Monte Carlo Study of Temperature and Bias Dependence of Spin Transport in GaAs

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Abstract. An ensemble Monte Carlo approach has been used to simulate spin relaxation in GaAs devices. Effect of varying temperature and applied bias on spin relaxation time has been studied in n-type bulk GaAs. Our results show that the spin relaxation times are longer at low temperatures and that increasing the applied bias yields enhancement of the spin polarization in the system.

1. Introduction
Semiconductor spintronic devices based on control and manipulation of electron spins are considered to be the future extension of present electronics. Spin lifetime of more than 100 ns has been experimentally observed in n-type semiconductors [1, 2]. Clearly, the longer the spin lifetime, the better and more reliable will be the spintronic devices. Study of spin transport in semiconductors has become extremely important for the development of the novel spin based devices, and GaAs is one of the widely studied materials both experimentally and theoretically for spin related phenomena [1]-[7]. In this paper we present a study of a three-dimensional, n-doped GaAs sample in which a spin-polarized current is electrically injected via a ferromagnetic contact. This study is conducted using Monte Carlo methods and we analyse the effect of varying temperature and applied bias on the decay of spin polarization within the GaAs sample.

2. Monte Carlo Method
The Ensemble Monte Carlo method has been used extensively in modeling charge transport in semiconductor materials and devices. It can be used to simulate specific devices and to include various scattering mechanisms, material properties and different boundary conditions, which makes it a highly flexible technique [8, 9]. This Monte Carlo method is a semiclassical approach in which the basic transport simulation in any semiconductor device begins with random generation of a free flight time for each particle which ends with a scattering event changing the energy and momentum of the particle. The process is then repeated for the next set of free flights. The free flight time is given by \( \tau = -\ln(r)/\Gamma \) where \( r \) is any random number between 0 and 1 and \( \Gamma \) is the total scattering rate (including self-scattering) calculated at the beginning of the simulation. In between the scattering events the charge carriers are considered to propagate along a classical trajectory and are influenced by external forces due to applied electric and magnetic fields. The equations of motion for the free flight make use of the electric
field obtained by solving the Poisson equation consistent with the device boundary conditions. At the end of each free flight the type of scattering responsible for terminating it is chosen by using a random number between 0 and \( \Gamma \), and then the new energy and momentum of the particle are calculated. The scattering mechanisms considered in our simulation are scattering between electrons and phonons and scattering of electrons with ionized impurities. Phonon scattering involves both acoustic and optical modes as well as absorption and emission of phonons. The corresponding scattering rates are calculated using Fermi’s Golden rule. Data sampling is done at regular time intervals \( \Delta t \) to allow for estimation of dynamic carrier parameters like position, velocity, energy as well as to update potentials and fields. The choice of this time interval \( \Delta t \) depends on the stability criteria \([9]\).

The next step is to integrate the spin dynamics in the Monte Carlo simulation. At the beginning of the simulation when positions and velocities are assigned to carriers, a single electron spin density matrix \( \rho_i \) is defined for each particle, \( \rho_i(t) = \begin{bmatrix} \rho_{i\uparrow\uparrow}(t) & \rho_{i\uparrow\downarrow}(t) \\ \rho_{i\downarrow\uparrow}(t) & \rho_{i\downarrow\downarrow}(t) \end{bmatrix} \).

During the free flight sequence the spin of each particle evolves coherently which can be represented as

\[
\rho_i(t + \tau) = e^{-i(\mathcal{H}_D)\tau/\hbar}\rho_i(t)e^{i(\mathcal{H}_D)\tau/\hbar}.
\]  

(1)

Here, \( \mathcal{H}_D \) is the spin dependent Hamiltonian to incorporate the spin-orbit mechanism responsible for the relaxation of spin polarization. In the present calculations we have included only Dyakonov-Perel (DP) mechanism for spin relaxation as, in n-type GaAs, Elliot-Yafet (EY) mechanism is less important \([1, 4, 7]\), at least in the range of temperatures and densities we consider. In DP mechanism, between the scattering events, electron spins precess with an effective, momentum dependent, Larmor frequency \( \Omega \). The direction of the momentum \( \mathbf{p} \) changes due to electron scattering events, which results in spin reorientation. In our simulation

\[
\mathcal{H}_D = \hbar \Omega \cdot \sigma,
\]  

(2)

where \( \Omega = \frac{\beta}{\hbar} \{ p_x(p_y^2 - p_z^2), p_y(p_z^2 - p_x^2), p_z(p_x^2 - p_y^2) \} \) \([10]\), \( \sigma \) are the Pauli spin matrices and \( \beta \) is the spin-orbit coupling constant.

Thus, the evolution operator in equation (1) is given by

\[
e^{-i(\mathcal{H}_D)\tau/\hbar} = \begin{bmatrix} \cos(\mathcal{A}\tau) - i\frac{\mathcal{B}}{\mathcal{A}}\sin(\mathcal{A}\tau) & -i\frac{\mathcal{C}}{\mathcal{A}}\sin(\mathcal{A}\tau) \\ -i\frac{\mathcal{B^*}}{\mathcal{A}}\sin(\mathcal{A}\tau) & \cos(\mathcal{A}\tau) + i\frac{\mathcal{C^*}}{\mathcal{A}}\sin(\mathcal{A}\tau) \end{bmatrix}.
\]  

(3)

