

Spin injection through an Fe/InAs interface

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The spin dependence of the interface resistance between ferromagnetic Fe and InAs is calculated from first principles for specular and disordered (001) interfaces. Because of the symmetry mismatch in the minority-spin channel, the specular interface acts as an efficient spin filter with a transmitted current polarization between 98% and 89%. The resistance of a specular interface in the diffusive regime is comparable to the resistance of a few microns of bulk InAs. Symmetry breaking arising from interface disorder reduces the spin asymmetry substantially, and we conclude that efficient spin injection from Fe into InAs can only be realized using high-quality epitaxial interfaces.

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Compared to magnetic multilayers, semiconductor heterostructures can be made with low defect concentrations, resulting in large transport mean free paths at low temperatures. The large Fermi wavelength of charge carriers in doped semiconductors then leads to finite-size effects and a host of phenomena related to the electron waves maintaining their phase coherence over long distances.¹ Current interest in spin injection into semiconductors is motivated by a desire to combine the control over transport phenomena possible in semiconductors using external gates with the additional spin degree of freedom in ferromagnetic metals which has given rise to such new phenomena as oscillatory exchange coupling, giant magnetoresistance (GMR), and junction (or tunnel) magnetoresistance (JMR or TMR).²

While spin injection from a magnetic semiconductor using optical detection techniques was successfully demonstrated some years ago,^{3,4} spin injection from a metallic ferromagnet into a semiconductor was only realized very recently.⁵ Schmidt *et al.*⁶ pointed out that a basic obstacle to spin injection in this case is the large difference in their conductivities; the spin-independent resistivity of a semiconductor such as InAs is much larger than either the majority- or minority-spin resistivity of a ferromagnetic metal (FM) such as Fe. The resistances added in series are dominated by the spin-independent semiconductor term. Schmidt *et al.* did not take into account the possibility of a spin-dependent interface resistance which, if sufficiently large, could generate a spin-dependent potential drop at the interface.^{7,8}

Qualitative arguments have been given for the existence of such a spin dependence,⁹ and a number of studies based on free-electron models have appeared.^{10,11} Transition-metal atoms are characterized by fivefold orbitally degenerate d states with a large Hund's rule exchange splitting leading to large spin magnetic moments. In a solid these ten d states form complex band structures and Fermi surfaces. The origin of the spin dependence of the interface resistance in magnetic multilayers lies in the difference between how the majority- and minority-spin states match to the spin-degenerate electron states in a nonmagnetic metal (NM).^{12,13} By expressing the (mis)matching at the FM/NM interface in terms of the reflection and transmission matrices of scatter-

ing theory,¹⁴ the corresponding resistances can be calculated within the framework of the Landauer-Büttiker transport formalism.¹⁷⁻¹⁹ Because free-electron models do not describe realistically the electronic structure and magnetism of transition-metal elements and their interfaces with other materials, we have calculated the spin-dependent transmission for the Fe/InAs(001) system including the full electronic band structures and derive the corresponding interface resistances. We argue that spin injection should be observable for specular interfaces. However, we also show that introducing disorder into the interface layer greatly reduces the spin asymmetry. We focus on the special case of Fe/InAs because it forms an Ohmic contact. Since there is no Schottky barrier between these two materials, it should be possible to realize much larger currents than for systems such as Fe/GaAs where electrons must tunnel through this barrier.⁵

To calculate transmission and reflection matrices without introducing arbitrary fitting parameters, we use the local-density approximation (LDA) of density functional theory. The present implementation is based on the surface Green's function method²⁰ formulated for tight-binding linear muffin tin orbitals (TB-LMTO's).²¹ Because a minimal basis set is used, we are able to model the disorder with lateral supercells. The calculations were carried out in two stages. First the electronic structure, spin densities, and potentials of Fe/InAs were determined self-consistently using the layered TB-LMTO surface Green's function method.²⁰ To take account of the 5% lattice mismatch between the bulk crystal structures ($a_{\text{Fe}}=2.866 \text{ \AA}$, $a_{\text{InAs}}=6.058 \text{ \AA}$), we assume Fe to be tetragonal with its in-plane lattice constant matched to that of the cubic InAs substrate. The vertical lattice constant is contracted so that the Fe unit cell volume is the same as for the bulk material. To achieve reasonable space filling for InAs in the atomic sphere approximation,²¹ empty spheres were introduced in the interstitial positions in both In and As layers. At the interface the atomic sphere radii were set to the bulk values ($r_{\text{Fe}}=1.41 \text{ \AA}$ and $r_{\text{InAs}}=1.49 \text{ \AA}$) and the Fe-InAs distance was chosen so as to realize the local space filling. The correct band gap for InAs (which is found to be metallic in a straightforward LDA calculation) was obtained using a "scissors-operator" correction term. To form an

