Spin injection and accumulation in inhomogeneous semiconductors

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Abstract

We present a study of spin transport in charge and spin inhomogeneous semiconductor systems. In particular, we investigate the propagation of spin-polarized electrons through a boundary between two semiconductor regions with different doping concentrations. We use a theoretical and numerical method, presented in this paper, based on a self-consistent treatment of a two-component version of the Boltzmann transport equation. We show that space-charge effects strongly influence the spin transport properties, in particular giving rise to pronounced spin accumulation and spin density enhancement.

Key words: spin transport, Boltzmann equation, space-charge effects, spin accumulation

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All-semiconductor spintronics has recently become feasible due to the availability of diluted magnetic semiconductors for spin injection[1,2] and the long spin relaxation lengths present in semiconductors. In order to realize semiconductor spintronic applications, issues of spin injection, transport, manipulation and detection need to be studied and understood. In particular, transport studies need to answer questions pertaining to propagation and scattering of spins across interfaces, effects of applied fields and inhomogeneous doping variations and the resulting built-in electric fields. Some very interesting studies in this direction have been published recently by several groups[3,4,5,6]. However, most of the investigations have been based on drift-diffusion approaches and in some cases without taking into account space-charge effects which can be very significant in semiconductor transport.

In this paper we present a theoretical formulation beyond drift-diffusion that is capable of describing charge and spin transport through strongly inhomogeneous semiconductor systems, as well as nonequilibrium effects. Our approach is based on the semiclassical Boltzmann transport equation, two spin-dependent electron distribution functions and a self-consistent description which allows us to fully take into account space-charge effects. In the following, we will present our model and describe a numerical method for the solution of the resulting non-linear system of differential equations. Subsequently, we will exemplify the versatility of our model as well as the importance of space-charge effects by calculating the spin transport properties of a spin and charge inhomogeneous system, in particular studying the transport across a doping interface. We show that spin accumulation and magnification of the spin density imbalance occurs around the space-charge region and compare our results with the charge homogeneous case.

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Our theoretical model is based on a two-component version of the Boltzmann transport equation, in the relaxation-time approximation, as follows:

\[
\frac{-eE(x)}{m^*} \frac{\partial f_\uparrow(x,v)}{\partial v} + v \frac{\partial f_\uparrow(x,v)}{\partial x} = \frac{f_\uparrow(x,v) - f_\uparrow^0(x,v)}{\tau_m} - \frac{f_\downarrow(x,v) - f_\downarrow^0(x,v)}{\tau_{sf}^{\uparrow\downarrow}},
\]

\[
\frac{-eE(x)}{m^*} \frac{\partial f_\downarrow(x,v)}{\partial v} + v \frac{\partial f_\downarrow(x,v)}{\partial x} = \frac{f_\downarrow(x,v) - f_\downarrow^0(x,v)}{\tau_m} - \frac{f_\uparrow(x,v) - f_\uparrow^0(x,v)}{\tau_{sf}^{\uparrow\downarrow}},
\]

where \(E(x)\) is the inhomogeneous electric field, \(f_{\uparrow(\downarrow)}^0\) is the local equilibrium distribution for the spin up(down) electrons, and where we have introduced two scattering times, \(\tau_m\) and \(\tau_{sf}\), for the momentum relaxation and spin flip times, respectively. The electron distributions \(f_{\uparrow(\downarrow)}^0\) are local equilibrium distribution functions to which electrons with spin up(down) relax with the scattering time \(\tau_m\). In our calculations we assume nondegenerate statistics and assume a Maxwell-Boltzmann distribution normalized with the local density of spin up(down) electrons as our local equilibrium distribution according to

\[
f_{\uparrow(\downarrow)}(x,v) = n_{\uparrow(\downarrow)} \left[ \frac{m^*}{2\pi k_B T} \right]^{1/2} \exp \left( -\frac{m^* v^2}{2 k_B T} \right),
\]

where \(T\) is the lattice temperature and \(k_B\) is the Boltzmann constant. The inhomogeneous, field, \(E(x)\), is coupled to the spin densities via the Poisson equation

