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Theory of tunneling magnetoresistance of Fe/GaAs/Fe(001) junctions

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We investigate theoretically spin-dependent transport through an epitaxial Fe/GaAs/Fe(001) tunnel junction with and without spin-orbit interaction. Calculations neglecting spin-orbit interaction and the effect of *d* orbitals on the GaAs band structure predict that the tunneling magnetoresistance (TMR) should increase with increasing thickness of GaAs barrier and approach values close to the perfect spin-valve limit. However, when *d* orbitals and, in particular, spin-orbit interaction is included the TMR ratio saturates rapidly with GaAs thickness to a rather modest value of about 30% when the Fermi level E_F lies in the middle of the GaAs gap. This unexpectedly small value cannot be explained by spin-orbit interaction alone. It is shown that the underlying reason for this is the presence of a resonance in the minority-spin band structure of the Fe/GaAs/Fe trilayer lying close to the center of the gap. Investigation of the dependence of the TMR on the height of the GaAs barrier (position of the Fermi energy E_F in the gap) shows that the TMR of a perfect junction is strongly enhanced when E_F lies at the resonance in the minority-spin channel. However, we show that any small asymmetry of the junction removes the TMR peak and reduces the TMR to small values, of the order of 50%, for a rather large interval of values of E_F in the vicinity of the middle of the GaAs gap. We thus conclude that the spin-orbit coupling leads to saturation of the TMR with GaAs thickness, but the saturation value is determined by the presence of the resonance.

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I. INTRODUCTION

Strong efforts have been made in the last decade to achieve injection of spin-polarized current into semiconductors. This work has been motivated by the goal of combining spintronics with conventional semiconductor-based microelectronics. However, the spin polarization obtained in early experiments on injection from a transition-metal ferromagnet, such as Fe, into a semiconductor was very low. This was explained by Schmidt *et al.*[1] who pointed out that in the diffusive regime the conductance mismatch between ferromagnet (FM) and semiconductor (SC) creates a "fundamental obstacle" to successful spin injection from a metallic ferromagnet to a semiconductor. This obstacle can be removed by inserting a tunneling spin-polarized slab between the FM and SC interfaces. Such a tunneling slab can be either an intrinsic Schottky barrier[2,3] or an extrinsic tunneling barrier.[4,5]

An alternative approach is to attempt to mimic the extraordinary success of spin-polarized tunneling in Fe/MgO/Fe junctions and work in the ballistic regime. In this regime the argument of Schmidt *et al.*,[1] based on a simple resistor model of the FM/SC/FM interface, does not apply. Experimentally such a regime can be realized, for example, in the case of a tunneling FM/SC/FM junction.[6,7] Some previous nonrelativistic *ab initio* calculations of spin-dependent transport in Fe/GaAs/Fe(001) trilayer predicted a strong magnetoresistance and a high polarization of the current at zero bias[8,9] approaching the ideal 100%. The reason for such a very high spin polarization in the ballistic regime is that majority-spin Δ_1 electrons incident from Fe perpendicular to the interface couple strongly to the Δ_1 band in GaAs. The majority-spin electrons can thus easily cross the Fe/GaAs interface. On the other hand, there is no such Δ_1 band present for minority-spin electrons in Fe and the Δ_2 state in Fe couples only weakly to the Δ_1 band in GaAs. The minority-spin electrons are, therefore, strongly reflected from the interface. These arguments suggest that a very high spin polarization in GaAs should be realized in the ballistic regime for a perfect Fe/GaAs(001) interface. However, Popescu *et al.*[10,11] showed that in a fully relativistic approach, the spin-orbit coupling effect leads to a reduction in the tunneling magnetoresistance (TMR). Their work revealed the importance of including spin-orbit coupling when studying spin-dependent transport through GaAs. Thus, even in the ballistic regime there exists a "fundamental physical obstacle" which prevents the expected near 100% spin polarization of electrons injected from Fe to GaAs from being achieved.

