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Role of electron-electron scattering on spin transport in single layer graphene

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In this work, the effect of electron-electron scattering on spin transport in single layer graphene is studied using semi-classical Monte Carlo simulation. The D'yakonov-P'erel mechanism is considered for spin relaxation. It is found that electron-electron scattering causes spin relaxation length to decrease by 35% at 300 K. The reason for this decrease in spin relaxation length is that the ensemble spin is modified upon an e-e collision and also e-e scattering rate is greater than phonon scattering rate at room temperature, which causes change in spin relaxation profile due to electron-electron scattering. [http://dx.doi.org/10.1063/1.4862674]

I. INTRODUCTION

Single layer graphene is a single two dimensional sheet in which carbon atoms are arranged in a honeycomb lattice. Interest in graphene related devices has grown significantly over the past few years because of its many outstanding properties, such as, high charge carrier mobility, large spin diffusion length, tunable band gap, low spin orbit interaction and unusual quantum Hall effect. Graphene shows tremendous potential for both electronics and spintronics applications because of its unique structural, optical, electronic and especially spintronics properties.

Over the past few years, significant amount of work, both experimental and theoretical, has been done on graphene.[1–6] Novoselov et. al.[7] isolated graphene for the first time after more than four centuries its invention and experimentally demonstrated its long mean free path. Further, in Ref. 8, Wallace theoretically derived the existence of Dirac like Fermionic states for single layer graphene. Many experimental studies have also focused extensively on the effect of chemical doping on spin relaxation in graphene.[9–12] In Ref. 13, the non-equilibrium Green's function technique was employed to study charge and spin transport in single layer graphene, and the authors also demonstrated, in subsequent work, that bi-layer graphene has a higher potential for spintronic applications.

Currently, there is lot of research going on in spin transport in graphene employing Monte Carlo technique.[14,15] However, the effects of e-e scattering have yet to be addressed. The problem was neglected until now because of its little importance in the theoretical research of conventional charge based semiconductor devices. The reason is that whenever an event of e-e collision occurs, the ensemble velocity of charge carriers is conserved. In such cases, only momentum is redistributed which has no direct consequence to current flow. However, unlike current, ensemble spin is modified upon e-e collision and hence e-e collisions have direct consequence on spin transport. Therefore, inter-carrier collisions in graphene deserve careful attention in the determination of properties which are related to spin transport. The e-e scattering rate was found by Das Sarma and he calculated the mean free path in graphene through the analysis of the quasi-particle self-energies.[17] In

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Ref. 18 many-body effect of e-e interactions in graphene has been taken into account using perturbative Green's function approach but at very low temperatures and also without electron-phonon relaxation.

Monte Carlo simulation study of spin transport in single and multilayer graphene has already been presented in previous works.[14,15] In Ref. 14 the authors studied spin transport in SLG with varying temperature using semiclassical monte carlo simulation. The authors reported spin relaxation length of 0.9 um at 300 K without inclusion of coulomb scattering due to electron electron interaction. However as the carrier density in the channel region increases the coulomb scattering becomes dominant scattering mechanism in SLG as reported in Ref. 16. In Ref. 15 authors studied Spin Relaxation in BLG using semiclassical monte carlo approach including only electron-phonon interactions. As the number of stacked layers increase the contribution of electron-electron scattering to overall scattering reduces due to screening effects. To the best of our knowledge, there has been no study of the effect of e-e scattering on spin transport in single layer graphene. In this work, a semiclassical Monte Carlo simulation study of the influence of e-e scattering on spin transport in single layer graphene is presented. The Monte Carlo method of modeling charge transport in semiconductors is reviewed in Ref. 19. In our work, we have modeled the transport using classical laws of motion, and calculated the scattering rates which are based on Fermi's golden rule. Spin relaxation mechanism which has been considered in this work is D'yakonov-Perel (DP). The present work is organized as follows. Firstly, we will discuss the modeling of spin transport in single layer graphene incorporating both electron-phonon and e-e scatterings and then present comparative results of the effect of e-e scattering on spin transport in single layer graphene.

II. MODEL

The Monte Carlo method for modeling of single layer graphene in the presence of acoustic phonon scattering, optical phonon absorption scattering and optical phonon emission scattering has been discussed extensively in Ref. 15. In our simulation, we have also included e-e scattering. Here, we will briefly describe the Monte Carlo method used to model spin transport in graphene. Initially, positions, velocities and spins are assigned to electrons in a random and uniform fashion so as to depict a real system. The electrons are introduced from the source with spin 1 aligned in the +z direction. Then, various scattering rates are calculated and the free flight time of the carriers is determined at the end of which scattering events are selected stochastically based on the relative probabilities of the scattering events. The velocities of the carriers after scattering are determined from their scattering rates and by the generation of random numbers. Finally, new scattering rates and free flight times are calculated using new velocities and energies of carrier and this process is repeated for a fixed number of steps. The spin of each carrier during the free flight time precesses around an effective magnetic field which is obtained from the spin-orbit Hamiltonian. Modeling of spin relaxation is done by the DP spin relaxation mechanism as mentioned in Ref. 14.