\[
\frac{d^2 \phi}{dx^2} = -\frac{e}{\epsilon_0} \left( N_D(x) - n_\uparrow(x) - n_\downarrow(x) \right),
\]

where \(\phi(x)\) is the electrostatic potential profile, \(\epsilon\) is the dielectric constant and \(N_D(x)\) is the donor profile, where we in the following assume unipolar transport, no acceptors and complete ionization of the donors. The spin up(down) electron densities in eqs. (2,3) are obtained from the distribution functions \(f_{\uparrow(\downarrow)}(x,v)\) via

\[
n_{\uparrow(\downarrow)}(x) = \int f_{\uparrow(\downarrow)}(x,v)dv.
\]

Equations (1-4) are coupled through the spin densities, the electric field, and the spin flip scattering term in the BTE equations, and thus, they need to be solved self-consistently. We use a numerical approach based on finite difference and relaxation methods, that we originally developed for the study of nonequilibrium effects in charge transport through ultrasmall, inhomogeneous semiconductor channels[7],[8]. As boundary conditions, we adopt the following scheme: For the potential, the values at the system boundaries are fixed to \(\phi(x_l) = V_b\) and \(\phi(x_r) = 0\) (\(l, r\) denote the left and right boundary of the sample, respectively), corresponding to an externally applied voltage \(V_b\). The *electron charge density* is allowed to fluctuate around the system boundaries subject to the condition of global charge neutrality, which is enforced between each successive iteration in the self-consistent Poisson-Boltzmann loop. The *spin density* at the boundary is determined by the degree of boundary polarization

\[
P = (n_\uparrow - n_\downarrow) / (n_\uparrow + n_\downarrow),
\]

for which the density at the boundary is defined according to \(n_{\uparrow(\downarrow)} = n/2(1 \pm P)\). For an unpolarized boundary, at which \(n_\uparrow = n_\downarrow\), care must be taken regarding to sample and/or contact size to ensure that any inhomogeneous spin density within the sample has decayed such that \(P = 0\) is valid at the unpolarized boundary. In addition, the size of the contacts has to be large enough, such that the electric field deep inside the contacts is constant and low. This allows us to use the analytical, linear response solution to the BTEs (1)

\[
f_{\uparrow(\downarrow)}(x_{l,r},v) = f_{\uparrow(\downarrow)}^0(x_{l,r},v) \left[ 1 - vE(x_{l,r})\tau_m / k_BT \right],
\]

as phase space boundary conditions at \(x_{l,r}\), where we use the local equilibrium distribution, \(f_{\uparrow(\downarrow)}^0(x_{l,r},v)\) and local electric field, \(E(x_{l,r})\), obtained from the previous numerical solution to the Poisson-Boltzmann iterative loop. At the velocity cut-off in phase space, we choose \(f_{\uparrow(\downarrow)}(x,v_{\text{max}}) = f_{\uparrow(\downarrow)}(x,-v_{\text{max}}) = f_{\uparrow(\downarrow)}^0(x,v)\), which is reasonable, since, in the calculations, we assume \(v_{\text{max}} \geq 30k_BT\). A more detailed description and discussion of our numerical method (described for pure charge transport) can be found in Ref. [7].

In the following we apply our model for the study of spin transport through a charge and spin inhomogeneous semiconductor structure. For this purpose, we use a 5 µm long GaAs sample, across which we apply a bias voltage \(V_b = -0.3\) V. We assume that electrons are spin-polarized with \(P = 1\) for \(x < -0.1\) µm (the sample is defined for \(-2.5 \leq x \leq 2.5\) µm) and that other parameters in the calculations are \(T = 300\) K, \(\tau_m = 0.1\) ps, \(\tau_{sf} = 1\) ns and \(\epsilon = 13.1\). Furthermore, we study two different structures, one charge homogeneous, with \(N_D = 10^{21}\) m\(^{-3}\), and one charge inhom-
with this region, however, the electric field is constant and inhomogeneous structures (solid lines), calculated at $x = 0.1 \mu m$ (vertical dotted line in the figure) and doping concentrations of $N_D/N_D^1 = 10^{21}/10^{22} \text{ m}^{-3}$ (thick lines).