There is also experimental evidence which indicates that the role of spin-orbit interaction in GaAs is important. In experiments on an Fe/GaAs/Fe junction a low TMR (Ref. 6) was measured even for an epitaxial structure.[7] The low polarization of the current measured in these experiments was attributed by the authors to spin-flip scattering taking place in the semiconductor. The importance of spin-orbit interaction in tunneling through GaAs was also confirmed by the recent observation of a strong tunneling anisotropic magnetoresistance in Fe/GaAs/Au tunnel junction.[12]

In this paper we investigate spin-dependent transport through a Fe/GaAs/Fe(001) tunnel junction in a tight-binding approach with and without spin-orbit interaction. Calculations neglecting spin-orbit interaction and the effect of *d* orbitals on the GaAs band structure predict that the TMR should increase with increasing thickness of GaAs barrier and approach values close to the perfect spin-valve limit. When *d* orbitals and, in particular, spin orbit is included, the TMR ratio is reduced, as was previously shown by Popescu *et al.*[10,11] However, their calculation was only for the Fermi level E_F located precisely in the middle of the GaAs gap. In fact, it is well known that Fe/GaAs has an interface state for minority-spin carriers lying very close to the middle of the gap which leads to a strong resonant enhancement of the minority-spin conductance.[9,13,14] It follows that this resonance should have a very strong effect on the TMR of an Fe/GaAs/Fe junction which could alter the results significantly depending on the precise position of E_F in the gap (GaAs barrier height). This, in turn, is dependent on factors such as interface quality. In this paper we pursue these ideas and explore the effect of spin-orbit coupling on the TMR of a GaAs junction as function of the GaAs thickness and the barrier height, i.e., position of E_F in the GaAs gap.

We find that the effect of spin-orbit coupling is to cause saturation of the TMR with GaAs thickness, however, the saturation value depends critically on the barrier height. For values of E_F far from the resonance the TMR is large (over 1000%) and the effect of spin-orbit coupling is to reduce it by about a factor of two. However, when E_F lies closer to the resonance the situation becomes more complicated. For a perfect symmetric junction the TMR has a large peak (about 5000%) at the resonance but is almost zero on either side of the peak. For a slightly asymmetric junction the TMR peak is removed and the TMR saturates to modest values. This complicated behavior of the TMR is analyzed in terms of the interplay between the spin-orbit coupling and the resonance in the conductance of the minority-spin channel.

II. MODEL

We describe the band structure of the Fe electrodes and GaAs interlayer using a tight-binding parametrization. The electron wave functions are decomposed in a basis of atomic orbitals and the Hamiltonian of the system is described by a set of parameters obtained by fitting to the experimental or *ab initio* calculated band structures. The Fe bands were fitted in a sp^3d^5 basis to the *ab initio* band structure of bcc Fe.[15] The valence bands of GaAs can be described using s and p electrons.[16] However, it has been shown by Vogl *et al.* that a simple sp^3 orbital basis is not sufficient to reproduce the shape of the conduction bands accurately.[17] The problem was first resolved by introducing an excited s state called s^* which greatly improved the effective masses of the conduction bands. Later work by Jancu *et al.*[18] showed that to accurately describe the band structure above the gap, d states must also be included. For the sake of comparison and to show the importance of these d states in the ballistic transport through GaAs, we performed our calculations using two alternative sets of parameters: (1) a simple model using an sp^3 orbital basis derived by Chadi and Cohen.[16] The parameters in this model were fitted to reproduce the experimental band gap and the effective masses of the valence bands.

(2) A more complete model employing an $sp^3d^5s^*$ orbital basis which was derived by Jancu *et al.*[18] The parameters of this model were fitted to the experimental band structure and also to density-functional theory calculations using local-density approximation (LDA)+GW approximation. The band structures for both these models are shown in Figs. 1(a) and 1(b).

