# Efficient Simulations of the Transport Properties of Spin Field-Effect Transistors Built on Silicon Fins

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**Abstract.** Significant progress in integrated circuits performance has been supported by the miniaturization of the transistor feature size. With transistor scalability gradually slowing down new concepts have to be introduced in order to maintain the computational speed increase at reduced power consumption for future micro- and nanoelectronic devices. A promising alternative to the charge degree of freedom currently used in MOSFET switches is to take into account the spin degree of freedom. We computationally investigate transport properties of ballistic spin field-effect transistors (SpinFETs). These simulations require a significant amount of computational resources. To achieve the best performance of calculations we parallelize the code for a shared-memory multi-CPU system. As the result of the optimization of the whole model a significant speed-up in calculations is achieved. We demonstrate that the [100] oriented silicon fins are best suited for practical realizations of a SpinFET.

## 1 Introduction

The outstanding increase of the computational speed in present integrated circuits is supported by the continuing miniaturization of the semiconductor device feature size. With scaling approaching its physical limits, the semiconductor industry is facing the challenge to introduce new innovative elements to increase integrated circuit performance. Employing spin as an additional degree of freedom is promising for boosting the efficiency of future low-power integrated electronic circuits. Indeed, the spin of an electron can change its orientation to opposite very fast by consuming an amazingly small amount of energy. Thus utilizing spin properties for future microelectronic devices opens a great opportunity to reduce power consumption.

The spin field-effect transistor is a future semiconductor spintronic device promising a performance superior to that achieved in the present transistor technology. SpinFETs are composed of two ferromagnetic contacts (source and drain) connected to the semiconductor channel. The ferromagnetic source (drain) contact injects (detects) spin-polarized electrons to (from) the semiconductor region.

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Thus ferromagnetic contacts play the role of polarizer and analyzer for the electron spin as described by Datta and Das [1]. Because of the non-zero spin-orbit interaction the electron spin precesses during the propagation through the channel. At the drain contact only the electrons with the spin aligned to the drain magnetization can leave the channel and contribute to the current. Current modulation is achieved by changing the strength of the spin-orbit interaction in the semiconductor region and thus the degree of the spin precession. The strength of the spin-orbit interaction can be controlled by applying the external gate voltage which introduces the structural inversion asymmetry. This is the dominant mechanism of the spin-orbit interaction in confined structures of III-V semiconductors. The corresponding effective Hamiltonian is in the Rashba form [2]

$$H_R = \frac{\alpha_R}{\hbar}(p_x\sigma_y - p_y\sigma_x), \tag{1}$$

where $\alpha_R$ is the effective electric field-dependent parameter of the spin-orbit interaction, $p_{x(y)}$ is the electron momentum projection on the $x(y)$ axis, $\sigma_x$ and $\sigma_y$ are the Pauli matrices.

Silicon is characterized by a weak spin-orbit interaction and long spin life time. It is therefore an attractive material for spin-driven applications. However, because of the weak spin-orbit interaction, silicon was not considered as a candidate for the SpinFET channel material. Recently it was shown [3] that thin silicon films in the SiGe/Si/SiGe structures have enhanced values of the spin-orbit interaction. It turns out, however, that the Rashba spin-orbit interaction in confined silicon structures is relatively weak and is approximately ten times smaller than the value of the dominant contribution which is of the Dresselhaus type with a corresponding effective Hamiltonian in the form

$$H_D = \frac{\beta}{\hbar}(p_x\sigma_x - p_y\sigma_y). \tag{2}$$

This term is due to interfacial disorder induced inversion symmetry breaking and depends almost linearly on the effective electric field [4]. For a built-in field of 50kV/cm, the strength of the Dresselhaus spin-orbit interaction is found to be $\beta \approx 2\mu$eVnm, which is in agreement with the value found experimentally [5], while $\alpha_R \approx 0.1\mu$eVnm. This value of the spin-orbit interaction in confined silicon systems is sufficient for application as SpinFET channels.

