Spin accumulation and decay in magnetic Schottky barriers

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Abstract

The theory of charge and spin transport in forward-biased Schottky barriers reveals characteristic and experimentally relevant features. The conductance mismatch is found to enhance the current induced spin-imbalance in the semiconductor. The GaAs|MnAs interface resistance is obtained from an analysis of the magnetic field dependent Kerr rotation experiments by Stephens et al. and compared with first-principles calculations for intrinsic interfaces. With increasing current bias, the interface transparency grows towards the theoretical values, reflecting increasingly efficient Schottky barrier screening.

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An obstacle to the direct injection of spins from a ferromagnetic metal (F) into a semiconductor (SC) is the so-called conductance mismatch [1]. Paradoxically, this problem is most severe for good electric contact, because most of the applied potential drop is then wasted over the highly resistive semiconductor and very little is left to spin-polarize the current in the magnetically active region. Selection rules at ballistic interfaces are responsible for a large interface spin polarization [2, 3] that allows significant spin accumulation in spite of the mismatch, but even small amounts of disorder have detrimental effects [3]. Use of ferromagnets with low conductances matched to those of the semiconductor [4] is another route, but many material problems, such as low critical temperatures for ferromagnetism, have still to be solved [5]. Spins can be effectively injected into a semiconducting base contact of a three-terminal spin-flip transistor [6] or by pumping spins into the semiconductor by ferromagnetic resonance [7], but none of these theoretical predictions have been confirmed experimentally yet. The spin polarization of the injected current can be increased by tunneling or Schottky barriers, both causing the applied potential to drop in the spin-selective region of the sample [1, 8, 9]. This feature has been employed in experiments that divide into two categories. In the first, hot electrons are injected into a metallic magnetic multilayer base in the forward bias regime. In the “spin-valve transistor” [10] this is achieved via a Schottky barrier; in “magnetic tunnel transistors”, tunneling barriers are used instead [11]. The second category of experiments concentrates on injecting spins from the ferromagnet into semiconductors by applying a reverse bias, reaching polarizations of 30 \% [12]. Here the spin current is the observable, measured by the circular polarization of the recombination luminescence of the injected electrons with thermalized holes.

Recently, Stephens et al. [13] investigated in forward-biased Schottky barriers not the hot electrons that traverse a ferromagnetic base as in Refs. [10, 11], but the cold ones that remain in the semiconductor. A significant bias-dependent spin accumulation in the semiconductor was observed by Kerr rotation. The interpretation as spin dependent reflection at the interface was supported by a simple parabolic band/step potential model. In this Letter we present a theoretical analysis based upon an adaptation of magnetoelectronic circuit theory [6, 14]. We find that the conductance mismatch has a beneficial effect on the size of the spin accumulation. Analyzing the Bloch equation that governs the spin accumulation in the presence of an applied magnetic field we find that the experimental results on the dephasing by a magnetic field (Hanle effect) can be used to extract the SC|F interface resistance.
We also present first-principle calculations of intrinsic interface transport parameters for disordered interfaces as a function of the SC Fermi energy.

The sample configuration is indicated in Fig. 1. We start with a discussion of an infinite planar Schottky barrier model between a degenerately n-doped semiconductor SC and a metallic ferromagnet F that is kept at low temperatures and biased with an electric particle current $I_C$. With increasing forward (positive) bias the semiconductor band edge is lifted relative to the ferromagnetic one. The ionized donor atoms are increasingly screened until at a bias close to the Schottky barrier height the semiconductor band edge at the interface comes close to the bulk Fermi energy of the semiconductor $\varepsilon_F$. The “flat-band” condition is defined asymptotically at a voltage close to the barrier height where the tunneling current and thus the electric field in the semiconductor start to become significant. Although the theory is valid for arbitrary material combinations we concentrate here on the sample investigated by Stephens et al., in which the GaAs is n-doped with densities of $\sim 10^{17}$ cm$^{-3}$. With an impurity scattering mean free path of $\sim 30$ nm the semiconductor is safely in the diffuse transport regime. The I-V characteristic in the forward bias shows a band tail close to the Schottky barrier and roughly Ohmic behavior at high bias with a resistance of 300 $\Omega$, indicating that the thin semiconductor layer limits the transport. Important parameters are the spin-flip diffusion length of $\ell_{sd} \simeq 2$ $\mu$m [16], and a flat-band depletion length of $\sim 20$ nm. Any residual band-bending is thus incorporated in the (quantum) interface resistance. The conductance of the high-density metallic ferromagnet MnAs is much higher than that of the semiconductor and disregarded. We concentrate on the dimensionless spin-dependent ($s = \uparrow, \downarrow$) occupation function $f_s(\varepsilon)$ in the semiconductor near the interface at an energy $\varepsilon$ from the band edge. The up spin direction $\uparrow$ is chosen parallel to the majority spin in the ferromagnet. Close to the flat band condition the energy of the electrons entering the metal is of the order of the Schottky barrier height, that is much larger than the semiconductor Fermi energy. The spectral spin current into the metal is therefore