The situation for the inhomogeneous sample is, however, the electric field is constant and inhomogeneous structures (solid lines), calculated at $x = 0.1 \mu m$ (vertical dotted line in the figure) and doping concentrations of $N_D/N_D^1 = 10^{21}/10^{22} \text{ m}^{-3}$ (thick lines).

In Fig. 1 we show the potential energy profiles (dashed lines) and electric field distributions (solid lines) for a homogeneous sample with $N_D = 10^{21} \text{ m}^{-3}$ for $x < 0.1 \mu m$, and $10^{22} \text{ m}^{-3}$ for $x > 0.1 \mu m$.

In Fig. 1 we show the potential energy profiles (dashed lines) and electric field distributions (solid lines) for the homogeneous (thin lines) and inhomogeneous (thick lines) sample, respectively. A potential barrier is formed at the interface between the two regions in the inhomogeneous sample, as a consequence of electrons diffusing from the highly doped right region to the lightly doped left region. Correspondingly, the electric field is peaked around the interface and a space-charge region of $0.5 \mu m$ is formed. Outside of this region, however, the electric field is constant with $|E_{\text{left}}| > |E_{\text{right}}|$. Naturally, for the homogeneous sample, the potential drops linearly over the sample and the electric field distribution is constant, as illustrated by the thin lines in Fig. 1.

In Fig. 2 we show the calculated spin density imbalance, $\Delta n_{\uparrow\downarrow}$, for the homogeneous (dashed lines) and inhomogeneous (solid lines) case, calculated at $V_b = -0.3 \text{ V}$ (thick lines) and $V_b = 0.3 \text{ V}$ (thin lines). The interfaces between the unpolarized and polarized segments occur at $x_p = -0.1 \mu m$ and $x_c = 0.1 \mu m$, respectively, as indicated by the vertical dotted lines. Inset shows the total charge density around the two interfaces, for $V_b = -0.3 \text{ V}$.

The situation for the inhomogeneous sample is, however, the electric field is constant and inhomogeneous structures (solid lines), calculated at $x = 0.1 \mu m$ (vertical dotted line in the figure) and doping concentrations of $N_D/N_D^1 = 10^{21}/10^{22} \text{ m}^{-3}$ (thick lines).

In Fig. 2 we show the potential energy profiles (dashed lines) and electric field distributions (solid lines) for a homogeneous sample containing a doping interface at $x = 0.1 \mu m$. Naturally, for the homogeneous structure can be described by 

$$\Delta n_{\uparrow\downarrow} = \frac{eE}{k_B T} + \sqrt{\frac{eE}{k_B T} + \frac{1}{[L_s^*(x)]^2}},$$

where $L_s = \sqrt{D \tau_{sf}}$ is the intrinsic spin-diffusion length in the absence of an electric field, and where $D = k_B T \tau_m/m^*$ obtained from the Einstein relation. From eq. (6) it follows that the spin-diffusion length is enhanced in the direction anti-parallel to an applied electric field and suppressed in the direction parallel to the field.\cite{4,5} Hence, the difference between the two dashed curves corresponding to the decay of $\Delta n_{\uparrow\downarrow}$ in the homogeneous sample, calculated at two bias voltages with opposite sign, can be explained by an exponential decay with a field-dependent diffusion length given by eq. (6).

The situation for the inhomogeneous sample is, however, the electric field is constant and inhomogeneous structures (solid lines), calculated at $x = 0.1 \mu m$ (vertical dotted line in the figure) and doping concentrations of $N_D/N_D^1 = 10^{21}/10^{22} \text{ m}^{-3}$ (thick lines).

In Fig. 2 we show the potential energy profiles (dashed lines) and electric field distributions (solid lines) for a homogeneous sample containing a doping interface at $x = 0.1 \mu m$. Naturally, for the homogeneous (dashed lines) and inhomogeneous (solid lines) case, calculated at $V_b = -0.3 \text{ V}$ (thick lines) and $V_b = 0.3 \text{ V}$ (thin lines). The interfaces between the unpolarized and polarized segments occur at $x_p = -0.1 \mu m$ and $x_c = 0.1 \mu m$, respectively, as indicated by the vertical dotted lines. Inset shows the total charge density around the two interfaces, for $V_b = -0.3 \text{ V}$.\cite{4,5} Hence, the difference between the two dashed curves corresponding to the decay of $\Delta n_{\uparrow\downarrow}$ in the homogeneous sample, calculated at two bias voltages with opposite sign, can be explained by an exponential decay with a field-dependent diffusion length given by eq. (6).