To calculate properties of the spin field-effect transistor we consider a model similar to [6,7]. Contrary to [6,7] we introduce the spin-orbit interaction in the Dresselhaus form. The effective mass Hamiltonian for the source and the drain contacts is taken in the form

$$\hat{H}_{source} = \frac{\hat{p}_x^2}{2m_f^*} + h_0\hat{\sigma_z}, \quad x < 0, \tag{3}$$

$$\hat{H}_{drain} = \frac{\hat{p}_x^2}{2m_f^*} \pm h_0\hat{\sigma_z}, \quad x > L, \tag{4}$$

where $m_f^*$ is the effective mass in the contacts, $h_0$ is the exchange splitting energy, and $\hat{\sigma_z}$ is the Pauli matrix; $\pm$ in (4) stands for the parallel and antiparallel configuration of the contact magnetization, respectively. For the silicon region the Hamiltonian reads

$$\hat{H}_S = \frac{\hat{p}_x^2}{2m_s^*} + \delta E_c - \frac{\beta}{\hbar}\hat{\sigma}_x \hat{p}_x + \frac{1}{2} g\mu_B B \hat{\sigma}^*, \tag{5}$$

for [100] oriented fins and

$$\hat{H}_S = \frac{\hat{p}_x^2}{2m_n^*} + \delta E_c - \frac{\beta}{\hbar}\hat{\sigma}_y \hat{p}_x + \frac{1}{2} g\mu_B B \hat{\sigma}^*, \tag{6}$$

for [110] oriented fins. Here $m_n^*$ is the subband effective mass, $\delta E_c$ is the band mismatch between the ferromagnetic and the silicon region, $\beta$ is the strength of the spin-orbit interaction, $g$ is the Landé factor, $\mu_B$ is the Bohr magneton, $B$ is the magnetic field, and $\hat{\sigma}^* \equiv \hat{\sigma}_x cos\gamma + \hat{\sigma}_y sin\gamma$ with $\gamma$ defined as the angle between the magnetic field and the transport direction.

To calculate the dependence of the transport properties on the spin-orbit interaction, we need the electron eigenfunctions in the ferromagnetic and the semiconductor regions. We are looking for a wave function in the left contact in the following form

$$\Psi_L(x) = (e^{ik_\uparrow x} + R_\uparrow e^{-ik_\uparrow x})\begin{pmatrix}1\\0\end{pmatrix} + R_\downarrow e^{-ik_\downarrow x}\begin{pmatrix}0\\1\end{pmatrix}, \tag{7}$$

$$\Psi_L(x) = R_\uparrow e^{-ik_\uparrow x}\begin{pmatrix}1\\0\end{pmatrix} + (e^{ik_\downarrow x} + R_\downarrow e^{-ik_\downarrow x})\begin{pmatrix}0\\1\end{pmatrix}, \tag{8}$$

where (7) describes a spin-up induced electron and (8) describes a spin-down induced electron, $k_{\uparrow(\downarrow)}$ is the wave vector of the spin-up(spin-down) electron, $R_{\uparrow(\downarrow)}$ are the corresponding reflection coefficients. For the right contact the wave function is given by

$$\Psi_R(x) = C_\uparrow e^{ik_\uparrow x}\begin{pmatrix}1\\0\end{pmatrix} + C_\downarrow e^{ik_\downarrow x}\begin{pmatrix}0\\1\end{pmatrix}, \tag{9}$$

where $C_\uparrow(\downarrow)$ are the transmission amplitudes. For the silicon region the wave function can be written as

$$\psi_S(x) = A_+ e^{ik_{x1}^{(+)}x}\begin{pmatrix}k_1\\1\end{pmatrix} + B_+ e^{ik_{x2}^{(+)}x}\begin{pmatrix}k_2\\1\end{pmatrix} \tag{10}$$