$$eI_s(\varepsilon) = G_s^I(\varepsilon) f_s(\varepsilon),$$  \hspace{1cm} (1)

where $G_s^I(\varepsilon)$ is the interface conductance at energy $\varepsilon$. The total current of spin $s$ is given integrating over energy

$$I_s = \int I_s(\varepsilon) \, d\varepsilon.$$  \hspace{1cm} (2)

We assume a charge current bias of $I_C = I_{\uparrow} + I_{\downarrow}$ and introduce the spin current $I_z = \ldots$
We assume in the following that energy relaxation is fast, such that the distribution function at the interface is thermalized with non-equilibrium chemical potentials $\mu_s$. At low temperatures, assuming local charge neutrality $\mu_\uparrow + \mu_\downarrow = 0$ and an interface conductance that does not vary rapidly on the scale of $\mu_s$:

$$eI_z = \int_0^{\varepsilon_F + \mu_\uparrow} G_\uparrow (\varepsilon) \, d\varepsilon - \int_0^{\varepsilon_F + \mu_\downarrow} G_\downarrow (\varepsilon) \, d\varepsilon$$

(3)

$$= eI_z^{(0)} + \frac{\mu_z}{2} G^I (\varepsilon_F),$$

(4)

$$eI_C = \int_0^{\varepsilon_F} G^I (\varepsilon) \, d\varepsilon + \frac{\mu_z}{2} p (\varepsilon_F) G^I (\varepsilon_F)$$

(5)

where $G^I = G^I_\uparrow + G^I_\downarrow$, $p = (G^I_\uparrow - G^I_\downarrow) / G^I$, $\mu_z = \mu_\uparrow - \mu_\downarrow$ is the spin accumulation at the interface and

$$eI_z^{(0)} = \int_0^{\varepsilon_F} p (\varepsilon) G^I (\varepsilon) \, d\varepsilon.$$

(6)

In the degenerate limit, assuming that the conductivity is proportional to the density, the magnetically active region of the semiconductor is determined by the up-stream spin-diffusion length $\ell_u = \ell_{sd} \left( \sqrt{1 + X^2} - X \right)$, where $X = 3eI_C / \left( 8G_0^{SC} \varepsilon_F \right)$ is a measure of the potential drop induced by the current over the (zero-bias) spin diffusion length $\ell_{sd}$ in terms of the linear bulk conductance $G_0^{SC} = S \sigma^{SC} / \ell_{sd}$ of a semiconductor cube with area $S$ and thickness $\ell_{sd}$ [17]. In spite of the reduced spin-diffusion length, the conductance of the spin-coherent region is increased compared to the zero-bias limit:

$$G^{SC} = G_0^{SC} \frac{\ell_u}{\ell_{sd}}$$

(7)

(not $G_0^{SC} \ell_{sd} / \ell_u$ as might be expected naively). We then arrive at the effective circuit in Fig. 2, according to which the spin current $I_z = I_\uparrow - I_\downarrow$ that flows from the semiconductor bulk to the interface reads

$$eI_z = \frac{eI_z^{(0)}}{1 + G^I / 2G^{SC}}$$

(8)

and the sign of $\mu_z = -eI_z / G^{SC}$ is opposite to that of $I_z$. A low conductance $G^{SC} \rightarrow 0$ suppresses the spin current [11], but not the spin accumulation! By reversing $I_C$ and keeping in mind that the interface conductance is in general much smaller and less bias dependent, similar equations hold as well for reversed-bias Schottky barriers. As mentioned above, most experiments on reverse bias junctions focus on the spin current. The conductance mismatch problem is reflected in Eq. [8], where a small semiconductor conductance is seen to suppress
the spin current. In Refs. [1, 9] it was pointed out that a significantly polarized spin current can only be achieved when the reverse-bias Schottky barrier conductance is sufficiently small. However, in this case the spin accumulation $\mu_z$ is suppressed, which explains why Stephens et al. [13] only detected spin accumulation with a forward bias.

