Spin-orbit fields in ferromagnetic metal/semiconductor junctions

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The existence of the spin-orbit fields induced by the interface structure in Fe/GaAs junctions is proven from first-principles calculations. While the underlying symmetry of the fields follows that of the interface, the specific realization of the symmetry depends on the electron momentum and energy. The calculated atomic-layer-resolved expectation values of the Bloch states’ spins show that the spin-orbit fields peak at the GaAs side of the interface. The employed technique is applicable to ferromagnetic junctions in general.

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To manipulate electron spins one usually resorts to the magnetic field. Recent experimental advances show that the relativistic spin-orbit interaction can do the job as well. Indeed, spin-orbit coupling appears as an effective magnetic force acting on the electron spin and, equally important, on the electron motion. These effective magnetic—more descriptively spin-orbit—fields emerge as a collective effect of individual atomic spin-orbit couplings in systems lacking space inversion symmetry. By employing first-principles techniques, here we uncover the microscopic structure of the spin-orbit fields.

We demonstrate the origin of their effective spectral description widely used to study magnetic, transport, and optical manifestations of spin-orbit phenomena in solids. We visualize the charming patterns of the microscopic spin-orbit fields, atomic layer by layer, and show their interface origin for the technologically important case of Fe/GaAs nanojunctions recently used in tunneling magnetoresistance experiments. These spin-orbit fields give important microscopic clues in searching for vertical tunneling and lateral magnetotransport phenomena in single ferromagnetic layer metal/semiconductor junctions in which the interface, not the bulk, dictates the magnetic symmetry.

In solid-state systems lacking space inversion symmetry spin-orbit coupling (SOC) is manifested on the spectral level as an effective magnetic field whose direction and magnitude depend on the electron momentum. In other words, spin-up and spin-down electrons of the same momentum have different energies. The most prominent examples are the Dresselhaus spin-orbit coupling describing the effects of the bulk inversion asymmetry (BIA) as in zinc-blende semiconductors, and the Bychkov-Rashba spin-orbit coupling describing the effects of the structure inversion asymmetry (SIA), as in asymmetric quantum wells. Apart from semiconductor structures, where the Bychkov-Rashba coupling has been extensively studied, it has also been investigated in metallic surfaces, in graphene on a Ni substrate, and in Au and Ag monolayers on W(110) substrates.

Here we go beyond the effective spectral description. We ask how the effective spin-orbit fields (SOFs) are distributed in real space, what is their typical magnitude, functional form, and symmetry pattern. We explore these issues on the example of Fe/GaAs junctions in which the phenomenon of tunneling anisotropic magnetoresistance (TAMR) was observed and explained in terms of the interface-induced spin-orbit fields. The magnetization direction in Fe makes for a nice control knob orienting the spin, while the magnetic anisotropy is determined by the interface symmetry, not by the symmetry of the bulk materials. These two features allow for investigating the microscopic nature of the spin-orbit fields. Such ferromagnetic metal/semiconductor junctions are useful for room temperature spin injection and magnetotransport.

In earlier studies of SOC effects in surfaces and interfaces the SOC parameters have been extracted by fitting the energy bands close to the Γ point, assuming a Bychkov-Rashba-type SOC. This procedure, however, requires a priori knowledge of the specific form of the SOF and applies only to very small k-vectors. Here we introduce a procedure to obtain the form of the SOF for any k-point directly from ab-inito data. We illustrate this on a Fe/GaAs slab, in which the magnetization is perpendicular to the layers. This configuration allows for a simple relation between the spin-expectation values and SOF. By computing the spin expectation values from first principles, the specific vector pattern of the SOF, unknown a priori, is obtained. The results show a highly anisotropic SOC, which takes on different forms, from the ones known in semiconductor physics to more exotic ones for states away from the Γ point. One fascinating outcome is the possibility of flipping the anisotropy axis of the SOF when going from one band to another, consistent with the bias-induced inversion of the TAMR observed in experiments.

In order to deduce the analytical form of the SOC Hamiltonian at low electronic momenta in our Fe/GaAs slab, we propose a general model from which the SOF
can be extracted when contrasted with the \textit{ab-initio} data. The non-centrosymmetric GaAs layer is of the $D_{2d}$ symmetry, thus exhibiting the BIA spin-orbit coupling. The interface lowers the symmetry to $C_{2v}$ with the twofold rotation axis $C_2$ along the growth direction [001] [25]. The $C_{2v}$ symmetry accounts for both the BIA and SIA; the spin-orbit field lies in the plane of the slab, perpendicular to the growth direction. The most general SOC Hamiltonian consistent with $C_{2v}$ symmetry can be written for the in-plane momenta around the Γ point as

$$H_{so} = \alpha(k_x, k_y)k_x \sigma_y + \beta(k_x, k_y)k_y \sigma_x,$$

where $k_x$ and $k_y$ are the components of the in-plane wave vector $k$, $\sigma_x$ and $\sigma_y$ are the Pauli matrices, and $x$ and $y$ correspond to the diagonal [110] and [110] crystallographic directions in GaAs, respectively. The functional parameters $\alpha$ and $\beta$ are even in the momenta

$$\begin{align*}
\alpha(k_x, k_y) &= \alpha^{(0)} + \alpha^{(1)} k_x^2 + \alpha^{(2)} k_y^2 + \ldots , \\
\beta(k_x, k_y) &= \beta^{(0)} + \beta^{(1)} k_x^2 + \beta^{(2)} k_y^2 + \ldots ,
\end{align*}$$