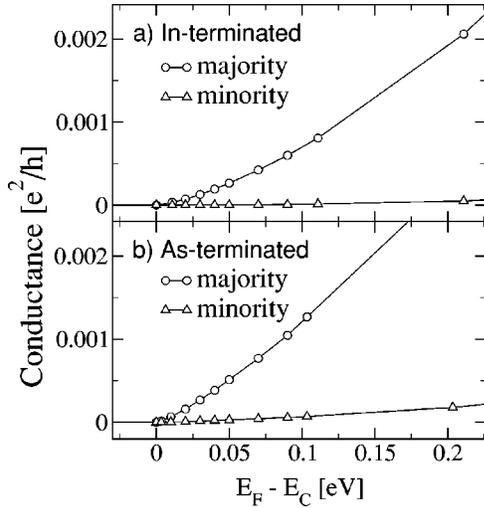


FIG. 1. Conductance of (a) In- and (b) As-terminated Fe/InAs interfaces (in units of e^2/h) as a function of the distance of the Fermi energy (E_F) from the bottom of the conduction band (E_C) for majority (\circ) and minority (\triangle) spins.

Ohmic contact, the Fermi level was positioned at the bottom of the InAs conduction band by using the coherent potential approximation (CPA) to substitute some of the trivalent In with quadrivalent Sn which acts as an electron donor. The atomic potentials were calculated self-consistently for the four monolayers of Fe and six layers of InAs closest to the interface.²² The CPA was also used to determine self-consistent potentials for disordered interfaces.²⁰ Using these potentials as input, the transmission coefficients $t_{\mu\nu}^\sigma(\mathbf{k}_\parallel)$ (μ and ν denote the incoming and transmitted Bloch waves, respectively) were calculated in a second step with a recently developed scheme based on the TB-LMTO method.¹⁹ To calculate the conductance, a summation must be carried out over the two-dimensional (2D) Brillouin zone (BZ). This was done with a \mathbf{k}_\parallel mesh density equivalent to 6.4×10^5 mesh points in the 2D BZ of a 1×1 interface unit cell.

In Fig. 1 the spin-dependent conductances for In- and As-terminated specular (\mathbf{k}_\parallel conserving) interfaces, $G_\sigma = \sum_{\mu, \nu, \mathbf{k}_\parallel} |t_{\mu\nu}^\sigma(\mathbf{k}_\parallel)|^2$, are shown as a function of the position of the Fermi energy (E_F) above the bottom of the conduction band (E_C) which is controlled by the doping in an experiment.²² For both terminations a large spin asymmetry is predicted. For $E_F - E_C = 0.02$ eV (corresponding to a doping concentration of about 10^{17} cm $^{-3}$, thus just in the metallic regime) the ratio G_\uparrow/G_\downarrow is about 110 for In and 18 for As termination and decreases slowly with increasing $E_F - E_C$. These ratios correspond to current polarization values [defined as $(G_\uparrow - G_\downarrow)/(G_\uparrow + G_\downarrow)$] of 98% and 89%, respectively.

The large spin dependence of the Fe/InAs interface scattering can be simply understood by analyzing the bulk band structures of both materials [shown in Fig. 2 for $\mathbf{k}_\parallel = 0$ (Γ point)]. Similar arguments have been used previously to analyze spin-polarized tunneling.^{15,16} The band structure of tetragonal Fe [Figs. 2(a) and 2(b)] differs slightly from the usual cubic case. However, the axial symmetry for the (001)

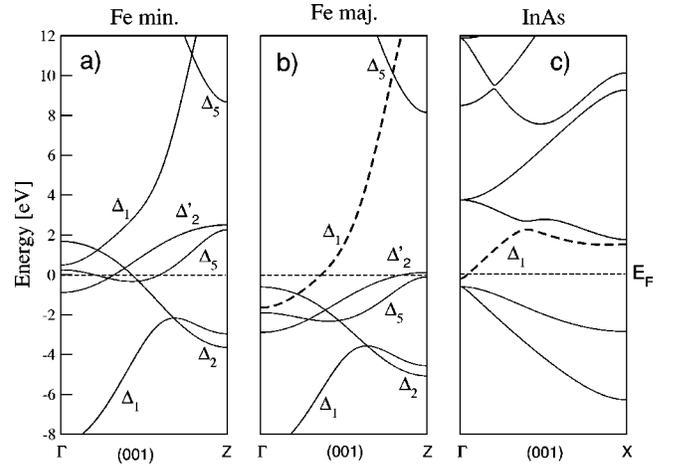


FIG. 2. Energy band structures of tetragonal Fe minority-spin states (a), majority-spin states (b), and InAs states (c) at $\mathbf{k}_\parallel = 0$ for $\mathbf{k} = (00k_z)$ perpendicular to the interface. The states with Δ_1 symmetry discussed in the text are shown as dashed lines.

