Spin-orbit induced anisotropy in the tunneling magnetoresistance of magnetic tunnel junctions

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The effects of the spin-orbit interaction on the tunneling magnetoresistance of magnetic tunnel junctions are investigated. A model in which the experimentally observed two-fold symmetry of the anisotropic tunneling magnetoresistance (TAMR) originates from the interference between Dresselhaus and Bychkov-Rashba spin-orbit couplings is formulated. Bias induced changes of the Bychkov-Rashba spin-orbit coupling strength can result in an inversion of the TAMR. The theoretical calculations are in good agreement with the TAMR experimentally observed in epitaxial Fe/GaAs/Au tunnel junctions.

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The tunneling magnetoresistance (TMR) effect refers to ferromagnet/insulator/ferromagnet heterojunctions, in which the magnetoresistance exhibits a strong dependence of the relative magnetization directions in the different ferromagnetic layers and their spin polarizations. Because of this peculiarly strong asymmetric behavior of the magnetoresistance, TMR devices find multiple uses ranging from magnetic sensors to magnetic random access memory applications.

It came as a surprise that the tunneling magnetoresistance may strongly depend on the absolute orientation of the in-plane magnetization directions with respect to a fixed crystallographic axis, as experimentally observed in Refs. 5,6,7. The phenomenon was termed tunneling anisotropic magnetoresistance (TAMR). Even more intriguing is the observation of the TAMR effect in heterojunctions such as (Ga,Mn)As/AlOx/Au and Fe/GaAs/Au sandwiches, where only one of the layers is magnetic, and for which the TMR effect is absent. It has been recognized that the origin of the TAMR effect is related to the spin-orbit interaction (SOI) 5,6,7,8,9,10. However, the nature and details of the underlying mechanism producing the TAMR remains a puzzle. In fact, it has become clear that the responsible mechanisms for the TMR can be different in different systems. The (Ga,Mn)As/Alumina/Au heterojunctions 5 and in (Ga,Mn)As nanoconstrictions 11 has been associated with the anisotropic density of states in the ferromagnet (Ga,Mn)As and was theoretically modelled by introducing strain effects. First-principle calculations for the case of an Fe(001) surface have recently demonstrated the appearance of the TAMR effect due to the shifting of the resonant surface band via Rashba SOI when the magnetization direction changes. Furthermore, it has recently been observed that the symmetry axis of the two-fold symmetry of the TAMR in Fe/GaAs/Au heterojunctions can be flipped by changing the bias voltage.

Here we formulate the model proposed to explain the experimental results of Ref. 9, in which the two-fold symmetry of the TAMR observed in epitaxial ferromagnet/semiconductor/normal metal junctions originates from the interface-induced $C_{2v}$ symmetry of the SOI arising from the interference of Dresselhaus and Bychkov-Rashba spin-orbit couplings. Such interference effects have already been investigated in lateral transport in 2D electron systems. The symmetry, which is imprinted in the tunneling probability becomes apparent in the contact with a magnetic moment.

Consider a ferromagnet/semiconductor/normal-metal tunnel heterojunction. The semiconductor is assumed to lack bulk inversion symmetry (zinc-blende semiconductors are typical examples). The bulk inversion asymmetry of the semiconductor together with the structure inversion asymmetry of the heterojunction give rise to the Dresselhaus 13,14,15,16 and Bychkov-Rashba 14 SOIs, respectively. The interference of these two spin-orbit couplings leads to a net, anisotropic SOI with a $C_{2v}$ symmetry which is transferred to the tunneling magnetoresistance when the electrons pass through the semiconductor barrier. The model Hamiltonian describing the tunneling across the heterojunction reads

$$H = H_0 + H_Z + H_{BR} + H_D. \quad (1)$$

Here

$$H_0 = -\frac{\hbar^2}{2}\nabla \left[\frac{1}{m(z)}\nabla\right] + V(z), \quad (2)$$

with $V(z)$ the conduction band profile defining the potential barrier along the growth direction ($z = 001$) of the heterostructure. The electron effective mass $m(z)$ is assumed to be $m = m_e$ in the central (semiconductor) region and $m = m_l = m_r \approx m_0$ (here $m_0$ is the bare electron mass) in the left (ferromagnetic) and right (normal metal) layers.

