our simulations and

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discuss the Monte Carlo method. Section 3 deals with the result and discussion. Section 4 concludes this paper.

2. Simulation model

To model spin transport in armchair GNR we use electronic bandstructure data obtained by the semiempirical method as reported in Refs. [16,17]. As described in previous section constraining one dimension of graphene sheet results in nanoribbons of armchair or zigzag type which give graphene its semiconducting properties. The perfect armchair GNR behaves as a semiconductor (finite band gap) for the armchair row $M \neq 3n+2$ (β and γ-type) while is a semi-metal for $M=3n+2$ (α-type). However, if the edge effects are taken into account the GNR are always semiconducting.

The GNR of armchair type can be categorized into α-,β-, and γ-ac GNRs based upon their electronic bandstructure as reported in Refs. [16,17]. α-ac GNRs are $N=8,11,14,\ldots$ and are gapless for perfect GNR. β-acGNRs are $N=9,12,15,\ldots$ and γ-acGNRs are $N=10,13,16,\ldots$ and have finite bandgap. For each ac GNR type, band gaps and electron effective masses are inversely proportional to the width of the GNR with a varying proportionality constant. The band gap versus width (W) relations for each type of ac GNR is given by the following equation:

$$\begin{aligned} E_{gap} &= 0.04\ \text{eV}/W\ (\text{nm})\ \text{for}\ \alpha-\text{acGNR} \\ &= 0.86\ \text{eV}/W\ (\text{nm})\ \text{for}\ \beta-\text{acGNR} \\ &= 1.04\ \text{eV}/W\ (\text{nm})\ \text{for}\ \gamma-\text{acGNR} \end{aligned} \quad (1)$$

Each type of ac GNRs follow an inverse relation of effective mass with the width given below,

$$\begin{aligned} m/m_0 &= 0.005/W\ (\text{nm})\ \text{for}\ \alpha-\text{acGNR} \\ &= 0.091/W\ (\text{nm})\ \text{for}\ \boldsymbol{\beta}-\text{acGNR} \\ &= 0.160/W\ (\text{nm})\ \text{for}\ \gamma-\text{acGNR} \end{aligned} \quad (2)$$

where m_0 is the free electron mass.

D'yakonov-Perel' (DP) relaxation [23] due to structural inversion asymmetry (Rashba spin–orbit coupling) and Elliott–Yafet (EY) relaxation [24] causes spin dephasing in graphene armchair nanoribbon. In the DP mechanism [23] electrons experience an effective magnetic field generated by the spin–orbit interaction. This magnetic field changes randomly every time the electron undergoes scattering event leading to spin dephasing. Temporal evolution of spin is given by the following equation [25,26]:

$$\frac{d\vec{S}}{dt} = \vec{\Omega}\ \vec{S} \quad (3)$$

where $\vec{\Omega}$ is the precession vector. The temporal evolution of the spin in a random time interval Δt is determined by $\vec{\Omega}$. The vector $\vec{\Omega}$ depends on electron wave vector and changes from one time interval to the next as electron wavevector dynamically evolves while it travel along the channel. This time evolution of the wavevector is determined from the Monte Carlo simulation [27–31]. Spin components $S_x(t+\Delta t)$, $S_y(t+\Delta t)$ and $S_z(t+\Delta t)$ are evaluated in each time interval Δt. Spin evolution terminates if any scattering event takes place in the middle of interval Δt. The wavevector state is updated based on the type of scattering event and $\vec{\Omega}$ is again calculated from the new wavevector, The spin evolution continues for the remainder of the time interval after new $\vec{\Omega}$ is calculated. The statistics about spin components is available at the end of time interval Δt. The analytical relation between the spin relaxation time τ_s and momentum relaxation time τ_p for DP relaxation is given by the following equation [32]:

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

Here Δ is the spin orbit splitting.

Spin flip scattering due to EY mechanism is taken into consideration along the lines [25,32]. The scattering rate due to this mechanism is given by the following equation:

$$\frac{1}{\tau_s^{EY}} = A\left(\frac{k_B T}{E_g}\right)^2 \eta^2 \left(\frac{1-\eta/2}{1-\eta/3}\right)^2 \frac{1}{\tau_p} \quad (5)$$

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 band gap and η is given by the following expression:

$$\eta = \frac{\Delta}{E_g+\Delta} \quad (6)$$

Here Δ is the spin orbit splitting.

We employ the Monte Carlo method to model spin transport in GNR. The Monte Carlo method involves determining free flight time by calculating the various scattering rates. During free flight period carriers are evolved according to classical transport equations after which they undergo scattering. The velocities of the carriers after scattering are calculated from their scattering rates and by the generation of random numbers. Finally, new scattering rates are calculated from the new velocities and energies of carriers and new free flight times are calculated. The process is repeated for a predetermined number of steps. During the free flight period, the spin of an individual carrier precesses around an effective magnetic field obtained from the spin–orbit Hamiltonian.

The magnitude of the average spin vector is computed using the following expression:

$$|<S>(x,T)| = \sqrt{<S_x>^2 + <S_y>^2 + <S_z>^2} \quad (7)$$

The spin dephasing length is defined as 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.

The major scattering mechanisms incorporated in our simulation are ionized impurity scattering, acoustic phonon scattering, optical phonon scattering and spin flip. For the scattering mechanisms discussed below the scattering events change the wavevector of a particle from $\mathbf{k}$ to $\mathbf{k}'$. The scattering due to phonons are assumed to be isotropic. For the initialized distribution of particles we solve the Poisson equation [21,26–29] after dividing the device into uniformly spaced grids along its length. Knowing the position of the particles the charge distribution in each grid is calculated and then Poisson equation is solved to get the local electric field at each grid. Finally using the energies of the particles the individual scattering rates for each of the particles is calculated. The electrons crossing over into the drain are reinjected at the source with polarized spin along the direction perpendicular to the layer of graphene.

3. Results and discussion

The length of the device simulated is 5 μm. The driving electric field considered is 1 kV/cm. The value electric field applied along the axis of the graphene to induce charge flow ensures that the parabolic approximation is valid. At high fields due to nonparabolicity of the bands the scattering to other bands lead to additional heating. For the value of driving electric field considered the transport in the channel is effectively drift diffusive [19,21]. The scattering mechanisms incorporated in our simulations include the ionized impurity scattering, the acoustic phonon scattering and the optical phonon scattering. The time step used in the simulation is 0.005 fs and the particles are evolved for 3×10^5 steps for steady state solution. The choice of value of time step Δt