The situation for the inhomogeneous sample is, however, different. The spin density imbalance, $\Delta n_{\uparrow\downarrow}$, has a non-monotonic spatial dependence: i) it in-
creases before the interface at \( x < -0.1 \, \mu m \) where the polarization is turned off, ii) past the interface, for \( x \geq -0.1 \, \mu m \), \( \Delta n_{\uparrow\downarrow} \) decreases, iii) a second steep increase occurs around the interface at \( x = 0.1 \, \mu m \) between the \( N_D = 10^{21} \, m^{-3} \) and \( N_D = 10^{22} \, m^{-3} \) regions of the sample, where a peak is formed, followed by a monotonic decrease toward 0 at the far-right side of the sample.

The origin of these features can be understood as follows: We can rewrite the spin density imbalance according to

\[
\Delta n_{\uparrow\downarrow} = n_{\uparrow} - n_{\downarrow} = n - 2n_{\downarrow},
\]

Far to the left of the sample, where \( P = 1, n_{\downarrow} = 0 \). Furthermore, the electric field and the charge density are constant and correspondingly, \( \Delta n_{\uparrow\downarrow} = n \). For a homogeneous sample, only the second term in eq. (7) has a spatial variation with a typical exponential decay as discussed above. However, in a charge inhomogeneous structure, both the spin and charge densities have a strong spatial dependence and hence, both terms in eq. (7) affect the overall spatial dependence of \( \Delta n_{\uparrow\downarrow} \).

The increase of \( \Delta n_{\uparrow\downarrow} \) for \( x < -0.1 \, \mu m \), where \( n_{\downarrow} \approx 0 \), is due to a pure charge pile-up of the total charge, \( n \), which is increasing from left-to-right due to the diffusion of electrons from the high-doping region to the low-doping region to the left (see inset in Fig. 2). For \( x > -0.1 \, \mu m \), spin relaxation gives rise to an increase of \( n_{\downarrow} \), the second term in eq. (7), and hence reduces \( \Delta n_{\uparrow\downarrow} \) as seen in the sudden drop in the spin density imbalance of Fig. 2. However, around the interface at \( x = 0.1 \, \mu m \), \( \Delta n_{\uparrow\downarrow} \) increases again, and a sharp peak emerges.

This peak can be explained in terms of the spatial dependence of the total charge \( n \). Close to the doping interface at \( x = 0.1 \, \mu m \), there is a sharp rise in the total charge density, as shown in the inset of Fig. 2, which occurs in order to accomodate the difference in doping concentrations between the two regions. In this region, the increase of the total charge \( n \) is much faster than the increase in \( n_{\downarrow} \) and hence, \( \Delta n_{\uparrow\downarrow} \) rises sharply, as given by eq. (6) and as seen in Fig. 2. Beyond the interface for \( x > 0.1 \, \mu m \), however, the total charge saturates at \( n \approx 10^{22} \, m^{-3} \) (see inset) and therefore, the gradual decrease of the \( \Delta n_{\uparrow\downarrow} \) peak for \( x > 0.1 \, \mu m \) is solely due to the increase in \( n_{\downarrow} \) due to the spin-flip term in eq. (1). We note that spin accumulation at a doping interface has been recently reported by Pershin and Privman [6].

From the above discussion and results it is evident that space-charge effects strongly influence the properties of semiconductor spin transport. In particular, we conclude that spin transport characteristics depend on several length scales, not only the electric-field dependent spin-diffusion lengths defined in eq. (6), but also the charge screening length, and the momentum relaxation length. Therefore, a self-consistent treatment such as ours is needed for an accurate description of the space-charge effects in semiconductor spintronics. We also note that the importance of band-bending effects on spin injection in the nonlinear regime of transport have been demonstrated in recent experiments [9].

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