The spin splitting due to the exchange field in the ferromagnetic layer is given by

$$H_Z = \frac{\Delta(z)}{2} \mathbf{n} \cdot \sigma. \quad (3)$$

Here $\Delta(z)$ represents the exchange energy, $\sigma$ is a vector whose components are the Pauli matrices, and $\mathbf{n}$ is a unit vector defining the spin quantization axis determined by
the in-plane magnetization direction in the ferromagnet. The Zeeman splitting in the semiconductor and normal metal can be neglected.

The Dresselhaus SOI can be written as \(^{15,16,17,18,19}\)

\[
H_D = \frac{\hbar}{2} \left( \sigma_x p_x - \sigma_y p_y \right) \frac{\partial}{\partial z} \left( \gamma(z) \frac{\partial}{\partial z} \right),
\]

(4)

where \(x\) and \(y\) correspond to the \([100]\) and \([010]\) directions, respectively. The Dresselhaus parameter \(\gamma(z)\) has a finite value \(\gamma\) in the semiconductor region, where the inversion bulk inversion asymmetry is present, and vanishes elsewhere. Note that because of the step-like spatial dependence of \(\gamma(z)\), the Dresselhaus SOI [Eq. (4)] implicitly includes the interface and bulk contributions.\(^{15}\)

The Bychkov-Rashba SOI due to the interface inversion asymmetry is incorporated in the model through the term\(^{20}\)

\[
H_{BR} = \frac{\hbar}{2} \sum_{i=l,r} \alpha_i (\sigma_x p_y - \sigma_y p_x) \delta(z - z_i),
\]

(5)

where, \(\alpha_i\) (\(\alpha_r\)) denotes the SOI strength at the left (right) interface \(z_i = 0\) (\(z_r = d\)). The Bychkov-Rashba SOI contribution inside the semiconductor can be neglected here.

Assuming that the in-plane wave vector \(k_z\) is conserved throughout the heterostructure, one can decouple the motion along the growth direction \((z)\) from the other spatial degrees of freedom. The \(z\) component of the scattering states in the left (ferromagnetic) region [eigenstates of the Hamiltonian (1)] with eigenenergy \(E\) can be written as

\[
\Psi^{(l)}_{\sigma} = \frac{e^{ik_z z}}{\sqrt{k_z}} \chi_\sigma + r_{\sigma,\sigma} e^{-ik_z z} \chi_{\bar{\sigma}} + r_{\sigma,-\sigma} e^{-ik_z z} \chi_{-\sigma},
\]

(6)

where \(z \leq 0\), \(\chi_{\sigma}\) represents a spinor corresponding to a spin parallel (\(\sigma = \uparrow\)) or antiparallel (\(\sigma = \downarrow\)) to the magnetization direction defined by the vector \(n\), and \(k_z\) is the corresponding \(z\) component of the wave vector in the left region. In the central (semiconductor) region \((0 < z < d)\) we have\(^{17,18}\)

\[
\Psi^{(s)}_{\sigma} = (A_{\sigma,i} e^{q_i z} + B_{\sigma,i} e^{-q_i z}) \zeta_i,
\]

(7)

where \(q_{\pm} = (1 \pm 2m_e^s \gamma k_z / \hbar^2)^{-1/2} q_0\) (with \(q_0\) being the \(z\) component of the wave vector in the barrier in the absence of SOI) and \(\zeta_i\) are spinors corresponding to spins parallel (+) and antiparallel (−) to the direction \(k_{\parallel} \times z\), which is the quantization direction in the barrier. In the right (normal metal) region \((z \geq 0)\) the scattering states read

\[
\Psi^{(r)}_{\sigma} = t_{\sigma,\sigma} e^{i\kappa(z-d)} \chi_{\sigma} + t_{\sigma,-\sigma} e^{i\kappa(z-d)} \chi_{-\sigma},
\]

(8)

where \(\kappa_{\sigma}\) is the corresponding \(z\) component of the wave vector in the right region. The expansion coefficients in Eqs. (6) - (8) can be found by applying standard matching conditions at each interface.\(^{10,19}\) Once the wave function is determined, the particle transmissivity can be calculated from the relation

\[
T_{\sigma}(E, k_{\parallel}) = \text{Re} |\kappa_{\sigma}| t_{\sigma,\sigma}|^2 + \kappa_{-\sigma} |t_{\sigma,-\sigma}|^2.
\]

(9)

The current flowing along the heterojunction then is

\[
I = \sum_{\sigma = \uparrow, \downarrow} I_{\sigma},
\]

(10)

where

\[
I_{\sigma} = \frac{e}{(2\pi)^3 \hbar} \int dE d^2 k_{\parallel} T_{\sigma}(E, k_{\parallel}) |f_i(E) - f_r(E)|,
\]

(11)

and \(f_i(E)\) and \(f_r(E)\) are the electron Fermi-Dirac distributions with chemical potentials \(\mu_i\) and \(\mu_r\) in the left and right leads, respectively.