Below we present the key results that we have used in our simulations. The energy momentum dispersion relation[15] for single layer graphene is given by

$$E(k) = \hbar v_F |k| \tag{1}$$

where k denotes the net momentum of electron and $v_F = 10^6$ m/s denotes the Fermi velocity in graphene.

In Ref. 20, Goodnick and Lugli have discussed the transport phenomenon in 3D systems in which they have included e-e scattering. In our work, we have used their model as reference and modified the results for 2D systems, such as, single layer graphene. The calculation of the e-e scattering rate requires a summation over carrier distribution functions of all electrons which have anti-parallel spin. This process is computationally not viable and has to be replaced by a more pragmatic approach. Hence, as proposed in Ref. 20, 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. The maximum value of e-e scattering rate in single layer

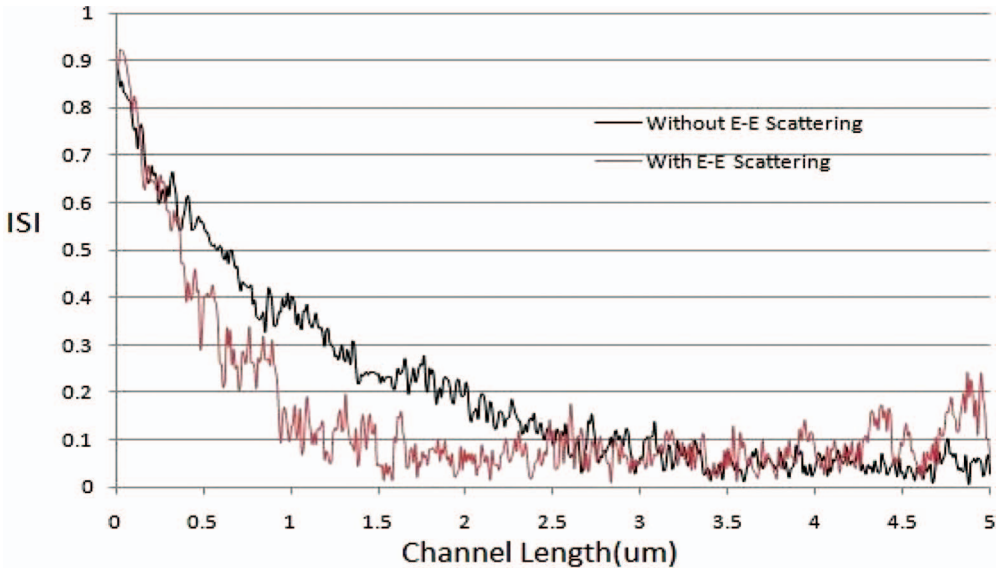

FIG. 1. |S| along the channel length at 300 K.

graphene is given by

$$\Gamma_{max} = \frac{2\pi^2 e^4 N_s \mathrm{IkI}}{\hbar^2(\varepsilon_r\varepsilon_0)^2 \mathrm{vF}} \frac{1}{q_0^2} \tag{2}$$

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.[21,22] Whenever an e-e scattering event is selected, a partner electron is selected from the ensemble by a method which is slightly different from the one described by Mosko-Moskova.[23] In this work, we have used a semi classical model so each electron is assigned a definite coordinate value for position. We try to make use of this information and the decision of the partner electron is done on the basis of least distance from the scattered electron.We randomly choose the scattering angle which helps in calculating the actual value of integrand. After that, a number is chosen randomly between zero and the maximum value, i.e., Γ_{max} and the e-e scattering is selected only if the integrand is greater than this number. If e-e scattering is rejected then the electron and its partner continue to move along their original paths.

III. RESULTS AND DISCUSSION

In an earlier work,[15] detailed study of the simulation of single layer graphene was presented. For single layer graphene, the length of the device simulated is 5 um and the width is 5 nm. The value of the Rashba parameter is taken to be $\eta = 0.005$ meV (V/nm). Potential difference between source and drain is 4 V. Spin is injected along z direction i.e. perpendicular to the plane of the graphene layer and 100% spin injection is considered. Simulation is performed with a basic time step of 0.005 fs and the particles are simulated for 1 million steps. Only the steady state data during the last 20,000 steps are taken and averaged to get the final result.