growth direction is the same as in the cubic structure. Therefore the bands along this direction are labeled by the same irreducible representations of the point symmetry group and have the same orbital character as their cubic counterparts. We first note that the only states available for transport in InAs are concentrated around the center of the 2D BZ. The \mathbf{k}_\parallel -resolved transmission coefficients are therefore nonzero only close to the zone center. At $\mathbf{k}_\parallel = 0$, the single occupied InAs conduction band state has Δ_1 symmetry. Comparing the Fe majority- and minority-spin band structures, we immediately notice that only the majority bands have a state with this symmetry at (or close to) the Fermi level. Because the point group of the Fe/InAs(001) interface does not contain a fourfold rotation axis, the Δ'_2 Fe states can also couple to the Δ_1 states in InAs. However, the Δ'_2 states consist of localized in-plane d_{xy} orbitals, so this coupling is expected to be much smaller than between Δ_1 states. Though this symmetry argument is only strictly applicable at $\mathbf{k}_\parallel = 0$, the majority channel is expected to dominate the conductance. The qualitative predictions are confirmed by the full calculation. For $E_F - E_C = 0.1$ eV, the transmission probability is plotted in Fig. 3 as a function of \mathbf{k}_\parallel for an In-terminated interface. For majority spins, it has a maximum value ~ 0.64 at the Γ point. For the minority spins it is a local minimum with a value almost two orders of magnitude smaller.

The above results are only applicable in the ballistic regime where the resistance is dominated by interface scattering. To address the more realistic diffusive regime, we need to determine the interface resistance encountered when a specular interface is embedded in diffusive Fe and InAs. To do this, we use the expression derived by Schep *et al.*:¹⁷

$$R_{\text{Fe/InAs}} = \frac{h}{e^2} \left[\frac{1}{\sum |t_{\mu\nu}|^2} - \frac{1}{2} \left(\frac{1}{N_{\text{Fe}}} + \frac{1}{N_{\text{InAs}}} \right) \right],$$

where the first term is the inverse of the Landauer-Büttiker conductance and $N_{\text{Fe(InAs)}}$ is the Sharvin conductance (in

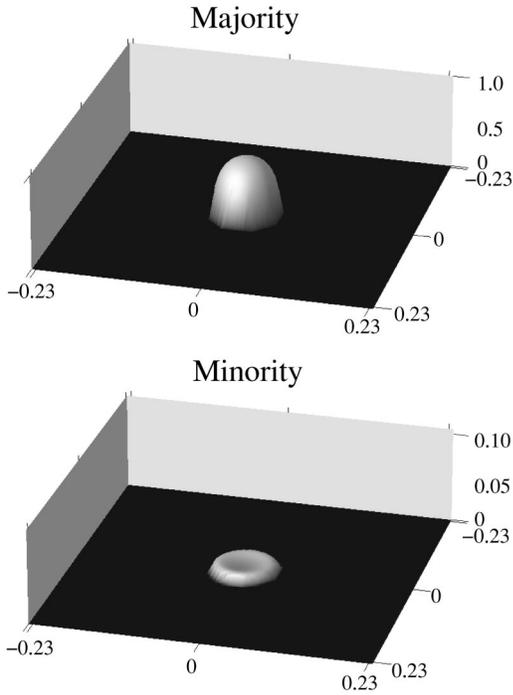


FIG. 3. The transmission probabilities as a function of k_{\parallel} for the In-terminated interface (the As-terminated case is qualitatively similar). The upper plot is for majority and the lower for minority spins. $E_F - E_C$ is equal to 0.1, and only the central 5% of the 2DBZ area is shown (the values on the horizontal axes are given in the units of $\sqrt{2}\pi/a_{\text{InAs}}$). Note that different vertical scales are used for majority and minority spins.

units of e^2/h) of Fe (InAs). Obviously, the Sharvin resistance correction is dominated by the contribution from the semiconductor.

