Spin transport in semiconductor quantum devices

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Abstract

We augmented an ensemble Monte-Carlo semiconductor device simulator [3] to incorporate electron spin degrees of freedom using a Bloch equation model to investigate the feasibility of spintronic devices. Results are presented for the steady state polarization and polarization decay due to scattering and spin orbit coupling for a III-V MOSFET device as a function of gate voltages, injection polarization and strain.

1. Theory

Following [4] we augmented a conventional Monte Carlo simulation of an InAlAs/InGaAs HEMT to incorporate electron spin.

Spin states described by the spin density matrix \( \rho(\mathbf{r}, t) \) given by \( \rho(\mathbf{r}, t) = \rho_{\uparrow}(\mathbf{r}, t) \rho_{\downarrow}(\mathbf{r}, t) \)

Where \( \rho_{\uparrow} \) and \( \rho_{\downarrow} \) are the probabilities of finding an electron in a spin up or spin down state and the diagonal elements \( \rho_{\uparrow\uparrow} \) and \( \rho_{\downarrow\downarrow} \) represent the coherences. This can be parameterised by a spin polarization vector \( \mathbf{S} = (S_x, S_y, S_z) \) where \( S_x \), \( S_y \) and \( S_z \) represents the Pauli matrices.

Spin polarization vector of the current \( \mathbf{S} = (S_x, S_y, S_z) \) was obtained by averaging the components of the spin polarization vectors of all electrons in a thin slice through the device channel located at position \( x = x_0 \) at time \( t \).

This is done at a temperature of 300K for gate voltages varying between threshold and saturation for each device.

The exponential operator can then be written as a scattering matrices

\[ e^{-iHt} = \sum_{\alpha, \beta} \frac{1}{\sqrt{2\pi}} \int d\mathbf{k} \left[ \begin{array}{c} \rho_{\alpha\beta}(\mathbf{k}, t) \end{array} \right] e^{i\mathbf{k}\cdot\mathbf{R}} \]

where \( \mathbf{k} = (k_x, k_y, k_z) \) is the wave vector and \( \mathbf{R} \) is the position vector.

This exponential operator can then be written as a scattering matrices

\[ \rho(\mathbf{r}, t) = \frac{1}{\sqrt{2\pi}} \int d\mathbf{k} \left[ \begin{array}{c} \rho_{\alpha\beta}(\mathbf{k}, t) \end{array} \right] e^{i\mathbf{k}\cdot\mathbf{r}} \]

Dyakonov-Perel-type spin dephasing was modelled using interaction Hamiltonians. For a structure was obtained by averaging the components of the spin polarization vectors of all electrons in a thin slice through the device channel located at position \( x = x_0 \) at time \( t \).

2. Method

The spin-augmented device simulator was used to simulate spin transport in an InGaAs/InAlAs MOSFET similar to those used in [3] (see Figs 10a) and 1b). The spin orbit coupling constant \( \Gamma = 2.56 \) eV nm and \( \Gamma = 0.56 \) eV nm for the unstrained case were obtained from the \( \Gamma \) calculations detailed in Section 4. The electrons were initially randomly polarised with the Bloch vectors evenly distributed across a sphere in real space caused by hyperfine coupling, based on the observation that Dyakonov-Perel mechanism is the dominant source of spin relaxation in GaAs[2] although such effects could easily be incorporated into the simulator.

3. Spin Transport Simulation Results

4. Strain effects

The effects of mechanical strain on the spin were investigated by means of \( \rho \) band-structure calculations. The method involves using Landau-Doppler perturbation theory to solve the Schrödinger equation about a point of high symmetry for a finite number of bands, accounting for the contribution from band interactions using physical parameters called Kane parameters for band contributions with Luttinger parameters obtained from experimental data.

Adaptation for strain: Following Bir, Pokus and Bühner [1]. An extra term is added to each element of the unstrained Hamiltonian created by replacing \( \rho_{\alpha\beta} \) and \( (\alpha', \beta') \) with \( \rho_{\alpha\beta} \) and \( (\alpha', \beta') \) unperturbed wave functions for each device.