We have considered two cases in our simulation – one, in which e-e scattering is not included and the other in which e-e scattering is included. In the first case, spin relaxation length is found to be 0.9 um while in the latter case it becomes 0.58 um. Hence e-e scattering causes a decrease of 35% in spin relaxation length which shows the significant influence of e-e scattering on spin transport in graphene. Figure 1 compares the magnitude of the spin plotted as a function of length along the channel for the two cases considered in our simulation. We have defined the spin relaxation length to be the distance from the source where the injected spin component reduces to 1/e of its value at the source end.

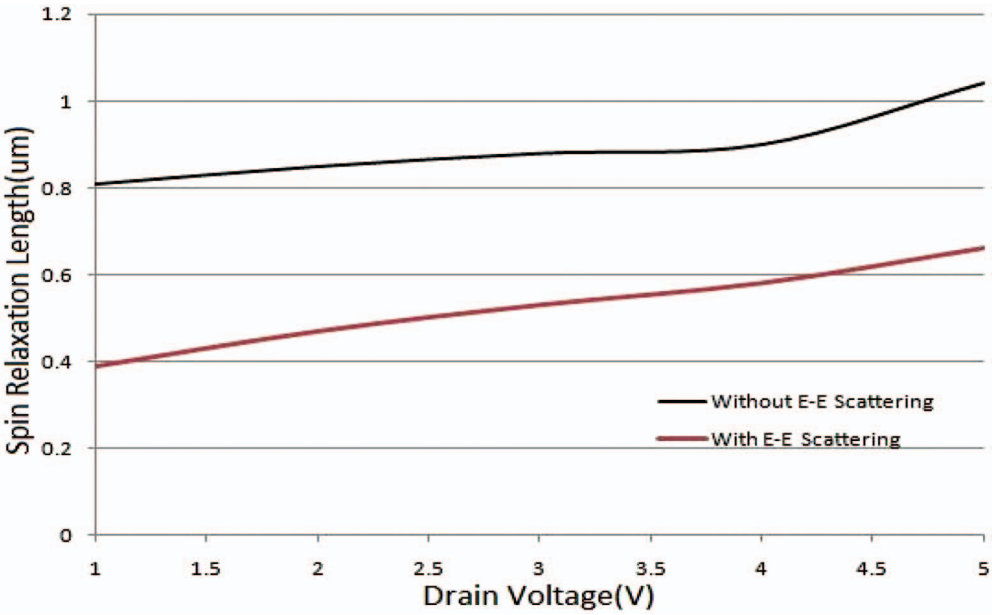

FIG. 2. Spin Relaxation length for different drain voltages.

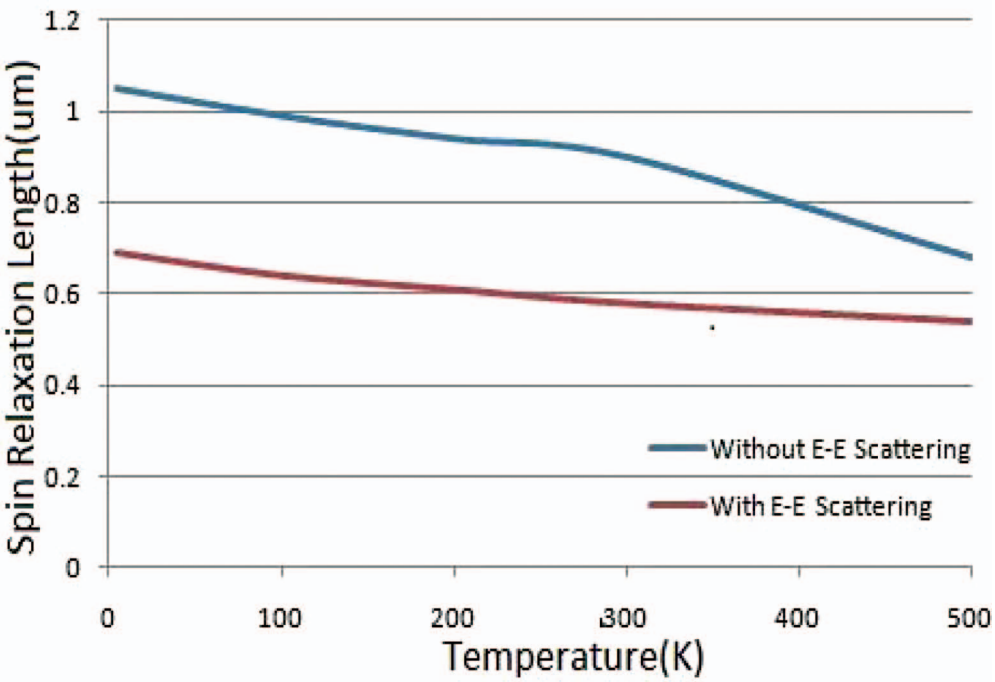

FIG. 3. Spin relaxation length for different temperatures, with and without e-e scattering.

