Spin depolarization in the transport of holes across $\text{Ga}_x\text{Mn}_{1-x}\text{As}/\text{Ga}_y\text{Al}_{1-y}\text{As}/p\text{-GaAs}$

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We study the spin polarization of tunneling holes injected from ferromagnetic GaMnAs into a p -doped semiconductor through a tunneling barrier. We find that spin-orbit interaction in the barrier and in the drain limits severely spin injection. Spin depolarization is stronger when the magnetization is parallel to the current than when it is perpendicular to it.

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Achieving the injection of spin-polarized current from a ferromagnetic material into a semiconductor is one of the challenges in spintronics.^{1,2} However, the conductivity mismatch between ferromagnetic metals and semiconductors prevents simple strategies of spin injection in the diffusive regime.^{3,4} At least two kinds of proposals have been suggested in order to circumvent this obstacle. The first, is the use of a tunnel barrier between the ferromagnetic source and the semiconductor.⁵ Second, is the use of diluted magnetic semiconductors (DMS) as a source.^{6,7}

Ferromagnetic diluted magnetic semiconductors materials like GaMnAs have raised enormous interest because of both their fundamental interest and their potential in spintronics proposals. One of the appealing features of GaMnAs and other DMS is that they can be integrated easily with other III-V-based heterostructures combining the magnetic and electronic functionalities. In this direction heterostructures based in GaMnAs have been grown that feature strong tunneling magnetoresistance effects.^{8,9} On the other side, the Curie temperature is still below room temperature although improvement in post-growth-annealing techniques^{10,11} in GaMnAs DMS shows the ability to obtain critical temperatures larger than 150 K.

In GaMnAs, Mn act as an acceptor that supplies holes responsible for the long-range ferromagnetic interaction between the Mn spins.¹²⁻¹⁴ Crucial in the understanding of the ferromagnetic phase of the material is the fact that the spin-orbit interaction for the valence-band holes is very strong ($\Delta \sim 340$ meV). This large spin-orbit coupling has several effects on the properties of magnetic GaMnAs: (i) There is a large correlation between the T_c and strength of the spin-orbit interaction.¹² (ii) Spin orbit, combined with strain effects due to the substrate-DMS lattice mismatch, determines the easy axis for the magnetization.¹⁵ (iii) Spin orbit is also responsible for the anisotropic magnetoresistance in bulk GaMnAs.^{16,17}

In this work we address the effect of spin-orbit coupling on the injection of a spin-polarized hole current from a DMS into a p -doped paramagnetic semiconductor, via an epitaxially grown tunnel junction, i.e., in the coherent regime. In particular, we want to analyze how the spin polarization is degraded and how the spin current polarization depends on the angle formed by the electrical current and the magneti-

zation. These two questions are relevant for the possible use of GaMnAs as a source of spin-polarized current. The system of interest consists of a ferromagnetic semiconductor and a nonmagnetic semiconductor separated by a tunnel barrier. In particular, the left electrode is GaMnAs, the right electrode is p -doped GaAs, and the barrier is GaAlAs. We consider that transport takes place by tunneling through a GaAlAs barrier of width d . In this configuration spin-orbit coupling is the same along the whole heterostructure. We also analyze the effect produced by the quenching of the spin-orbit coupling only at the drain or both at the drain and the barrier. We anticipate the following main conclusions of this work:

(1) Spin-orbit coupling, both at the drain and at the barrier, significantly reduces the spin polarization of carriers injected into the nonmagnetic electrode.

(2) Spin injection depends significantly on the angle between the current flow and the magnetization of the source electrode. When the magnetization at the source is parallel to the electrical current, the depolarization effect is stronger than for the case of source magnetization perpendicular to the current.