Spin-Orbit Coupling: After calculating the band energies as a function of applied strain. The Dresselhaus and Rashba constants can be approximated using the inter-band energies at the \( \Gamma \) point along with 3 Kane parameters [2].

We investigated the effects of strain by calculating the change in spin orbit coupling for applied strain in three crystallographic directions [001], [110] and [111] corresponding to a lattice difference of between \( \Gamma \) and \( \Gamma \) of the unstrained lattice, the results from this are plotted in Figure 6.

5. Conclusion and Outlook

We have demonstrated the successful inclusion of electron spin into a realistic model of a transistor. Figure 4 shows that the average magnetisation starts off at a high value at the source which rapidly decays as the elecrons pass through the channel, followed by a partial magnetisation recovery due to spin refocusing as the electrons slow down to enter the drain. From Figure 4a) we see the magnetisation is sensitive to changes in gate voltages and to a lesser extent source-drain voltage this gives us a potential handle for control as the amount of magnetisation detected at the drain can be controlled by varying the gate voltage.

Mechanical strain also has a large effect on the spin as the increasing strain changes the symmetries of both the lattice and quantum well increasing the amount of spin orbit coupling. This strain sensitivity has the potential to be used in a sensor whereby measuring the spin at the drain gives an indirect measure of the amount of molecular strain in the channel.

Future work is now under way to investigate spin transport in different materials such as Si and the effects of low temperatures on the magnetisation decay and recovery.

References


Figure 1: (a) 3D model of InGaAs/InAlAs MOSFET device showing spin polarization of electrons along n-channel with \( (\uparrow \downarrow, \uparrow \downarrow) \) spin in the [001], [110] and [111] directions. (b) Cross section of the 25 nm gate length, n-channel InGaAs/InAlAs MOSFET.

Figure 2: Plots of the I-V characteristic and confinement potential obtained from the III-V MOSFET simulation.

Figure 3: Magnetisation \( |\delta| \) at the drain edge \( (r = 20\, \text{nm}) \) see Figure 1(b) and azimuth angle \( \theta \) (rotation in the x-y plane) as a function of gate voltage.

Figure 4: Magnetization vs position along the channel for varying Gate and Source-Drain voltages for x-polarized spin injection taken at \( t = 5\, \text{ps} \), i.e. after a steady state was reached.

Figure 5: (a) Magnetization vs Gate voltage and (b) Magnetization vs source-drain voltage.

Figure 6: (a) Magnetisation \( |\delta| \) at the drain edge \( (r = 20\, \text{nm}) \) see Figure 1(b) and azimuth angle \( \theta \) (rotation in the x-y plane) as a function of applied uniaxial strain in the [001], [110] and [111] directions.

Figure 7: Rashba and Dresselhaus mean field vectors \( \mathbf{H}_R \) and \( \mathbf{H}_D \) obtained by averaging over all particles in this slice across the channel for a single Monte Carlo run \( (\rho_{\uparrow}, \rho_{\downarrow}) \). The z-axis is in-plane perpendicular to the channel but for the vector plots the axes have been rotated so that \( \mathbf{x} \) is in the vertical direction for visual clarity.

Figure 8: Rashba and Dresselhaus mean field vectors \( \mathbf{H}_R \) and \( \mathbf{H}_D \) obtained by averaging over all particles in this slice across the channel for a single Monte Carlo run \( (\rho_{\uparrow}, \rho_{\downarrow}) \). The z-axis is in-plane perpendicular to the channel but for the vector plots the axes have been rotated so that \( \mathbf{x} \) is in the vertical direction for visual clarity.

Figure 9: (a) Magnetization vs position along the channel for varying Gate and Source-Drain voltages for x-polarized spin injection taken at \( t = 5\, \text{ps} \), i.e. after a steady state was reached.