

# Spin Transport in Nanowires

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## Abstract

We study high-field spin transport of electrons in a quasi one-dimensional channel of a *GaAs* gate controlled spin interferometer (SPINFET) using a semiclassical formalism (spin density matrix evolution coupled with Boltzmann transport equation). Spin dephasing (or depolarization) is predominantly caused by D'yakonov-Perel' relaxation associated with momentum dependent spin orbit coupling effects that arise due to bulk inversion asymmetry (Dresselhaus spin orbit coupling) and structural inversion asymmetry (Rashba spin orbit coupling). Spin dephasing length in a one dimensional channel has been found to be an order of magnitude higher than that in a two dimensional channel. This study confirms that the ideal configuration for a SPINFET is one where the ferromagnetic source and drain contacts are magnetized along the axis of the channel. The spin dephasing length in this case is about  $22.5\mu\text{m}$  at lattice temperature of 30K and  $10\mu\text{m}$  at lattice temperature of 77K for an electric field of 2kV/cm. Spin dephasing length has been found to be weakly dependent on the driving electric field and strongly dependent on the lattice temperature.

## 1 Introduction

Spin transport in semiconductor nanostructures has attracted significant research interest due to its promising role in implementing novel devices which operate at decreased power level and enhanced data processing speed. Additionally, spin is considered to be the ideal candidate for encoding qubits in quantum logic gates [3] because spin coherence time in semiconductors [2] is much longer than charge coherence time [4].

In this paper, we study spin transport of electrons in a quasi one-dimensional structure. In the past, we established [14] that in a SPINFET configuration where the ferromagnetic source and drain contacts are magnetized *along* the axis of the quasi one-dimensional channel, the spin dephasing time ( $\tau_s$ ) is about 3 ns for an electric field of 2kV/cm and 10 ns for an electric field of 100V/cm, at a (lattice) temperature of 30K. Spin dephasing time was much less when the contacts were magnetized along any other direction. In the present work, we highlight the spatial variation of spin polarization along the channel for this “large  $\tau_s$ ” configuration using a multi-subband Monte Carlo simulator.

This paper is organized as follows: in the next section, we describe the theory followed by a brief description of the Monte Carlo simulator in section III and results in section IV. Finally we conclude in section V.

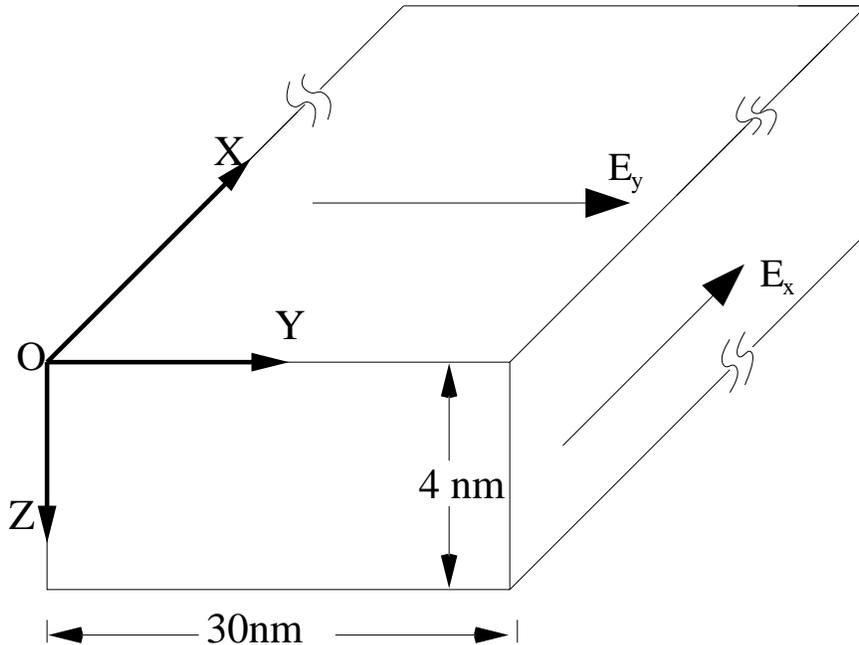


Figure 1: Geometry of the nanowire and axis designation (not drawn to scale)

## 2 Theory

Fig.1 shows the schematic of the quasi one-dimensional semiconductor structure. An electric field  $E_x$  is applied along the axis of the quantum wire to induce current flow. In addition, there could be another transverse field  $E_y$  to cause Rashba spin-orbit interaction. Such a field is indeed present in some spintronic devices e.g. a spin interferometer proposed in [7]. Spin polarized electrons are injected at one end of the wire from a half-metallic contact with the spin vector oriented along the wire axis. Our goal is to investigate how the injected spin polarization decays along the channel as the electrons traverse the quantum wire under the influence of electric fields  $E_x$  and  $E_y$  while being subjected to various elastic and inelastic scattering events.