The TAMR refers to the changes of the tunneling magnetoresistance \(R\) when varying the magnetization direction \(n\) of the magnetic layer with respect to a fixed axis. Here we assume the magnetoresistance \(R_{[110]}\), measured when \(n\) points in the \([110]\) crystallographic direction as a reference. The TAMR is then given by

\[
\text{TAMR}_{[110]}(\theta) = \frac{R(\theta) - R_{[110]}}{R_{[110]}} = \frac{I_{[110]} - I(\theta)}{I(\theta)},
\]

(12)

where \(\theta\) is the angle between the magnetization direction \(n = (\cos \theta, \sin \theta, 0)\) and the \([100]\) crystallographic axis. We also find it useful to define the tunneling anisotropic spin polarization (TASP) as

\[
\text{TASP}_{[110]}(\theta) = \frac{P_{[110]} - P(\theta)}{P(\theta)}.
\]

(13)

The TASP measures the changes in the tunneling spin polarization\(^{2,4,17}\) \(P = (I_{-} - I_{+}) / I\) (which is a measurable quantity accounting for the polarization efficiency of the transmission) when rotating the in-plane magnetization in the ferromagnet.

For a concrete demonstration of the proposed theoretical model we performed zero-temperature calculations of the TAMR in an epitaxial Fe/GaAs/Au heterojunction similar to that used in the experimental observations reported in Ref. \(^{4}\). We use the value \(m_e = 0.067 m_0\) for the electron effective mass in the central (GaAs) region. The barrier width and high (measured from the Fermi energy) are, respectively, \(d = 80 \ \text{Å}\) and \(V_b = 0.75 \ \text{eV}\), corresponding to the experimental samples in Ref. \(^{4}\). For the Fe layer a Stoner model with the majority and minority spin channels having Fermi momenta \(k_{F\uparrow} = 1.05 \times 10^8 \text{ cm}^{-1}\) and \(k_{F\downarrow} = 0.44 \times 10^8 \text{ cm}^{-1}\) respectively, is assumed. The Fermi momentum in Au is taken as \(k_F = 1.2 \times 10^8 \text{ cm}^{-1}\).\(^{24}\) We consider the case of relatively weak magnetic fields (specifically, \(B = 0.5 \text{ T}\)). At high magnetic fields, say, several Tesla, our model is invalid as it does not include cyclotron effects relevant...
when the cyclotron radius becomes comparable to the barrier width.

The Dresselhaus spin-orbit parameter in GaAs is \( \gamma = 24 \, \text{eV} \, \text{Å}^3 \).\(^{16,17,18}\) The values of the Bychkov-Rashba parameters \( \alpha_l \) and \( \alpha_r \) [see Eq. (3)] are not known for metalsemiconductor interfaces. Due to the complexity of the problem, a theoretical estimation of such parameters requires first principle calculations including the band structure details of the involved materials, which is beyond the scope of the present paper. Here we assume \( \alpha_l \) and \( \alpha_r \) as phenomenological parameters. In order to investigate how does the degree of anisotropy depend on these two parameters we performed calculations of the ratio \( R_{[110]} / R_{[\bar{1}10]} \) (which is a measure of the degree of anisotropy)\(^2\) as a function of \( \alpha_l \) and \( \alpha_r \). The results are shown in Fig. 1 where one can appreciate that the size of this ratio (and, consequently, of the TAMR) is dominated by \( \alpha_l \). Then, since the values of the TAMR are not very sensitive to the changes of \( \alpha_r \) we can set this parameter, without loss of generality, to zero. This leaves \( \alpha_l \) as a single fitting parameter when comparing to experiment. Such a comparison is shown in Fig. 2(a) for different values of the bias voltage. The agreement between theory and experiment is very satisfactory. The values of the phenomenological parameter \( \alpha_l \) are determined by fitting the theory to the experimental value of the ratio \( R_{[\bar{1}10]} / R_{[110]} \) and this is enough for our theoretical model to reproduce the complete angular dependence of the TAMR, i.e., the proposed model is quite robust. Assuming that the interface Bychkov-Rashba parameters are voltage dependent\(^4\) (unlike \( \gamma \), which is a material parameter) we perform the same fitting procedure for the available experimental data corresponding to different bias voltages and extract the bias dependence of \( \alpha_l \) [see the inset in Fig. 2(a)], from which we estimate the value \( \alpha_l \approx 23 \, \text{meV} \, \text{Å}^2 \) at zero bias. This value is comparable to the corresponding value of the interface Bychkov-Rashba parameter \( \alpha_l \approx 27 \, \text{meV} \, \text{Å}^2 \) obtained from a five level \( k \cdot p \) model\(^{25}\) for an InAs/GaAs interface. Selecting InAs/GaAs for comparison with Fe/GaAs we only wish to show that our fitted values have reasonable magnitude, not differing too much from known values in semiconduc-