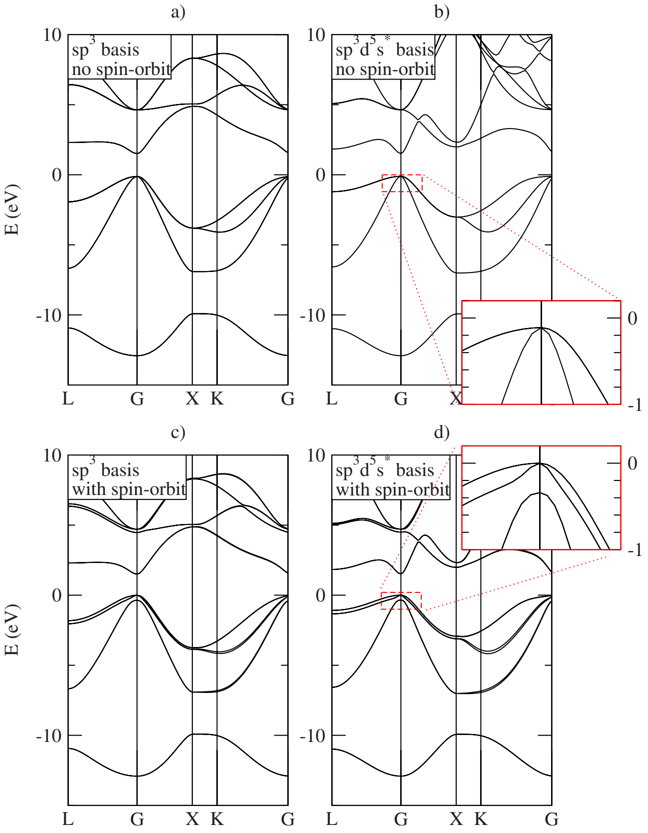


FIG. 1. (Color online) Band structure of GaAs for the two sets of tight-binding parameters with and without spin-orbit coupling: (a) sp^3 basis without spin orbit, (b) $sp^3d^5s^*$ basis without spin orbit, (c) sp^3 basis with spin orbit, and (d) $sp^3d^5s^*$ basis with spin orbit.

Spin-orbit coupling strongly affects the band structure of GaAs. The splitting Δ_{so} of the valence bands at the $\bar{\Gamma}$ point due to spin-orbit coupling is 0.35 eV.[19] Such a large splitting cannot be neglected when compared to the band gap, which is 1.52 eV for GaAs. We have, therefore, included the spin-orbit coupling by adding a spin-orbit term to the intra-atomic p-orbital elements of our tight-binding Hamiltonian. The spin-orbit Hamiltonian is given by $\xi_X \hat{\mathbf{L}}.\hat{\mathbf{S}}$, where $\hat{\mathbf{L}}$ is the orbital moment operator, $\hat{\mathbf{S}}$ is the spin moment operator, and ξ_X is the spin-orbit parameter for atom X. This Hamiltonian can be found in Ref. 20. The spin-orbit parameters ξ_{Ga} and ξ_{As} for our two sets of bands are given by Chadi[19] and Jancu *et al.*,[18] respectively. The band structures obtained when adding spin-orbit interaction to both models are shown in Figs. 1(c) and 1(d).

Since the spin-orbit term in the Hamiltonian mixes up the majority- and minority-spin channels, we expect it to have a strong influence on the ballistic spin transport through GaAs even in the absence of spin-flip scattering. To demonstrate its effect, we have performed two parallel transport calculations, one with spin-orbit coupling included and the other with spin-orbit coupling omitted.

We consider a perfect Fe/GaAs/Fe tunnel junction oriented in the (001) direction with As-terminated interface (Fig. 2). The lattice constant of the zinc-blend structure of GaAs is almost exactly the double of the lattice constant of

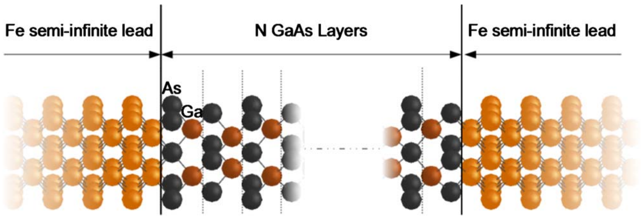


FIG. 2. (Color online) Geometry of the model Fe/GaAs/Fe junction.