In reality, the spin and spatial wavefunctions of the electrons are coupled together via *spin-orbit coupling* Hamiltonian and hence spin dephasing (or depolarization) rates are functionals of the electron distribution function in momentum space. The distribution function in momentum space continuously evolves with time when an electric field is applied to drive transport. Thus, the dephasing rate is a dynamic variable that needs to be treated self-consistently in step with the dynamic evolution of the electrons' momenta. Such situations are best treated by Monte Carlo simulation.

Following Saikin [12], we describe electron's spin by standard spin density matrix formalism [6]:

$$\rho_\sigma(t) = \begin{bmatrix} \rho_{\uparrow\uparrow}(t) & \rho_{\uparrow\downarrow}(t) \\ \rho_{\downarrow\uparrow}(t) & \rho_{\downarrow\downarrow}(t) \end{bmatrix} \quad (1)$$

which is related to the spin polarization component as

$$S_n(t) = Tr(\sigma_n \rho_\sigma(t)) \quad (2)$$

where  $n = x, y, z$  and  $\sigma_n$  denotes Pauli spin matrices. We *assume* that in a small time interval  $\delta t$  no scattering takes place and the electron accelerates very slowly due to the driving electric field

(in other words,  $E_x \delta t$  is sufficiently small). During this interval  $\delta t$  we describe electron's transport by a constant "average wavevector":

$$k = \frac{k_{initial} + k_{final}}{2} = k_{initial} + \frac{qE_x \delta t}{2\hbar} \quad (3)$$

During this interval, the spin density matrix undergoes a unitary evolution according to

$$\rho_\sigma(t + \delta t) = e^{-\frac{iH_{so}(k)\delta t}{\hbar}} \rho_\sigma(t) e^{\frac{iH_{so}(k)\delta t}{\hbar}}, \quad (4)$$

where  $H_{so}(k)$  is the momentum dependent Hamiltonian that has two main contributions due to the bulk inversion asymmetry (Dresselhaus interaction) [8]

$$H_D(k) = -\beta \langle k_y^2 \rangle k \sigma_x, \quad (k \equiv k_x) \quad (5)$$

and the structural inversion asymmetry (Rashba interaction) [11]

$$H_R(k) = -\eta k \sigma_z. \quad (6)$$

The constants  $\beta$  and  $\eta$  depend on the material and, in case of  $\eta$ , also on the external electric field  $E_y$  that breaks inversion symmetry. Equation (4) describes a rotation of the average spin vector about an effective magnetic field given by the magnitude of the average wavevector ( $k$ ) during the time interval  $\delta t$ . The assumption of constant  $k$  implies that spin dynamics is coherent during  $\delta t$  and there is no dephasing (reduction of magnitude) since the evolution is *unitary*. However, the electric field  $E_x$  changes the value of the average wavevector  $k$  from one interval to the other. Also, the stochastic scattering event that takes place between two successive intervals changes the value of  $k$ . These two factors produce a distribution of spin states that results in effective dephasing. Thus the evolution of the spin polarization vector  $\vec{S}$  (with components  $S_x$ ,  $S_y$  and  $S_z$ ) can be viewed as coherent motion (rotation) coupled with dephasing/depolarization (reduction in magnitude). This type of dephasing is the D'yakonov-Perel' relaxation which is a dominant mechanism for spin dephasing in one-dimensional structures.

Another spin dephasing mechanism is the Elliott-Yafet relaxation [9] which causes instantaneous spin flip during a momentum relaxing scattering. However, in quasi one-dimensional structures momentum relaxing events are strongly suppressed because of the one-dimensional constriction of phase space for scattering. So we can neglect this effect as a first approximation.

The third important spin dephasing mechanism, known as Bir-Aronov-Pikus mechanism accrues from exchange coupling between electrons and holes. This effect is absent in unipolar transport.

Apart from these three, spin relaxation may take place due to magnetic field caused by local magnetic impurities, nuclei spin and other spin orbit coupling effects. However, in this work we consider only the D'yakonov-Perel' mechanism which is the most important spin dephasing mechanism in quantum wires of technologically important semiconductors like *GaAs*.