Theoretical approach: The system considered is formed by three well-defined regions along the growth direction (z). The *left region* (L) is the source for the spin-polarized current and is formed by GaMnAs. The *barrier region* (B) is formed by GaAlAs, while the *right region* (R) is a paramagnetic p -doped semiconductor, for example, Be-doped GaAs. The valence bands of this system are described in a $\mathbf{k} \cdot \mathbf{p}$ framework by means of a Hamiltonian having three parts,

$$\begin{aligned} H^L &= H_{\mathbf{k},\mathbf{p}}^L + J_{pd} N_{Mn} \text{Sm} \vec{\Omega} \cdot \vec{s}, \\ H^B &= H_{\mathbf{k},\mathbf{p}}^B + \Delta V^{L-B}, \\ H^R &= H_{\mathbf{k},\mathbf{p}}^R + \Delta V^{L-R}. \end{aligned} \quad (1)$$

$H_{\mathbf{k},\mathbf{p}}^L$, $H_{\mathbf{k},\mathbf{p}}^B$, and $H_{\mathbf{k},\mathbf{p}}^R$ are six-band Kohn-Luttinger Hamiltonians for L , B , and R , respectively.^{12,13} Ternary compounds GaMnAs and GaAlAs are described a virtual-crystal approximation (VCA). We use the same Kohn-Luttinger parameters to describe the electronic properties of GaAs, GaMnAs, and GaAlAs, i.e., $H_{\mathbf{k},\mathbf{p}}^R = H_{\mathbf{k},\mathbf{p}}^L = H_{\mathbf{k},\mathbf{p}}^B$.

In GaMnAs exchange interaction couples the spin of

valence-band holes with the spin of the Mn ions, which are randomly located in the cation sublattice. In the mean field and VCA,¹² the disordered exchange interaction is replaced by a homogeneous effective Zeeman field. This approach accounts for a number of experimental observations. The second term of H^L describes the coupling of the holes to the effective field. There, J_{pd} is the exchange coupling, N_{Mn} the Mn ion density, S the spin of a Mn ion, m the average polarization of the Mn spins, $\vec{\Omega}$ the orientation of the magnetization, and $\vec{s}$ the spin of the holes. In this theoretical framework, the ferromagnetic electrode is characterized by the density of Mn and the density of holes. For a given set of parameters in the model we obtain the spin polarization of both Mn and holes.¹⁴

The GaAlAs barrier and p -doped GaAs drain are described by means of $k \cdot p$ Hamiltonians with shifts ΔV^{L-B} and ΔV^{L-R} with respect to the top of the valence band of the ferromagnetic semiconductor. The precise value of the barrier height ΔV^{L-B} depends on the Al content in the barrier, which is typically in the range between 20% and 40%. The conduction-band offset between GaAs and AlAs is, at the Γ point, close to 1 eV. Therefore, we report results for an intermediate value (30%) of $\Delta V^{L-B}=300$ meV and we have checked that the results do not change qualitatively for barriers in the mentioned range. The shift ΔV^{L-R} permits to have a different carrier density in the p -doped region with a common Fermi energy across the heterostructure. Our rigid-band model neglects band-bending effects across the interfaces.¹⁸

Charge and spin transport are studied in the scattering formalism.^{19–21} The quantum states of the electrodes are described by a band index n and a wave vector $\mathbf{k}$, in the framework of the six-band $\mathbf{k} \cdot \mathbf{p}$ approximation. These states are a linear combination of p -like orbitals with total angular momenta $J=3/2$ and $J=1/2$. In the presence of spin-orbit coupling, the spin is not a good quantum number so that the quantities conserved in the tunneling process are the energy, E , and the parallel component of the wave vector, $k_{\parallel}$.^{19,20} An incoming plane-wave state from L , $|n, E, k_{\parallel}; L\rangle$, is transmitted to a plane wave $|n', E, k_{\parallel}; R\rangle$ at R with a transmission amplitude $t_{n,n'}^{k_{\parallel}}(E)$. As the group velocity in the left and right regions are in general different, the transmission probability from a state $|n, E, k_{\parallel}; L\rangle$ to a state $|n', E, k_{\parallel}; R\rangle$ reads¹⁹