We also observed the spin relaxation length for different electric field between source and drain. When drain voltage increases from 1 V to 5 V, spin relaxation length increases from 0.81 um to 1.05 um when e-e scattering is not considered and it increases from 0.39 um to 0.66 um when e-e scattering is considered.The reason for this change in spin relaxation length on changing drain voltage is that the drift velocity of carriers increases as the electric field between source and drain increases. Figure 2 shows the variation of spin relaxation length with respect to different drain voltages for the two cases.

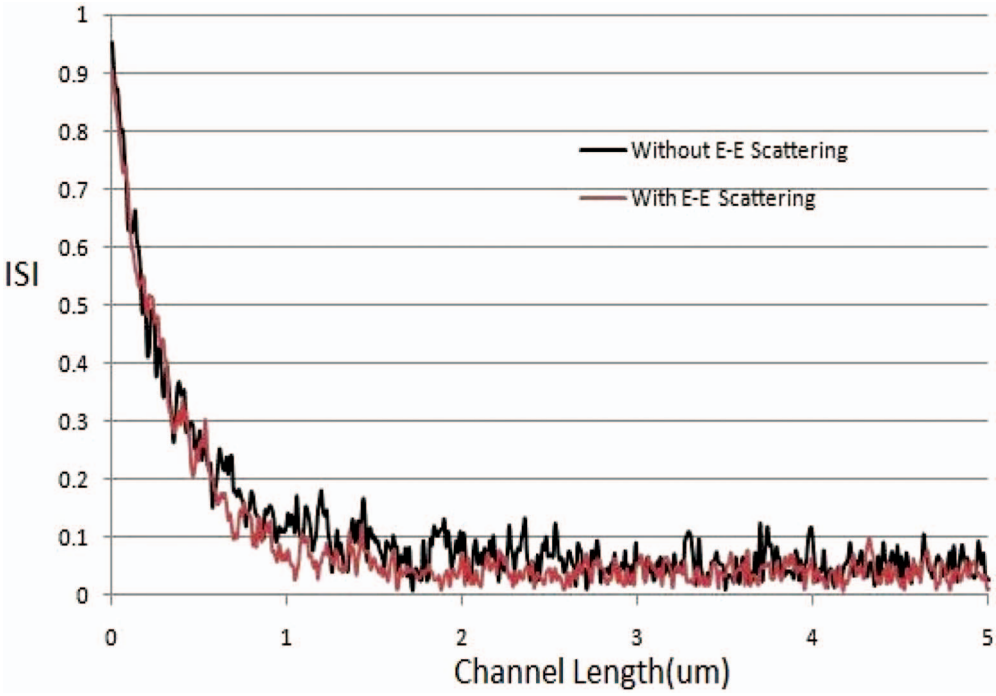

FIG. 4. |S| along the channel length at 1000 K, with and without e-e scattering.

Effect of temperature on spin relaxation profile has also been observed in monolayer graphene. Figure 3 shows the variation of spin relaxation length for different temperature. Simulation results indicate significant decrease in spin relaxation length at lower and room temperature when e-e scattering is included while at higher temperature spin relaxation length remains almost same on including e-e scattering. This variation happens because at lower temperature phonon scattering rate is lower than e-e scattering rate hence spin relaxation length decreases drastically on including e-e scattering. At higher temperature, phonon scattering increases and becomes comparable to e-e scattering and hence spin relaxation length remains almost same on including e-e scattering. Figure 4 shows the magnitude of spin along the length of the channel at 1000K which shows that spin relaxation length remains same even on including e-e scattering.

IV. CONCLUSION

In this work, we have studied the effect of e-e scattering on spin transport in single layer graphene using Monte Carlo method. We have included e-e scattering along with acoustic phonon scattering, optical phonon emission and optical phonon absorption scatterings. Our simulation results (Figure 1) indicate that spin relaxation length in single layer graphene decreases by 35% on including e-e scattering at 300 K. This variation in spin relaxation length occurs because phonon scattering rate is lesser than e-e scattering rate at room temperature. At high temperature, spin relaxation length remains same even on including e-e scattering because phonon scattering becomes comparable to e-e scattering. Besides (Figure 2) we conclude that spin relaxation length increases with increasing drain voltage due to the increased drift velocity of carriers.

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