The values of the expansion parameters $\alpha^{(i)}$, $\beta^{(i)}$ ($i = 0, 1, 2, \ldots$) determine the specific form of the SOF. For example if $\alpha^{(0)} = -\beta^{(0)} (\alpha^{(0)} = \beta^{(0)})$, $H_{so}$ reduces in the limit of small $k = |k|$ to the well known as Bychkov-Rashba field (linearized Dresselhaus SOCs). By introducing the SOF field

$$\mathbf{w}(k_x, k_y) = \left( \begin{array}{c} \beta(k_x, k_y) k_y \\ \alpha(k_x, k_y) k_x \\ 0 \end{array} \right),$$

Eq. (1) can be rewritten as $H_{so} = \mathbf{w}(k) \cdot \mathbf{\sigma}$, where $\mathbf{\sigma}$ is the vector of Pauli matrices.

When the magnetization is perpendicular to the layers the in-plane components of the spin are influenced by the SOC only. Since the exchange field dominates over the SOC, the spin is quantized largely along the magnetization direction, and the expectation values of the transverse components of the spin $\langle s \rangle$ can be obtained by considering $H_{so}$ as a perturbation. First order perturbation theory gives

$$\langle s_x \rangle = w_x / \Delta; \quad \langle s_y \rangle = w_y / \Delta,$$

where $\Delta$ is the exchange splitting energy and $\hbar = 1$. Using these relations, we can determine the specific form of $\mathbf{w}$, which provides an effective spatially averaged SOF of the system.

The small lattice mismatch between Fe (2.87 Å) and GaAs (5.65 Å) allows for the smooth epitaxial growth of Fe on a GaAs (001) surface. Early investigations of the stability of 1 × 1 Fe/GaAs interfaces within density functional theory [25] revealed that when more than two atomic layers of Fe are deposited on a GaAs (001) surface, the flat or partially intermixed interfaces are more stable than the fully intermixed one. The large $pd$ hybridization lowers the cohesive energy [26] and, therefore, the antibonding bonds between Fe and As are more stable than the Fe-Ga bonds. While the density functional calculations indicate that the As-terminated flat interface is more stable than the partially intermixed one [25], a recent Z-contrast scanning transmission electron microscopy reported a single plane of alternating Fe and As atoms at an Fe/AlGaAs interface [27]. Here we consider an ideal structure with an As-terminated flat interface. Our slab, encased in a 6 Å vacuum, contains 9 (001) atomic layers of GaAs with the diagonal lattice spacing $d = a/\sqrt{2} = 3.997$ Å and three atomic planes of bcc Fe.

The electronic structure of the ideal Fe/GaAs slab has been calculated using the full potential linearized augmented plane waves (LAPW) technique [28] and a generalized gradient approximation for the exchange-correlation functional [29]. The SOC has been treated by solving the Dirac equation for the core electrons, while the valence electrons are treated within second variational method.

The band structure of the Fe/GaAs heterostructure along the high symmetry lines connecting the S − Γ − X points in the Brillouin zone (BZ) is shown in Fig. 1 for a magnetization orientation along the [001] direction. Atomic-like contributions to the states coming from the interface atoms are emphasized by filled (red) and open (blue) circles for spin-up and spin-down, respectively.

![Figure 1: Calculated band structure for the Fe/GaAs slab and magnetization along [100]. The states with spin-up (spin-down) at the Fe/GaAs interface are emphasized with red filled (blue open) circles whose radii are proportional to the corresponding charge density at the interface. The inset shows the As-terminated flat 1 × 1 interface model assumed in the study.](image)

We now explore the SOF in our heterostructure. We take bands ($n = 1, \ldots, 5$) close to the Fermi level (see the band labels in Fig. 1) and calculate the expectation values of the transverse spin components close to the Γ point. Thus by keeping only the linear terms in $k$ of the SOF and fitting $w_x / \Delta$ and $w_y / \Delta$ to the \textit{ab-initio} data for $\langle s_x \rangle$ and $\langle s_y \rangle$, respectively, we can determine the band-resolved Bychkov-Rashba-type, $\alpha = (\alpha^{(0)} - \beta^{(0)}) / 2$, and
Dresselhaus-type, $\gamma = (\alpha^{(0)} + \beta^{(0)})/2$, parameters. They are shown in Table I. Interestingly, the product $\alpha \gamma$ changes sign from band $n = 1$ to $n = 2$, indicating a flipping of the symmetry axis of the SOF (compare left and right panels in Fig. 2). While typically the ratio $\alpha/\gamma$ is measured [30], here by choosing $\Delta = 2$ eV, which is within $\pm 20\%$ range of the exchange splitting of the $\Gamma_{12}$ and $\Gamma_{25}'$ states in bcc Fe, we obtain absolute values for $\alpha$ and $\gamma$. The extracted values are similar to those found in semiconductors [3].

