Investigation of Spin-Polarized Transport in GaAs Nanostructures

Brian D. Tierney†, Timothy E. Day, and Stephen M. Goodnick

Department of Electrical Engineering and Center for Solid State Electronics Research
Arizona State University, Tempe, AZ 85287-5706

e-mail: brian.tierney@asu.edu

Abstract. A spin field effect transistor (spin-FET) has been fabricated that employs nanomagnets as components of quantum point contact (QPC) structures to inject spin-polarized carriers into the high-mobility two-dimensional electron gas (2DEG) of a GaAs quantum well and to detect them. A centrally-placed non-magnetic Rashba gate controls both the density of electrons in the 2DEG and the electronic spin precession. Initial results are presented for comparable device structures modeled with an ensemble Monte Carlo (EMC) method. In the EMC the temporal and spatial evolution of the ensemble carrier spin polarization is governed by a spin density matrix formalism that incorporates the Dresselhaus and Rashba contributions to the D’yakonov-Perel spin-flip scattering mechanism, the predominant spin scattering mechanism in AlGaAs/GaAs heterostructures from 77-300K.

1. Introduction

A necessary condition toward realizing spintronic logic elements is the ability to electrically inject spin polarized carriers into the active region of the device. One such proposal incorporates a nanomagnet above a QPC structure, where the QPCs act as efficient spin filters [1], thus eliminating the need for cumbersome external magnetic fields or dilute ferromagnetic semiconductor materials. We investigate a similar scheme by fabricating a spin modulator structure utilizing magnetized split gates as QPCs, shown schematically in Fig. 1(a). The actual device is shown in Fig. 1(b).

![Fig. 1: (a) Device schematic and (b) Optical micrograph of the fabricated spin device.](image-url)
In Fig. 1, the two magnetic split-gates act as an injector and detector of spin-polarized carriers in the 2DEG structure in the GaAs quantum well. The device is predicted to exhibit a low resistance state when the magnetization vectors of the two pairs of split-gates (QPCs) are aligned and a high resistance state when anti-aligned. The centrally placed gate serves to control the density and spin precession of the spin-polarized carriers in lieu of an external magnetic field via the Rashba effect. The Rashba effect is a relativistic phenomenon in which the necessary effective in-plane magnetic field needed to lift the spin degeneracy is induced via an electric field applied normal to the plane of electron confinement, i.e., in the heterostructure growth direction.

2. Theoretical Model

An ensemble Monte Carlo (EMC) technique is used to model electronic and spin transport and the associated decay of the polarization after injection. In the EMC, the random motion of charge carriers in the semiconductor is simulated as free flights subjected to forces that accelerate the carriers during free flight, and instantaneous scattering events that randomize the velocity. The scattering rates are calculated quantum mechanically from perturbation theory [2]. In the EMC simulation the electrons in the quasi-2DEG are treated using the same multi-subband approach of earlier models [3]. 2D scattering due to polar optical and acoustic phonons are included for the quantum well electrons. Bulk mode phonons are assumed in all cases. Additionally, the simulation incorporates the Pauli Exclusion Principle in the scattering rates through a self-scattering rejection technique, allowing simulation at low temperatures.

The dominant spin relaxation mechanism in the present simulation regime is the D’yakonov-Perel mechanism. The spin polarization of each carrier is governed by a time dependent spin density matrix given as [4]

$$\rho(t) = \begin{pmatrix} 1 + P_x(t) & P_y(t) - i P_z(t) \\ P_y(t) + i P_z(t) & 1 - P_x(t) \end{pmatrix}$$

where $P_x$, $P_y$, and $P_z$ are the components of the polarization vector. For each carrier within the EMC, the density matrix given by Eq. (1) evolves in time as

$$\rho(t+\delta t) = e^{-i(H_R+H_D)\delta t/\hbar} \rho(t) e^{i(H_R+H_D)\delta t/\hbar}.$$  

(2)

The terms $H_R$ and $H_D$ in Eq. (2) refer to the Rashba and Dresselhaus contributions, respectively, to the momentum-dependent spin-splitting in the Hamiltonian. In the 2DEG, adequate approximations to the Rashba and Dresselhaus terms are typically given as [4]

$$H_R = \eta \left( k_x \sigma_z - k_y \sigma_y \right),$$  

(3)

$$H_D = \gamma \left( k_x \sigma_y - k_y \sigma_x \right).$$  

(4)

The $\vec{k}$ terms in Eqs. (3)-(4) refer to the in-plane momentum and the $\sigma$ terms are the Pauli matrices. The nature of the proportionality constant, $\eta$ in Eq. (3) is controversial [5]. It is dependent on local electric fields in the quantum well, even if only to a small extent. We thus set $\eta = \alpha E_{local}$ where $\alpha = 5.33 eV \cdot \AA^2 / V$ and $E_{local}$ is the electric field along the growth direction in the quantum well evaluated at various points along the 2DEG channel. In Eq. (4), $\gamma_i = \beta \langle k_i^2 \rangle$ where $i$ denotes the subband index and the quantity $\langle k_i^2 \rangle$ is calculated for each subband using only the equilibrium wavefunctions, as an approximation, and noting that $k \rightarrow -i \nabla z$. $\beta$ is $29 eV \cdot \AA^3$.