![FIG. 1: Values of the ratio \( R_{[110]} / R_{[\bar{1}10]} \) as a function of the interface Bychkov-Rashba parameters \( \alpha_l \) and \( \alpha_r \).](image1)

![FIG. 2: (a) Angular dependence of the TAMR in an Fe/GaAs/Au tunnel heterojunction for different values of the bias voltage \( V_{bias} \). Solid lines corresponds to our theoretical results while symbols represent the experimental data (conveniently mirrored) as deduced from Ref. 4. The values of the phenomenological parameter \( \alpha_l \) have been determined by fitting the theory to the experimental values of the ratio \( R_{[\bar{1}10]} / R_{[110]} \) for each value of \( V_{bias} \). The extracted bias dependence of \( \alpha_l \) is shown in the inset. (b) Angular dependence of the TAMR for different barrier widths.](image2)
where $\langle k \rangle$ represents average over $k_{ij}$. Note that the first order term vanishes after average over $k_{ij}$ since $w(k_{ij}) = -w(-k_{ij})$. Taking into account Eqs. (12), (15), and (16) one obtains the following approximate expression for the TAMR

$$T_{a} = \frac{\langle \alpha \gamma T^{(2)}(k_{ij}) \rangle}{\langle T^{(0)}(k_{ij}) \rangle} \propto \alpha \gamma \langle \sin(2\theta) \rangle - 1,$$

where the arguments of the expansion coefficients $T^{(0)}$ and $T^{(2)}$ have been omitted for brevity. The angular dependence in Eq. (17) is consistent with that found experimentally, as well as that obtained from the full theoretical calculations [see Fig. 2(b)]. One can clearly see from Eq. (17) that bias-induced changes of the sign of the Bychkov-Rashba parameter $\alpha_1$ lead to an inversion of the TAMR. When $\alpha_1 \gamma = 0$, the two-fold TAMR is suppressed. To put in words, the Bychkov-Rashba (or Dresselhaus) term by itself cannot explain the observed $C_{2v}$ symmetry. The suppression of the TAMR is approximately realized in Fig. 2(a) for the case of a bias voltage of 50 mV.

The above model neglects the contribution of the spin-orbit-induced symmetries of the involved bulk structures. Say, Fe exhibits a four-fold anisotropy, which should be reflected in the tunneling density of states. The fact that this is not seen in the experiment suggests that this effect is smaller than the two-fold symmetry considered in our model.

Another system parameter that can influence the size of the TAMR is the width of the barrier. The angular dependence of the TAMR for the case of $V_{bias} = -90$ meV is displayed in Fig. 2(b) for different values of the barrier width $d$. As clearly seen in Fig. 2(b), our model predicts an increase of the TAMR when increasing the width of the barrier.

Finally, we show the angular dependence of the TASP [see Eq. (13)] in Fig. 3 for different values of the bias voltage. The anisotropy of the tunneling spin polarization indicates that the amount of transmitted and reflected spin at the interfaces depends on the magnetization direction in the Fe layer, resulting in an anisotropic spin local density of states at the Fermi surface and showing spin-valve-like characteristics.

In summary, we have formulated a theoretical model in which the two-fold symmetry of both the TAMR and the TASP in epitaxial ferromagnet/semiconductor/normal-metal heterojunctions originates from the interplay between the Dresselhaus and Bychkov-Rashba SOIs. Our theoretical results for epitaxial Fe/GaAs/Au heterojunctions are in good agreement with the available experimental data.

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Eq. (5) can be well justified at semiconductor interfaces. We propose it here as a phenomenological model for metal/semiconductor interfaces, as the simplest description of the interface-induced SOI symmetry. For metallic surfaces the Bychkov-Rashba SOI has already been investigated. We assume that electrons with small transverse momenta $p_x$ and $p_y$ have sizable tunneling probabilities, justifying the linear character of the SOI.

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