We can recast (4) in the following form for the temporal evolution of the spin vector:

$$\frac{d\vec{S}}{dt} = \vec{\Omega} \times \vec{S}. \quad (7)$$

where the so-called "precession vector"  $\vec{\Omega}$  has two components  $\Omega_D(k)$  and  $\Omega_R(k)$  due to the bulk inversion asymmetry (Dresselhaus interaction) and the structural inversion asymmetry (Rashba interaction) respectively:

$$\Omega_D(k) = \frac{2a_{42}}{\hbar} \left( \frac{\pi}{W_z} \right)^2 k \quad (8)$$

$$\Omega_R(k) = \frac{2a_{46}}{\hbar} E_y k \quad (9)$$

where  $a_{42}$  and  $a_{46}$  are material constants and  $W_z$  is the dimension of the wire along  $z$  direction. In our work we take  $a_{42} = 2 \times 10^{-29}$  eV-m<sup>3</sup>,  $a_{46} = 4 \times 10^{-38}$  C-m<sup>2</sup> and  $E_y = 100$  kV/cm which are reasonable for *GaAs* – *AlGaAs* heterostructures. Solution of (7) is straightforward and analytical expressions for  $S_x(t)$ ,  $S_y(t)$  and  $S_z(t)$  can be obtained quite easily (see [14]). We note that spin is conserved for every individual electron during  $\delta t$ , i.e.

$$S_x^2(t + \delta t) + S_y^2(t + \delta t) + S_z^2(t + \delta t) = S_x^2(t) + S_y^2(t) + S_z^2(t) \quad (10)$$

### 3 Monte Carlo Simulation

The average value of the wavevector in a time interval  $\delta t$  depends on the initial value of the wavevector  $k_{initial}$  at the beginning of the interval. Intervals are chosen such that a scattering event can occur only at the beginning or end of an interval. The choice of scattering events and the wavevector state after the event (i.e. the time evolution of the wavevector) are found from a Monte Carlo solution of the Boltzmann transport equation in a quantum wire [1]. The following scattering mechanisms are included: surface optical phonons, polar and non-polar acoustic phonons and confined polar optical phonons. A multi-subband simulation is employed; upto six subbands can be occupied in the  $y$  direction and only one transverse subband is occupied along the  $z$  direction even for the highest energy an electron can reach. This is because the width of the wire ( $y$ -dimension) in our simulation is 30 nm and the thickness ( $z$  dimension) is only 4 nm. Hard wall boundary conditions are applied. The details of the simulator can be found in [1].

We solve (7) directly in the Monte Carlo simulator. The simulation has been carried out in the absence of any external magnetic field, although the Monte Carlo simulation allows inclusion of such a field.

### 4 Results and Discussion

We consider the case when the electrons are injected at the left end ( $x = 0$ ) of the quantum wire with their spins initially polarized along the axis of the wire (i.e along  $x$  axis). In order to maintain current continuity, as soon as an electron exits from the right end of the wire, it is re-injected at the left end. The spin polarization of this electron is re-oriented along  $x$  direction.

#### 4.1 Effect of driving electric field:

In Fig.2, we show how the magnitude of the “average spin vector”  $\langle S \rangle$  (defined later) decays along the channel for four different values of the driving electric field  $E_x$ . For this study, we have set lattice temperature = 30K and length of the channel = 40  $\mu$ m.

The quantity  $\langle S \rangle$  is calculated as follows: at each point  $x$  along the channel we compute “ensemble average” of the spin components during the entire evolution time  $T$ . Mathematically, this can be expressed as

$$\langle S_i \rangle(x, T) = \frac{\sum_{t=0}^T \sum_{n=1}^{n_x(x,t)} S_{i,n}(t)}{\sum_{t=0}^T n_x(x, t)}. \quad (11)$$

Here  $i$  denotes the components  $x$ ,  $y$  and  $z$ ,  $n_x(x, t)$  denotes number of electrons in a bin of size  $\delta x$  centered around  $x$  at time  $t$ ,  $S_{i,n}(t)$  denotes the  $i$  th component of spin corresponding to the  $n$  th electron and is derived from equation (7). The “average spin vector” is defined as:

$$\langle S \rangle(x, T) = \left[ \langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 \right]^{\frac{1}{2}} \quad (12)$$

Fig.2 is the snapshot of this “time-averaged ensemble spin polarization” ( $\langle S \rangle$ ) along the channel for  $T = 5$  ns. It has been found (though not shown) that  $\langle S \rangle$  is almost independent of the evolution time  $T$  for  $T \geq 5$  ns. So we can deem Fig.2 as “steady state” spin polarization along the channel.

We note that the decay characteristic resembles an exponential trend. Therefore we define the spin dephasing length ( $l_s$ ) as the distance (measured from left end) where  $\langle S \rangle$  decays to  $\frac{1}{e}$  times its initial value of 1. For  $E_x = 2$  kV/cm (or voltage across the channel =  $V_{DS} = 8$  volts),  $l_s \sim 22.5\mu\text{m}$ .