$$+ A_- e^{ik_{x1}^{(-)}x}\begin{pmatrix}k_3\\-1\end{pmatrix} + B_- e^{ik_{x2}^{(-)}x}\begin{pmatrix}k_4\\-1\end{pmatrix}, \tag{11}$$

where $k_{x1(2)}^{+(-)}$ are the wave vectors corresponding to the Hamiltonian (5) in case of a [100]-oriented fin or (6) in case of a [110]-oriented fin. The coefficients $k_1, k_2, k_3, k_4$ are calculated depending on the fin orientation. For a [100]-oriented fin the coefficients are

$$k_1 = -\frac{\frac{iBg\mu_B \sin(\gamma)}{2} - \frac{Bg\mu_B \cos(\gamma)}{2} + \beta k_{x1}^{(+)}}{\sqrt{\left(\frac{Bg\mu_B \cos(\gamma)}{2} - \beta k_{x1}^{(+)}\right)^2 + \left(\frac{Bg\mu_B \sin(\gamma)}{2}\right)^2}}, \tag{12}$$

$$k_2 = -\frac{\frac{iBg\mu_B \sin(\gamma)}{2} - \frac{Bg\mu_B \cos(\gamma)}{2} + \beta k_{x2}^{(+)}}{\sqrt{\left(\frac{Bg\mu_B \cos(\gamma)}{2} - \beta k_{x2}^{(+)}\right)^2 + \left(\frac{Bg\mu_B \sin(\gamma)}{2}\right)^2}}, \tag{13}$$

$$k_3 = \frac{\frac{iBg\mu_B \sin(\gamma)}{2} - \frac{Bg\mu_B \cos(\gamma)}{2} + \beta k_{x1}^{(-)}}{\sqrt{\left(\frac{Bg\mu_B \cos(\gamma)}{2} - \beta k_{x1}^{(-)}\right)^2 + \left(\frac{Bg\mu_B \sin(\gamma)}{2}\right)^2}}, \tag{14}$$

$$k_4 = \frac{\frac{iBg\mu_B \sin(\gamma)}{2} - \frac{Bg\mu_B \cos(\gamma)}{2} + \beta k_{x2}^{(-)}}{\sqrt{\left(\frac{Bg\mu_B \cos(\gamma)}{2} - \beta k_{x2}^{(-)}\right)^2 + \left(\frac{Bg\mu_B \sin(\gamma)}{2}\right)^2}}. \tag{15}$$

We compute the current through the device as

$$\begin{aligned} I^{P(AP)} =& \frac{e^2}{h} \int_{\delta E}^{\infty} \left[ T_{\uparrow}^{P(AP)}(E) + T_{\downarrow}^{P(AP)}(E) \right] \\ & \left\{ \frac{1}{1 + e^{\frac{E - E_F}{kT}}} - \frac{1}{1 + e^{\frac{E - E_F + eV}{kT}}} \right\} dE, \end{aligned} \tag{16}$$

where $k$ is the Boltzmann constant, $T$ is the temperature, and $V$ is the voltage. The transmission coefficients are determined by applying the standard boundary conditions at the ferromagnetic/silicon interfaces. The spin-up ($T_{\uparrow}^{P}$) and spin-down ($T_{\downarrow}^{P}$) transmission coefficients for the parallel configuration of the contact magnetization are defined as

$$T_{\uparrow}^{P} = |C_{\uparrow}|^2 + \frac{k_{\downarrow}}{k_{\uparrow}} |C_{\downarrow}|^2, \tag{17}$$

$$T_{\downarrow}^{P} = \frac{k_{\uparrow}}{k_{\downarrow}} |C_{\uparrow}|^2 + |C_{\downarrow}|^2. \tag{18}$$

For the anti-parallel configuration of the contact magnetization the transmission probabilities are given by

$$T_{\uparrow}^{AP} = \frac{k_{\downarrow}}{k_{\uparrow}} |C_{\uparrow}|^2 + |C_{\downarrow}|^2, \tag{19}$$

$$T_{\downarrow}^{AP} = |C_{\uparrow}|^2 + \frac{k_{\uparrow}}{k_{\downarrow}} |C_{\downarrow}|^2. \tag{20}$$