We now turn to the spin-accumulation in the presence of a variable in-plane magnetic field, taking the magnetization of F to be parallel to the $z-$direction and the magnetic field $B$ in the $y-$direction. The magnetic-field induced non-collinearity of spin accumulation and magnetization creates a spin transfer torque on the ferromagnet, thus opens new decay channels [14] proportional to the spin-mixing conductance $G^{I \uparrow \downarrow}$ at the Fermi energy. The Bloch equation for the spin accumulation $\langle \mu \rangle = (\mu_x, \mu_y, \mu_z)$ can be written

$$-T^I d|\mu\rangle \over dt = \Gamma |\mu\rangle + \frac{2e|I_z\rangle}{G_I},$$

(9)

where $T^I = 2e^2D/G^I$ is the interface relaxation time in terms of the (single spin) semiconductor energy density of states $D$ in the magnetically active volume.

$$\Gamma = \begin{pmatrix} \eta_r + \xi & \eta_i & T^I\omega \\ -\eta_i & \eta_r + \xi & 0 \\ -T^I\omega & 0 & 1 + \xi \end{pmatrix},$$

(10)

where $\eta_r = 2 \text{Re} G^{I \uparrow \downarrow}/G^I$, $\eta_i = 2 \text{Im} G^{I \uparrow \downarrow}/G^I$, $\xi = 2G^{SC}/G^I$ and the Larmor frequency $\omega = g_e\mu_B B/\hbar$ in terms of the g-factor $g_e$ and the Bohr magneton $\mu_B$. Eq. (9) holds when the relaxation rate of the electron orbital degrees of freedom is sufficiently larger than $\omega$. The source term is the current bias applied to the semiconductor. $\langle I_z \rangle = \left(0, 0, I_z^{(0)} \right)$. The stationary state solution for the Bloch equation, $|\mu\rangle = \Gamma^{-1}2e|I\rangle/G_I$, is easily obtained analytically. The spin accumulation at the interface reads:

$$\langle |\mu\rangle = \left(\frac{-(\eta_r + \xi)\omega/T^I, \eta_i\omega/T^I, -(\eta_r + \xi)^2 - \eta_i^2}{[(\eta_r + \xi)^2 + \eta_i^2] (1 + \xi) + (\eta_r + \xi)\omega^2} \right) \frac{2eI_z^{(0)}}{G^I},$$

(11)

Stephens et al. [13] found the component of the spin accumulation normal to the interface $\mu_x$ well represented by a Lorentzian $A\omega / (\omega^2 + T^{-2})$. This form also follows from our rate equations with

$$\left(\frac{T^I}{T}\right)^2 = \left[(\eta_r + \xi)^2 + \eta_i^2 \right] \frac{1 + \xi}{\eta_r + \xi},$$

(12)

and $A = -2eI_z^{(0)}/ (G^IT^I)$. In the limit of a highly resistive semiconductor, $\xi \ll 1$, and taking $\eta_i = 0, \eta_r = 1$, we find that $T \to T^I$ and $AT \to \mu_z (\omega = 0)$, i.e. the zero field spin...
accumulation. It is therefore possible to obtain information about the interface conductance from the experimental spin dephasing time.

The MnAs|GaAs systems has been studied intensively [15], but not much is known about the electronic transport properties. Epstein et al. [18] reported that the conductance polarization is opposite to the magnetization direction, i.e. \( p < 0 \). We compute MnAs|GaAs (100) interface conductances \( G^I(\varepsilon) \) for the ZincBlende (\( \alpha \)) structure [19] by scattering matrix calculations with a first-principles tight-binding basis [3], assuming flat-band conditions with a Schottky barrier height of 0.8 eV (see Fig. 3). We find large differences between clean, and on a monolayer scale, alloy-disordered interfaces, e.g. the interface polarization changes sign when the interface becomes increasingly dirty. The negative polarization found in [18] is thus consistent with non-ideal interfaces. These features are quite similar to results for Fe|InAs that does not have a Schottky barrier [3]. We also note that in the regime considered here we calculate an \( \eta_r \simeq 1 \) in all cases and \( \eta_i \simeq 0 \) (0.35) for clean (disordered) interfaces. We parametrize the estimated interface conductance in terms of the SC Sharvin conductance \( G_{Sh}(\varepsilon_F) / S = (2e^2/h)(2m^*\varepsilon_F)/(4\pi\hbar^2) \) times a transparency parameter that at 12 meV is found to be \( \kappa = 0.27 \) for clean and dirty interfaces.