bcc Fe and we have thus assumed in our calculations that there is a perfect match between the bulk Fe and GaAs lattices. It follows that we can introduce a common unit cell in a plane parallel to the Fe/GaAs interface and work in a representation that is Bloch-type in plane and atomiclike in the perpendicular direction. At the interface, the As atoms fill half of the first nearest-neighbor sites of the bcc Fe. The tight-binding hopping parameters between the Fe and As atoms were determined from Harrison's formula.[21]

The conductance was calculated in the linear-response regime using the Kubo-Landauer formula which was applied to a junction consisting of semi-infinite Fe leads separated by a slab of GaAs. The total conductance G is obtained by summing the transmission probability at the Fermi level (E_F) of electrons with parallel wave vector $k_\parallel$ over the whole two-dimensional (2D) Brillouin zone

$$G = \frac{e^2}{h}\sum_{k_\parallel} T(E_F,k_\parallel). \tag{1}$$

The details of the method are described in Ref. 22. The optimistic TMR is defined by

$$\mathrm{TMR} = \frac{G_\mathrm{P} - G_\mathrm{AP}}{G_\mathrm{AP}}, \tag{2}$$

where G_P is the conductance when the magnetizations of the electrodes are parallel (P) and G_AP is the conductance when the magnetizations of the electrodes are antiparallel (AP).

III. SATURATION OF THE TMR AS A FUNCTION OF GaAs THICKNESS

In this section we study the TMR as a function of GaAs thickness for different tight-binding parametrizations with and without spin-orbit coupling. We consider undoped GaAs and place the Fermi level E_F in the middle of the GaAs gap, in agreement with self-consistent LDA calculations[9–11] on similar perfect epitaxial junctions. Our results for this system using the $sp^3d^5s^*$ orbital basis with spin-orbit coupling are qualitatively in agreement with those of Popescu *et al.*

In Fig. 3 we show the TMR ratio calculated using the two sets of tight-binding parameters discussed in Sec. I. For each set of parameters, we present our results for the cases when the spin-orbit interaction is included and omitted. The TMR ratio is plotted as a function of the thickness of the GaAs layer. Because of the small gap in GaAs, states distributed over the whole 2D Brillouin zone contribute to the tunneling through a thin layer of GaAs for both parallel and antiparallel configurations. This explains the complex behavior of the TMR calculated for small thicknesses of GaAs, and, in particular, the result that the TMR is negative for a few planes of GaAs. However, in the following, we concentrate on experimentally relevant larger thicknesses where the main contribution to transmission comes from states near the $\bar{\Gamma}$ point and a consistent physical picture emerges.

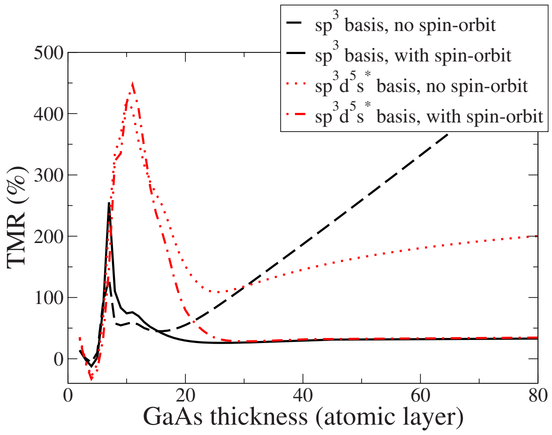


FIG. 3. (Color online) TMR as a function of GaAs thickness for the two sets of tight-binding parameters, with and without spin-orbit coupling, when E_F is in the middle of the GaAs gap.