The conductance is defined as

$$G^{P(AP)} = \lim_{V \to 0} \frac{I^{P(AP)}}{V}. \tag{21}$$

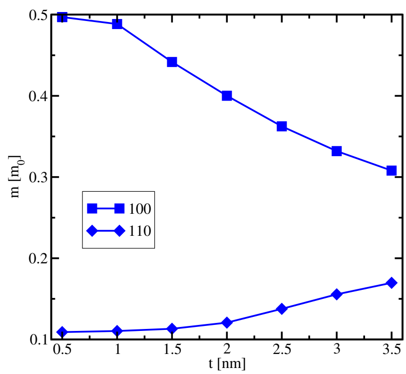


**Fig. 1.** Ground subband effective mass dependence on t in [100] and [110] fins

Finally, the tunneling magnetoresistance (TMR) is defined as

$$\mathrm{TMR} \equiv \frac{G^P - G^{AP}}{G^{AP}}. \tag{22}$$

## 2 Simulations

We investigate the dependence of the conductance through the silicon SpinFET on the physical parameters. In order to calculate the conductance one has to determine the wave vectors, compose the system of equations corresponding to the boundary conditions, and solve the obtained system of linear equations to determine the transmission coefficients for the spin-up and spin-down electrons. These calculations must be performed for the parallel and the anti-parallel configuration of the contact magnetization for each energy point of the half-infinite integrand (16). It follows from (21) that the integral evaluated numerically describes the conductance for a single point of the conduction band mismatch $\delta E_c$, at a single value of temperature $T$. Thus to investigate the transport properties of the silicon SpinFET at various parameter values a huge amount of calculations must be carried out. To reduce the simulation time the code for the model must be heavily optimized and parallelized.

The usual techniques for parallelization are divided into two groups - parallelization in case of shared-memory and parallelization in case of distributed memory systems. The advantage of shared-memory parallelization is that it guarantees uniform access to the memory for each process. This means that the time spent for data manipulation in the memory is approximately the same for each process. The advantage of distributed calculations is that the number of processors used for the calculations is not limited to the number of processors on a single node. In our simulations the code is parallelized with the OpenMP library. Because of the absence of the correlation between the conductances at different energy points the whole calculations are distributed between a large number of

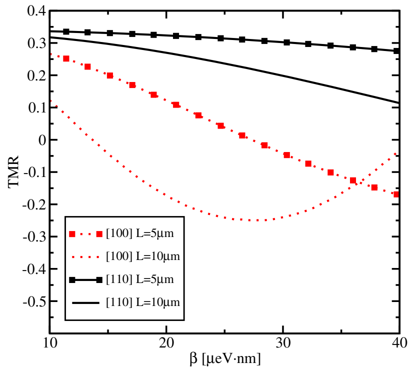


**Fig. 2.** Tunneling magnetoresistance dependence on the value of the Dresselhaus spin-orbit interaction for a magnetic field orthogonal to the transport direction. The source and the drain contact polarization $P$ =0.4, the delta-function barrier strength $z$ =5.

computing threads. Thus the time spent for the calculations is reduced proportionally to the number of parallel threads. Although threads perform calculations in parallel, the time spent by each thread to fulfill the tasks is not the same. Therefore one has to take proper care of a uniform distribution of the computational load between the threads. This problem is crucial for obtaining the maximum possible speed-up. Since OpenMP provides a possibility to control the amount of calculations for each thread in the run-time mode, the problem of the uniform distribution of the computational load is solved by standard tools.

## 3 Results

We have improved the performance of the code by utilizing the OpenMP approach. The results of using the parallel implementation are presented in Table 1. The actual speedup of the code is very close to the ideal speedup, in which the increase of the number of processors (cores) twice leads to the decrease in the computing time twice, due to the already mentioned fact that there is no correlation between the calculations of the conductances.