$$T_{n,n'}^{k_{\parallel}}(E) = |t_{n,n'}^{k_{\parallel}}(E)|^2 \frac{v_{n'}(E, k_{\parallel}; R)}{v_n(E, k_{\parallel}; L)}, \quad (2)$$

where $v_n(E, k_{\parallel}; L/R)$ is the group velocity, along the z direction perpendicular to the interfaces, of the state $|n, E, k_{\parallel}; L/R\rangle$. In our calculation, only incoming and transmitted states with positive group velocity are considered. In this approach, the linear conductance of the heterostructure can be obtained as a sum over all transmission channels, $G = (e^2/h) \sum_{n,n',k_{\parallel}} T_{n,n'}^{k_{\parallel}}(E_F)$.

In the following, we study the degradation of the spin polarization of carriers passing from the source (GaMnAs) to a paramagnetic drain. We define the spin polarization of the transmitted current,

FIG. 1. Spin polarization η_{tr} as a function of the bulk polarization of GaMnAs along two different directions.

$$\eta_{tr} = 2 \frac{\sum_{n,n',k_{\parallel}} T_{n,n'}^{k_{\parallel}}(E_F) \langle n', k_{\parallel}; E_F; R | s | n', k_{\parallel}; E_F; R \rangle}{\sum_{n,n',k_{\parallel}} T_{n,n'}^{k_{\parallel}}(E_F)}, \quad (3)$$

where s is the component of the hole spin along $\vec{\Omega}$. We have verified that η_{tr} along other directions vanishes. This quantity describes the spin polarization of the coherently transmitted holes. Inelastic events which can result in further spin relaxation after tunneling are not included in our approach.

Results: In Fig. 1, we show the spin polarization of the transmitted current, η_{tr} , as a function of the bulk polarization of GaMnAs, η_0 . At this point it is convenient to distinguish between the bulk polarization of GaMnAs, η_0 , and the polarization of the holes in the Fermi surface of this material, η_F .²² The carrier density at the ferromagnetic source is fixed,

FIG. 2. Spin polarization η_{tr} as a function of the bulk polarization of GaMnAs along two different directions. Results are for zero spin-orbit coupling only at R (circles) or at R and B (squares). The dashed line shows the spin polarization at the Fermi level of GaMnAs.

FIG. 3. Spin polarization η_{tr} as a function of the barrier width d for magnetization along two different directions.

$p_L = 0.1 \text{ nm}^{-3}$, while two different values of p_R are considered. Two different magnetization orientations of the ferromagnetic electrode are studied, either parallel or perpendicular to the current flow, chosen along z . The results in Fig. 1 are obtained with the same spin-orbit coupling constant, $\Delta = 0.34 \text{ eV}$, in all three regions. It is notorious that η_{tr} is significantly smaller than the bulk polarization of the injector. The depolarization is stronger when the carriers are polarized parallel to the current (z) (open circles) than when they are

polarized along x , i.e., perpendicular to the current (black circles). This effect is larger in the case with lower density p_R of carriers in the p -GaAs. The feature appearing in η_{tr} for $\eta_0 \approx 0.8$, for current perpendicular to the magnetization, coincides with the complete depopulation of a band of minority-spin carriers in GaMnAs.

The strong depolarization of coherently injected spins is produced by three mechanisms:

First: Reduction of the spin polarization at the Fermi surface. At small bias, only electrons at the Fermi level are injected. As it happens, the hole spin polarization at the Fermi energy η_F is smaller than the bulk spin polarization η_0 (dashed line of Fig. 2). The ratio η_F/η_0 is roughly 0.9 for $\eta_0 < 0.65$ and even larger as η_0 approaches 1. Therefore, this effect is small in general.