In the above equation,

\[
\mathcal{A} = \frac{\beta}{\hbar^2} \{ [p_x(p_y^2 - p_z^2)]^2 + [p_y(p_z^2 - p_x^2)]^2 + [p_z(p_x^2 - p_y^2)]^2 \}^{1/2},
\]

\[
\mathcal{B} = [p_x(p_y^2 - p_z^2)] - i[p_y(p_z^2 - p_x^2)],
\]

\[
\mathcal{C} = [p_z(p_x^2 - p_y^2)], \text{ and}
\]

\[
\mathcal{D} = \{ [p_x(p_y^2 - p_z^2)]^2 + [p_y(p_z^2 - p_x^2)]^2 + [p_z(p_x^2 - p_y^2)]^2 \}^{1/2}.
\]

The normalized spin polarization density can be written as

\[
P_{\alpha} = \Sigma_i Tr(\sigma_{\alpha\beta_i})/\Sigma_i Tr(\rho_i).
\]  

(4)

After each scattering event the particle momentum is updated and hence its Larmor frequency \( \Omega \). The spreading of these frequencies as the simulation proceeds ultimately causes the spin polarization to decay. In our simulation we consider the lowest conduction band in the effective mass approximation.
3. System

We have simulated a simple spin-transport device consisting of a 3-dimensional n-type GaAs sample sandwiched between a ferromagnet (FM) and a non-magnetic material (NM) as shown in Fig. (1). It is a layered structure with electrical spin injection from the ferromagnet into the semiconductor layer. The presence of the FM and NM layers is simulated by implementing a fully polarized \( \rho_i(0) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \) and an unpolarized \( \rho_i(0) = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix} \) spin reinjection from the left and right-end side respectively, into the GaAs layer. A bias is applied to the GaAs layer. Charge neutrality condition is implemented i.e. when an electron exits the GaAs layer, a new particle is reinjected at the other end of the device with a thermal velocity. The electric-field profile along the x direction is computed self-consistently at each time step via a coupled Poisson-Monte Carlo solution. Spin dynamics is calculated via the evolution of the spin polarization vector according to Eqs.(1-4).

![Figure 1. Sketch of the studied system](image)

4. Results

Values of the spin-orbit coupling parameter \( \beta \), reported in the literature show a wide variation. Our studies on the temperature dependence of spin relaxation time in n-type bulk GaAs yields similar results to the ones obtained recently by Jiang et al. [7] using a kinetic spin Bloch equations approach when the same values of \( \beta \) are used. Similar to [7], we also find a good agreement with experimental results in [1] for temperatures greater than 20 K with \( \beta = 8.2 \ eV\text{Å}^3 \). Following [7] have used \( \beta = 23.9 \ eV\text{Å}^3 \) for the range of temperatures and densities considered in the simulation results presented here.

![Figure 2. Variation of spin polarization with bias (a) at the start and (b) at the end of the simulated n-type GaAs layer at different temperatures after 20ps.](image)
In this section we analyze the effect of varying temperature and applied bias on the spin relaxation time in an n-type GaAs sample. The GaAs layer is uniformly doped with a carrier density of $1 \times 10^{17} \text{ cm}^{-3}$ and its length is taken as $0.1 \mu\text{m}$. The total number of simulated particles is 200000 and the sampling time step is $\Delta t = 0.1 \text{fs}$. Each simulation is run for 200000 time steps, i.e. for 20 ps. Figure (2) shows the temperature and bias dependence of spin relaxation for the n-doped GaAs layer. The spin polarization decreases with the increasing temperature. For a particular temperature an increase in applied field enhances the spin polarization in the system. Figure (2a) is plotted for the spin polarization (as defined by Eq (4) ) at the left end of the GaAs layer [11] whereas Fig. (2b) shows the residual spin polarization at the right end of the GaAs layer [11] after a simulation time of 20 ps. Our results agree with the experimental [1, 6] and theoretical [5, 7] results which also predict that spin relaxation time decreases with increase in the temperature of the system.

**Figure 3.** Spin polarization over the device length after 20 ps at 300 K and for varying applied bias.

**Figure 4.** Spin polarization averaged over the device vs bias after 20 ps and for three different temperatures.
In the high temperature regime, the effect of temperature on DP mechanism of spin relaxation is mainly determined by inhomogeneous broadening which is proportional to $T^3$ [7].

The spin dephasing is considerably affected by the applied fields. We note that even though the injection condition from the FM interface is 100% polarization, the spin polarization close to the FM interface is decreased to less than 80% for no applied fields due to particle diffusion. This value decreases to about 20% at the end of the device. This can be seen in Fig. (3) in which we have plotted the spin polarization over the whole length of device after 20 ps, for a temperature of 300 K and for varying applied bias. At high applied fields the spin polarization is enhanced and at the end of the simulation more spin-coherence is retained in the system (approx. 50% at the right end of the GaAs sample for a bias of 0.036 V). This seems in agreement with the high-field effect predicted in [12]. We also have calculated the average spin polarization in the system at the end of the simulation time and this is shown in Fig. (4). It is seen that for zero applied bias the system has an average of 50% spin polarization and this increases to nearly 80% for high bias (0.036 V) at 300 K. A similar trend is seen for lower temperatures but the system retains more spin-coherence in these cases, up to $\sim 85\%$ at 200 K.

5. Conclusions
Spin relaxation in GaAs has been analyzed using the ensemble Monte Carlo technique incorporating various scattering mechanisms. We have analyzed the effects of temperature and applied bias on electrically injected spin polarization. Our results show that increasing temperature reduces the spin relaxation times whereas high applied bias corresponds to a longer spin memory in the system.

6. Acknowledgments
Authors would like to thank Marco Saraniti, Jeremy Coe and Phil Hasnip for helpful discussions. The use of White Rose Grid Computational Resources at the University of York is gratefully acknowledged. This work is supported by EPSRC through grant number EP/F016719/1.

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