Earlier, spin transport of electrons in III-V semiconductor quantum well and heterostructures was carried out by Bournel et al. [15] and Privman et al. [12, 13]. Typical spin dephasing length was found to be  $\sim 1\mu\text{m}$ . In our present study we observe *an order of magnitude increase* in spin dephasing length. This is due to suppression of momentum relaxing events in one dimension (i.e. electron-phonon scattering) that also suppresses D’yakonov-Perel’ spin relaxation.

We also note from Fig.2 that spin polarization along the channel is weakly dependent on driving electric field  $E_x$ . At higher applied voltage (e.g.  $E_x = 4$  kV/cm), drift velocity is larger compared to the case when  $E_x = 2$  kV/cm. This effect leads to slight increase in the spin dephasing length. Also at high electric field, scattering probability increases which tends to decrease the spin dephasing length. We observe that for  $E_x = 6$  kV/cm or 8 kV/cm the later effect dominates over the first, leading to smaller  $l_s$ .

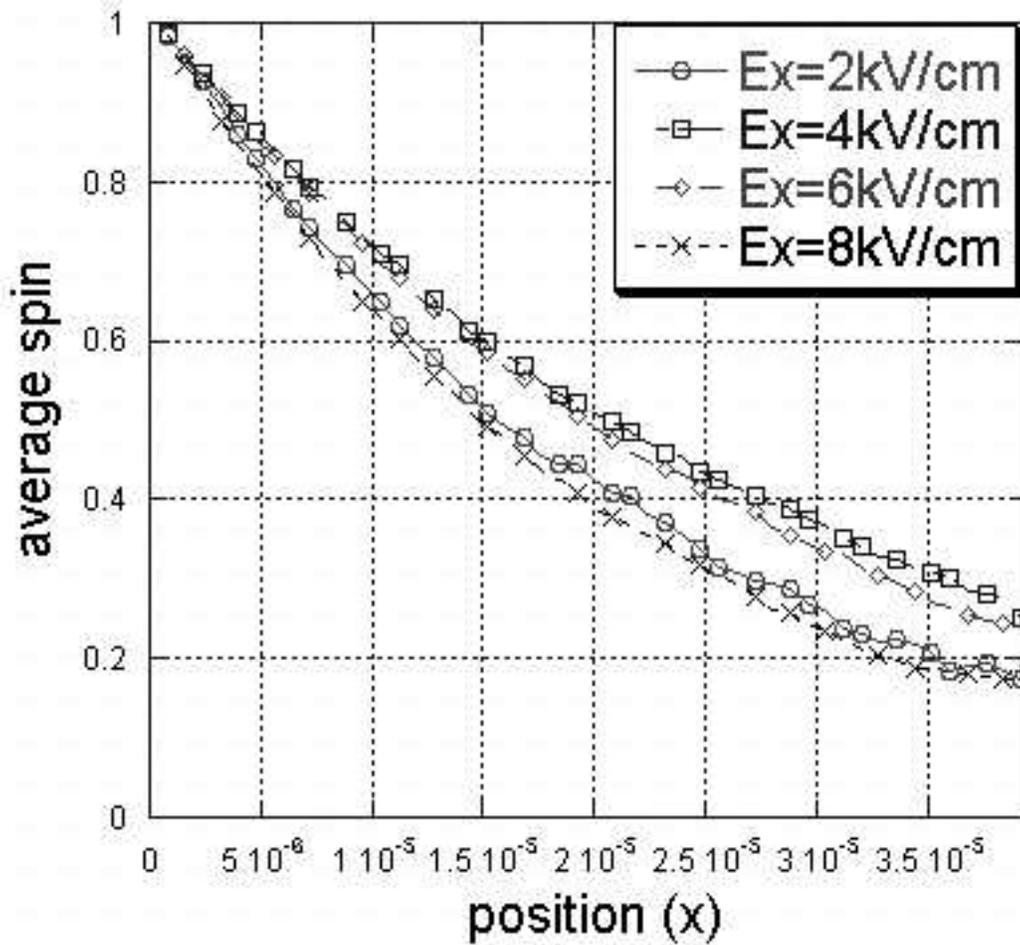


Figure 2: Spatial dephasing of ensemble average spin vector in *GaAs* quantum wire at 30K for various driving electric fields. Spins are injected with their polarization initially aligned along the wire axis. Position  $x$  is measured in meters.