Second: Spin-orbit coupling at the barrier and the drain. Figure 2 shows η_{tr} when spin-orbit coupling is removed either in the p -doped GaAs region or both in the barrier and p -doped region. The spin injection rate is significantly higher than the case of Fig. 1, showing that spin-orbit interaction is detrimental for successful spin injection. This is corroborated by the fact that polarizations are larger (lower depolarizations) when spin-orbit coupling is removed both at the barrier and the p -doped semiconductor. As in the case of Fig. 1, depolarization is stronger when carriers are polarized along the current direction. The directional dependence is also weaker, indicating that in the case of Fig. 1 it comes from the the spin-orbit interaction of both electrodes and barrier.

Third: Spin mixing and spin filtering in the barrier. Even in the absence of spin-orbit interaction in the barrier, tunnel probability can be spin dependent. This is known as spin filtering and accounts for the difference between the squares (spin orbit only in the source) and the dashed line in Fig. 2. In order to clarify the effect of the barrier in the depolarization, Fig. 3 shows η_{tr} as a function of the barrier width. The set of parameters is 0.733 for the polarization of GaMnAs (slightly below the kink in Fig. 2), $p_L = p_R = 0.1 \text{ nm}^{-3}$. We give results for the two orientations of the polarization as in Figs. 1 and 2, and both with and without spin-orbit coupling at R . All the curves have the same qualitative behavior: for $d=0$ the results for different orientations of m must coincide. For increasing, but still small values of d , band mixing effects become important and the curves for $m \parallel x$ and $m \parallel z$ separate from each other. For further increase of d , these two curves saturate becoming flat with d .

Let us discuss what is the physical origin of the large difference observed for depolarizations along the two orientations x and z . In the top of the GaAs valence band, the spin-orbit coupling creates a momentum-dependent effective Zeeman field that causes the hole angular momentum to align parallel or antiparallel to the wave vector.²³ This is evident in the spherical approximation to the Luttinger Hamiltonian, where the spin-orbit coupling is proportional to $-(\mathbf{k} \cdot \mathbf{J})^2$, J_i being the matrices for the angular momentum $3/2$. For a given $\mathbf{k}$ the eigenvalues are the heavy and light bands, both with $\mathbf{J}$ parallel or antiparallel to $\mathbf{k}$.²⁴ Because of the spin-orbit coupling, the Zeeman splitting is larger for states with $\mathbf{k}$ parallel to the magnetization than for states with $\mathbf{k}$ perpendicular to it [Fig. 4(a)]. In particular, for $\mathbf{k}$ parallel to the magnetization the heavy holes have spin $\pm 1/2$

FIG. 4. (Color online) Expectation value of the spin component along the direction of the polarization (z direction) in a contour at the Fermi level of GaMnAs, for two different values of η_0 . The filled/white circles depict positive/negative direction. The magnitude of spin is proportional to the circle size.

and an energy splitting $J_{pd}N_{Mn}Sm$, whereas states with $\mathbf{k}$ perpendicular to the magnetization are practically degenerated. This asymmetry reflects in the tunneling transport. For finite spin-orbit coupling, in a tunneling process only the energy and the component of the wave vector perpendicular to the current is conserved, and states with different parallel components of the wave vector and different spin polarization, can be mixed. This mixing results in a loss of spin polarization in the tunneling process. In Fig. 4 we see that the region of the Fermi surface, where states with different polarization can be mixed, is larger when tunneling current and magnetization are parallel (k_x constant) than when they are perpendicular (k_z constant). Therefore, the degradation of the spin current is bigger in the parallel case, as shown in all the results in Figs. 1–3 being that the perpendicular configuration is optimal for injecting spin.

In summary, spin-orbit coupling has a strong influence on

the spin injection of holes from ferromagnetic GaMnAs into p -doped GaAs via a tunneling barrier. First, spin-orbit interaction reduces severely the efficiency of spin injection. Therefore, prospects of hole spin injections seem better for materials with small spin-orbit-like Si or GaN. Second, the spin injection rate depends on the angle between current flow and magnetization. In particular, spin injection is significantly larger for samples magnetized parallel to the interfaces of the heterostructure.

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