Calculations in the presence of temperature require high accuracy. Therefore, the adaptive methods from the GNU Scientific Library [8] have been used for the numerical integration.

We consider square silicon fins with [100] or [110] orientation, with (001) horizontal faces. The parabolic band approximation is not sufficient in thin and narrow silicon fins. In order to compute the subband structure in silicon fins we employ the two-band **k·p** model, which has been shown to be accurate up to 0.5eV above the conduction band edge. The resulting Schrödinger differential equation, with the confinement potential appropriately added in the Hamiltonian, is discretized using the box integration method and solved for each value of the conserved momentum $p_x$ along the current direction using efficient numerical algorithms available through the Vienna Schrödinger-Poisson framework

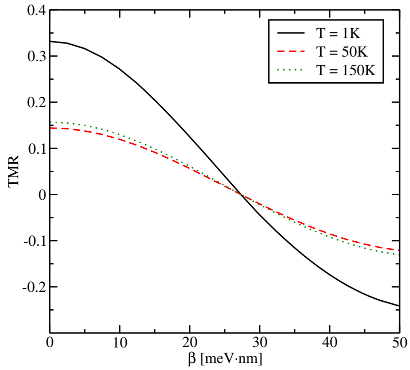


**Fig. 3.** Tunneling magnetoresistance dependence on the value of the Dresselhaus spin-orbit interaction for a semiconductor channel of length L=5$\mu m$; the spin polarization $P$ in the source and the drain contacts is $P$ =0.4; the strength $z$ of the delta-function-like barriers at the contacts between the channel and source/drain $z$ =5, the voltage $V$ =0.001V, and the effective mass in the ferromagnetic region $m_s^*$=0.438$m_0$

**Table 1.** Calculation time (seconds) depending on the number of processors and the number of points

| Number of Processors | N = 24 | N = 48 | N = 96 |
|---|---|---|---|
| 1 | 1036 | 2057 | 4129 |
| 2 | 549 | 1094 | 2198 |
| 4 | 286 | 570 | 1138 |
| 8 | 160 | 318 | 633 |

(VSP) [9]. The dependence of the effective mass of the ground subband on $t$ in [100] and [110] fins is shown in Fig. 1.

Some results obtained with our simulation procedure are shown in Fig. 2 and Fig. 3. For the channel we chose the silicon fins with [100] and [110] orientations and square cross-section with (001) horizontal faces. Fig. 2 shows the dependence of the TMR for the [100] and [110] oriented fins with a thickness $t$ =1.5nm on the value of the spin-orbit interaction $\beta$. The fins with [100] orientation show a stronger dependence on $\beta$ compared to the [110] oriented fins. The reason of the stronger dependence is that the influence of the spin-orbit interaction on the conductance is determined by the wave vector $k_D = m_n^* \beta / \hbar^2$. As the effective mass value for the [110] oriented fins is smaller compared to the [100] oriented fins, the same variation of $k_D$ results in a larger variation of $\beta$ in case of the [110] oriented fins. Thus the [100] oriented fins are preferred for silicon SpinFETs. Fig. 3 demonstrates the dependence of the TMR on the spin-orbit interaction at various temperatures. One can see that the oscillatory amplitude of the TMR survives even at T=150$K$. This fact is encouraging for utilizing silicon as the semiconductor channel material in SpinFETs at room temperature.

## 4 Conclusion

We investigated the transport properties of SpinFETs and show that silicon can be considered as a promising material for spin-driven applications. We sketch our way to speed-up the calculations by employing an efficient parallelization scheme. We show that because of the Dresselhaus form of the spin-orbit interaction the TMR of silicon fins can be modulated by the spin-orbit interaction even at relatively high temperatures. We demonstrate that because of the larger subband effective mass the [100] oriented silicon fins are best suited for the realization of a SpinFET.

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