For $E_F - E_C = 0.02$ eV we obtain values of $R^{\text{maj}} = 5.5 \times 10^4$ and $R^{\text{min}} = 7.1 \times 10^6$ $\text{f}\Omega \text{ m}^2$ for In termination and 2.1×10^4 , respectively, 5.2×10^5 $\text{f}\Omega \text{ m}^2$ for As termination. All these resistances are much larger than the resistances seen by electrons originating in the ferromagnetic layer within a spin-flip diffusion length of the interface⁶ which underlines the importance of interface properties (and not the bulk polarization) for injecting spins. Spin injection can occur in diffusive systems when the interface resistance is spin dependent and comparable to the resistance of the semiconductor layer.^{7,8} Within the free-electron model (with $m_{\text{eff}} = 0.04$) and assuming Thomas-Fermi screening of the impurity potential²³ we estimate the low-temperature resistivity of InAs with doping of 10^{17} cm^{-3} to be $\rho_{\text{InAs}} = 0.3 \times 10^{-4} \Omega \text{ m}$. The thickness L of InAs has a resistance comparable to the interface resistance $R_{\text{Fe/InAs}}$ when $L \sim R_{\text{Fe/InAs}}/\rho_{\text{InAs}}$ which yields values ranging from 0.7 μm (majority spin, As termination) to 240 μm (minority spin, In termination).

The large spin dependence of specular interface scattering discussed so far results directly from the symmetry of the Bloch states on either side of the interface. It is important to know whether the corresponding spin asymmetry will survive the interface disorder which is invariably present at real

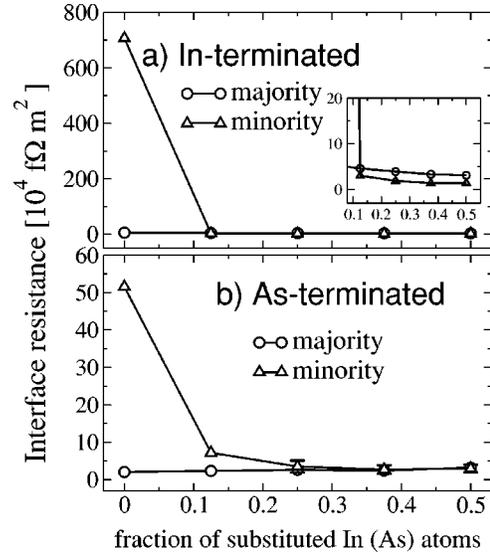


FIG. 4. Interface resistances for (a) In and (b) As termination as a function of the fraction of interfacial In or As atoms substituted by Fe for majority (\circ) and minority (\triangle) spins. The inset in (a) shows the same data with a blown-up ordinate scale. For both terminations the symmetry-induced spin asymmetry is strongly reduced by disorder.

interfaces. To address this question we performed calculations with 2×2 lateral supercells containing 8 In (As) atoms and 16 Fe atoms and introduced symmetry breaking by randomly replacing some of the interfacial In(As) atoms with iron. Figure 4 shows the majority- and minority-spin interface resistances as a function of the fraction of In (As) atoms which were replaced. The spread of values obtained for different configurations is indicated, where applicable, by vertical error bars. For both terminations we see a relatively weak variation in the majority channel. However, the large values of minority-spin interface resistances are suppressed by interface disorder and soon assume values comparable to the majority-spin values. This result suggests that the realization of the strong spin-filtering effect predicted in our calculations for In-terminated specular interfaces (and independently by Wunnicke *et al.*²⁴ for Fe/GaAs and Fe/ZnSe) requires very considerable care in preparing the interfaces. Since our findings are based on symmetry arguments, they should be equally applicable to epitaxial Fe/GaAs (Ref. 5) or Fe/AlGaAs (Ref. 25) if the Schottky barrier is sufficiently thin that carrier injection does not occur by thermionic emission over the barrier. When tunnel barriers composed of amorphous oxides are used for spin injection,²⁶ the symmetry arguments are most likely no longer valid. Such systems need to be studied in more detail.

The finding that disorder strongly *reduces* the high resistance of the minority-spin electrons by opening new transport channels which are symmetry forbidden for specular interfaces is quite similar to what was found for the Fe/Cr system by Xia *et al.*¹⁹

In conclusion, we have studied the transport properties of Fe/InAs(001) interfaces, taking into account the full elec-

tronic structure of both materials, and found strong spin selectivity of the transport through these interfaces provided that they are grown epitaxially with a very high degree of perfection.

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