In order to make contact with Stephens et al. [13] the above results for the planar junction have to be adapted to the experimental geometry in Fig. 1. For GaAs with doping density \( n = 10^{17} \text{ cm}^{-3} \), we take a mobility 3000 cm²/(Vs), an effective mass \( m^* = 0.067m_e \), and spin-flip diffusion length \( \ell_{sd} \simeq 2 \mu\text{m} \) [16], that is significantly larger than the film thickness \( d^{SC} = 0.5 \mu\text{m} \). The measured excess spin-dephasing rates \( T^{-1} \) at applied currents \( I_C \) are listed in the table. Close to the interface, the up-stream spin-flip diffusion length is not significantly reduced, so not only the whole \((\simeq 5 \times 50 \mu\text{m}^2)\) area under the conducting contact is spin coherent at all currents, but also strips on both sides with widths of the order of \( \ell_{sd} \) and \( \ell_u \), respectively. The drift effect on the available density of states is small, but it significantly affects the resistance of the spin coherent region. Due to the thin layer thickness of the GaAs, lateral spin diffusion may be disregarded. The results in the table are obtained assuming that \( \eta_i = 0, \eta_r = 1 \).

The experimental longevity of spins is striking and can only be explained by a reduced interface conductance. Any spin-flip process disregarded here, caused, e.g., by heating [16] due to high currents, would correspond to even smaller transparencies. The small \( \kappa \) at small bias reflects the residual Schottky barrier that is not yet completely screened. At
TABLE I: Experimental results for the spin dephasing rate $1/T$ at selected current bias $I_C$ from Ref. 13 and the estimates of device parameters according to the discussion in the text. $R^{SC}$ and $SR^I$ are the $SC$ bulk resistance of the magnetically active region and the interface resistance for the given bias. $\kappa$ is the transparency parameter that measures the interface conductance in unit of the $SC$ Sharvin conductance.

| $I_C$ (mA) | $R^{SC}$ (Ω) | $SR^I$ ($\frac{\Omega \text{m}^2}{10^{-9}}$) | $\kappa$ |
|------------|---------------|-----------------|--------|
| 0.3        | 0.25          | 43              | 25     | 0.004  |
| 1.1        | 1.2           | 63              | 5.2    | 0.014  |
| 2.7        | 6             | 111             | 1.1    | 0.074  |

higher bias these remnants should disappear and the spin-dephasing time should be governed by the intrinsic interface. At higher bias the interface conductances deduced from the experiments grow to about one third of the intrinsic first-principles results. An energy-averaged interface transparency is accessed by the electrical current itself. Disregarding the small term proportional to $\mu_z$ in Eq. (5), the current according to the first-principles conductances and a contact area of $250 \mu\text{m}^2$ should be $I_C \simeq 25 \text{mA}$. At the experimental currents of $I_C \lesssim 3 \text{mA}$ the average $\kappa$ is thus smaller than that at the Fermi energy obtained from the Hanle effect. This can be explained by an energy dependent $\kappa$ that decreases strongly when approaching the band edge. These remaining puzzles might be related to the measured spatial inhomogeneity of the current induced spin accumulation and thus interface conductance.

Stephens et al. 13 estimate the spin accumulation to be 10% of the Fermi energy from nuclear polarization data compared to an estimate of $\sim 15\%$ based on the first-principles results for disordered interfaces. The spin accumulation is found to saturate and even decrease again with large $I_C$. A probable reason is a reduced spin-flip diffusion length, either by heating or by a large drift contribution at higher bias.

In summary, we demonstrate how a transport property, the semiconductor–ferromagnet interface conductance, can be measured optically on an absolute scale. The conductance mismatch is found to favor spin injection into semiconductors in forward-biased magnetic Schottky barriers. At low bias the interface-mediated spin-decay is much weaker in the experiments 13 than expected from intrinsic SC|F interfaces. At higher bias the agreement
becomes better, indicating that the interface approaches (but does not reach) the Ohmic limit as calculated from first-principles. Experiments that determine the spin accumulation on an absolute scale would be of great help to refine the present analysis. The observed negative polarization [13, 18] can be explained by disorder at the interfaces. A systematic study as a function of semiconductor thickness could shed more light on the spin-decoherence in the non-linear transport regime.

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FIG. 1: Schematic drawing of the magnetic forward-biased Schottky diode of Stephens et al. [13]. The particle current $I_C$ is injected from the semiconductor film SC of thickness $d$ into the ferromagnet F through a contact area S. The excited spin accumulation diffuses back into the semiconductor over the spin-diffusion length $\ell_{sd}$ without bias and up-stream diffusion length $\ell_u$ against the bias. The spin accumulation in the semiconductor is plotted for $p > 0$. 
FIG. 2: Magneto electronic circuit for a current biased magnetic Schottky barrier in the absence of a magnetic field.
FIG. 3: Intrinsic conductance of a specular (left) and disordered (right) $\alpha$—MnAs/GaAs (100) interface at flat band conditions as a function of the excess energy in the GaAs conductance band and calculated from first principles [3].