The coupling of Eqs. (3)-(4) to the EMC is given through the $\vec{k}$ terms. At each time-step $\delta t$ in the EMC, the $\vec{k}$ terms in Eqs. (3)-(4) are updated after a carrier undergoes momentum scattering. The quantum mechanical probability of transmission through the QPCs is given by [6]

$$T_n(E) = \frac{1}{2} e^{-\beta |E-E_n|}$$  

(6)
where 
\[ E_n(x) = E_s(1 - \alpha x^2) \]  
(7) 
assumes a quadratic subband dispersion about the center of the QPC saddle potential and \( \beta \) for the \( n^{th} \) mode is 
\[ \beta_n = \frac{2m^*}{\hbar^2 E_s}. \]  
(8)

To validate our model, we simulated the temporal evolution of the spin polarization in k-space, corresponding to the 2DEG formed in an AlGaAS/GaAs modulation doped heterostructure. In Fig. 2(a), the simulated relaxation times for various crystallographic orientations are approximately 50 ps, which are consistent with experimental data [7] for our ground state confinement energy of \( \sim 22 \) meV. In Fig. 2(b), spin relaxation rates, as determined by the EMC are compared to experimental data for various well widths. The difference between the curves is likely due to higher carrier energies in the EMC compared to those of the optically excited carriers in the experiment.

3. Device Simulation
Initially we choose to model the QPC in Fig. 3, as a comparable component of the structure depicted in Fig. 1. The 2D↔3D transitions are accounted for in similar fashion to that described in [8]. The 3D scattering mechanisms include polar optical, acoustic, inter-valley phonons and impurity scattering. The self-consistent Schrodinger-Poisson problem is solved at equilibrium to obtain the confinement energies and 2D scattering rates. The particle energies are initially given by a Maxwell-Boltzman distribution. During a fixed free-flight time step of 0.5 fs, the particles are accelerated by the electric field. After completing a free-flight, a particular type of momentum scattering may occur, depending on the probability of occurrence relative to other mechanisms and to the probability that scattering will happen after the free-flight time. The spin density matrix for each particle is updated at the end of a free-flight. Poisson’s equation is solved every few femtoseconds to update the potential. Furthermore, all injected particles are assigned a chosen spin polarization.

The decoherence of an initial 100% polarized ensemble, polarized transverse to both the transport and growth direction, is shown in Fig. 4 for the 2DEG plane of the device depicted in Fig. 3. No quantum mechanical transmission is modeled in this case. Fig. 5 depicts the polarization in the 2DEG for a QPC structurally similar to that of Fig. 3 but with a length and width of 400nm. \( V_{ds} = 0.05V, \ V_{gs} = 0.4V \) (relative to the -0.8V Schottky barrier) here. Particles at the source are initially assigned a randomly chosen \( P_y = +1 \) or -1 polarization. \( P_x, P_z \) are initially zero. The transmission coefficient formalism is utilized for particles at the center of the QPC (200nm from the source). A magnetic field of 0.5 T is assumed to exist at this point across the QPC, resulting in Zeeman splitting. The color scheme indicates the degree of \( P_y \). Spin-down particles (blue peaks) are seen to be reflected. To make spin discrimination easier to see in this initial study, the GaAs g-factor was artificially enhanced by factor of 5. However, the fast de-phasing of the transmitted spin-up particles is in part due to unpolarized particles being injected at the drain. The conductance vs. gate voltage is shown in Fig 6.
y-axis $\rightarrow$ DRAIN

Figure 5. QPC with transmission coefficient modeled. $V_{gs} = -0.4V$, $T = 77K$. Initial polarization is randomly chosen to be in the $+/\ y$ direction. Spin down particles (blue) are reflected.

Figure 6. Conductance vs. Gate Voltage for the QPC of Fig. 5 with Zeeman splitting at the QPC. Negative values are likely due to EMC noise. Further resolution and a lower temperature is needed to show possible quantized conductance.

4. Conclusion. We have fabricated a spin modulator device, currently being tested, and simulated spin-polarized transport in a QPC with a semiclassical EMC in conjunction with a quantum mechanical QPC transmission formalism. A more complete study of the QPC problem, perhaps with higher g-factor materials such as InAS will follow.

References

[1] Gilbert M J and Bird J P, *Appl. Phys. Lett.*, 77, 1050-1052.
[2] C. Jacoboni, P. Lugli, The Monte Carlo Method for Semicond. Device Sim. ,SpringeVerlag,Vienna,1989.
[3] S.M. Goodnick and P. Lugli, *Phys. Rev. B* 37, 1988, 2578-2588.
[4] S. Saikin et al., *J. Appl. Phys.*, 94, No. 3, 2003, 1769-1775.
[5] W. Zawadzki and P. Pfeffer, *Semicond. Sci. Technol.*, 19, 2004.
[6] D.K. Ferry, S.M.Goodnick, Transport in Nanostructures, Cambridge University Press, UK, 1997.
[7] A. Malinowski et al., *Phys. Rev. B*, 62, No. 19, 2000, 13034-13039
[8] H. Ueno et al.,Proceedings of Intl.Workshop on Physics and Computer Modeling of Devices Based on Low-Dimensional Structures, pp. 85-89, IEEE Computer Society Press, 1996.