| band label $n$ | 1  | 2  | 3  | 4  | 5  |
|---------------|----|----|----|----|----|
| $\alpha/\gamma$ | -0.934 | 1.161 | 1.504 | 0.805 | 1.866 |
| $\alpha$ [eVÅ] | -0.033 | 0.125 | 0.091 | -0.010 | 0.090 |
| $\gamma$ [eVÅ] | 0.035 | 0.108 | 0.060 | -0.013 | 0.048 |

TABLE I: Band-resolved Bychkov-Rashba-type and Dresselhaus-type spin-orbit coupling parameters. The states close to the Fermi level (see labels in Fig. 1) and momenta close to the $\Gamma$ point with $k = \pi/100d$ are considered for fitting the values. The exchange splitting $\Delta = 2$ eV.

We now concentrate on the two bands in vicinity of the Fermi level. The left panel in Fig. 2 corresponds to band $n = 1$, while the right one to the $n = 2$. The three different cases, $k = \pi/50d, \pi/8d$ and $\pi/5d$, are considered for the plots of SOF, $\mathbf{w}(k)$ (bottom parts), and the polar plots of the field strength $w = |\mathbf{w}(k)|$ (upper parts) in units of the exchange splitting $\Delta$. Close to the $\Gamma$ point the SOF resemble the interference of Bychkov-Rashba-type and Dresselhaus-type SOCs (see Fig. 2a). However, away from the $\Gamma$ point higher in $k$ terms become relevant and more exotic patterns in the SOF manifest (see Figs 2b,c). Starting with $k = \pi/50d$, where linear terms in the SOF are dominant, the cubic terms in the SOF are already present for $k = \pi/8d$, and they get more pronounced together with terms of fifth and higher orders for $k = \pi/5d$. Those terms we have to include for fitting the SOF field model (see curves in polar plots in Fig. 2) to the ab-inito data (circles). The $C_{2v}$ symmetry of the SOF is preserved for all $k$.

In order to investigate from where the major contribution to the SOC in Fe/GaAs heterostructure comes, we calculate the layer-resolved SOF. In Fig. 3 we plot the Bychkov-Rashba-type and Dresselhaus-type parameters for each atomic layer within our slab for two bands, $n = 1, 2$. The values have been obtained by fitting the linearized SOF to the ab-inito data. By studying the nature of the bands we find that the band $n = 1$ exhibits an interface character, while the band $n = 2$ is a surface state corresponding to the As-terminated (001) surface of the slab (see also band character in the vicinity of the $\Gamma$ point in Fig. 1). In both cases the maximal values of the SOC parameters are near the Fe/GaAs interface, and especially, at the next nearest Ga atom plane as can be seen in Fig. 3. The maximal effect of the SOC is shifted to the GaAs region due to the fact that the interface As plane is in direct contact to the Fe and gets strongly polarized due to the proximity effect. Consequently, the in-plane spin components, and therefore, the SOF components are considerably reduced. Figure 3 also reveals that the main contribution to the SOF comes from the interface even in the case of the surface band ($n = 2$).

The SOFs may look different for different geometries,
growth directions and/or different materials compositions (say, Fe/GaAs/Au) \cite{24}, but the methodology presented here can be applied to rather generic cases. The SOF symmetry is crucial for fully understanding spin-injection from ferromagnets into semiconductors as well as magnetic and transport anisotropic properties in such junctions. This interface vector field can be observed by X-ray magnetic circular dichroism, while its manifestations are to be seen in magnetotransport experiments which effectively sample, with certain weights, the whole $k$-space.

The extracted magnitudes of $\alpha$ and $\gamma$ are within the range found in semiconductors \cite{2}. However, the magnitude of the SOC parameters can differ considerably from band to band. Similarly for the sign. This has observable consequences in transport properties of Fe/GaAs heterojunctions such as the TAMR \cite{2}. It has already been proposed that the $C_{2v}$ symmetry of the TAMR in ferromagnet/semiconductor-based tunnel junctions originates from the interference between Bychkov-Rashba-type and Dresselhaus-type SOCs and that the sign of the TAMR is determined by the product $\alpha \gamma$ (here $\alpha$ and $\gamma$ refer to the average values of the corresponding SOC parameters) \cite{2,3}. It has also been suggested that the sign of $\alpha \gamma$ (and therefore that of the TAMR) could be tuned by an external bias \cite{3,24}. This possibility is consistent with our results, in particular for the bands $n = 1, 2$, where the product $\alpha \gamma$ changes sign.

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