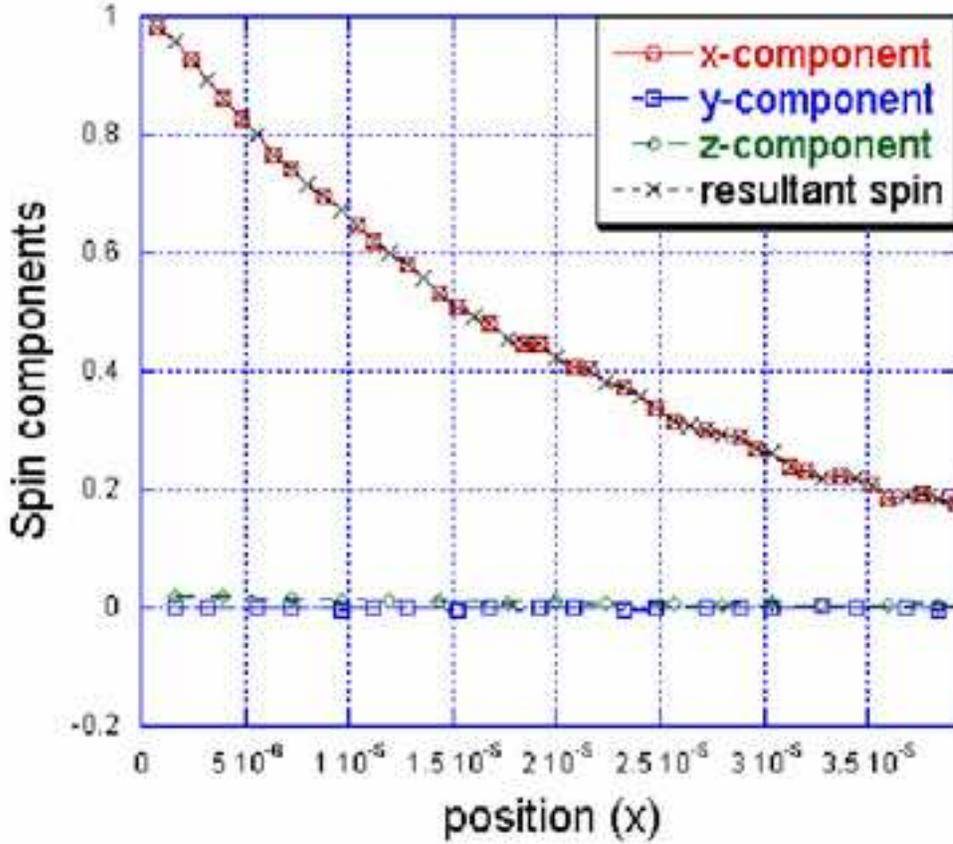


Figure 3: Spatial dephasing of the  $x$ ,  $y$  and  $z$  components of spin in the  $GaAs$  quantum wire structure at 30K. The driving electric field ( $E_x$ ) is 2kV/cm and the spins are injected with their polarization initially aligned along the wire axis. Position  $x$  is measured in meters.

#### 4.2 Decay of spin components:

Fig.3 shows how the average spin components (defined as  $\langle S_i \rangle$  in (11)) decay along the channel. The driving electric field  $E_x = 2\text{kV/cm}$  and the lattice temperature is 30K. Since, initially the spin is polarized along the  $x$  direction, the ensemble averaged  $y$  and  $z$  components remain near zero and the ensemble averaged  $x$  component decays along the channel. The decay of the ensemble averaged  $x$  component is indistinguishable from the decay of  $\langle S \rangle$  (defined in (12)) shown in Fig.3.

It is interesting to note that the spatial decay of the  $x$  component along the channel is monotonic with no hint of any oscillatory component which generally manifests for  $y$  and  $z$  polarized injections (not shown in this paper but see [14]). The oscillatory component is a manifestation of the coherent dynamics (spin rotation) while the monotonic decay is a result of incoherent dynamics (spin dephasing or depolarization). There is a competition between these two dynamics determined by the relative magnitudes of the rotation rate ( $\Omega$ ) and the dephasing rate. For the  $x$  component, the rotation rate is weak because it is solely due to Rashba interaction which is weak. Hence the dephasing dynamics wins handsomely resulting in no oscillatory component.

## 5 Conclusion

In this paper, we have shown how spin dephases in a quasi one dimensional structure. It has been found that the spin dephasing length is  $\sim 10\mu\text{m}$  in a *GaAs* 1-D channel at liquid nitrogen temperature which is an *order of magnitude* improvement over two dimensional channels. This effect can be exploited in the design of a gate controlled spin interferometer where the suppression of spin dephasing is a critical issue.

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