When GaAs is described in a simple sp^3 basis without spin-orbit interaction, its band structure is rather similar to that of MgO but with a much smaller gap. In that case, it has already been shown in previous work on Fe/MgO/Fe(001) tunneling junction[22,23] that the TMR of a perfect junction should increase with increasing insulating layer thickness. In fact, such a behavior is seen in Fig. 3. We can easily explain this result by considering the symmetry of electron states mediating perpendicular tunneling. At the Fermi level, majority-spin electrons in Fe traveling at the $\bar{\Gamma}$ point (perpendicular tunneling) in states with $\Delta_1(sp_z,d_{z^2})$ symmetry can couple strongly to $\Delta_1(sp_z)$ states in GaAs. On the other hand, minority-spin electrons are only in states with $\Delta_2(d_{xy},d_{x^2-y^2})$ and $\Delta_5(p_x,p_y,d_{xz},d_{yz})$ symmetries [see Fig. 4(a)]. In a simple sp^3 basis the Δ_5 states decay more rapidly in the GaAs tunnel barrier than the Δ_1 states [see the complex band structure of GaAs in Fig. 4(b)]. Thus when the Fe electrodes have parallel magnetizations, the majority-spin Δ_1 channel is the main source of tunneling current. In the antiparallel configuration, a majority-spin Δ_1 electron can tunnel through the barrier as in the parallel case but for symmetry reasons discussed above cannot be injected into the electrode with the opposite magnetization and is thus reflected at the second interface.

Away from the $\bar{\Gamma}$ point, these state symmetry and selection rules are broken. However, the current in the antiparallel configuration is much lower than in the parallel configuration and the TMR thus grows rapidly with increasing GaAs thickness. This effect becomes more pronounced as the barrier thickness increases and electrons with $k_\parallel$ near $\bar{\Gamma}$ quickly become the principal source of tunneling current. Such a behavior is illustrated in Fig. 5(a) which depicts the distribution of partial conductances in the 2D Brillouin zone. Figure 5(a)

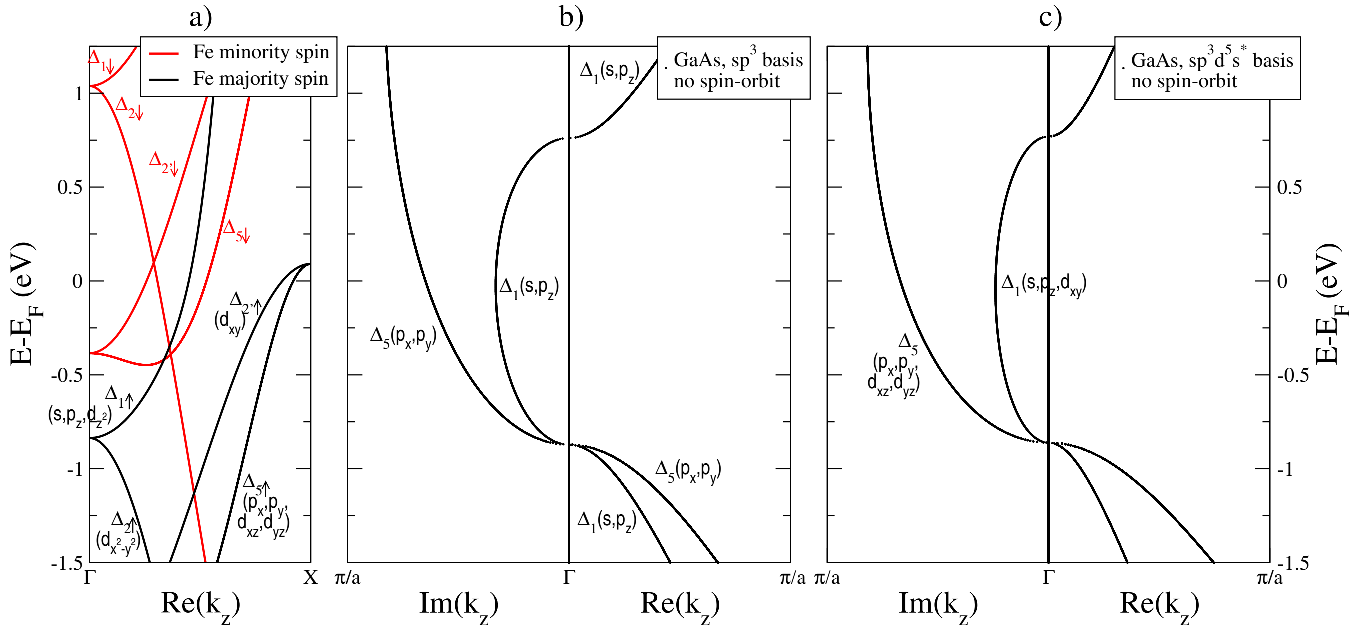
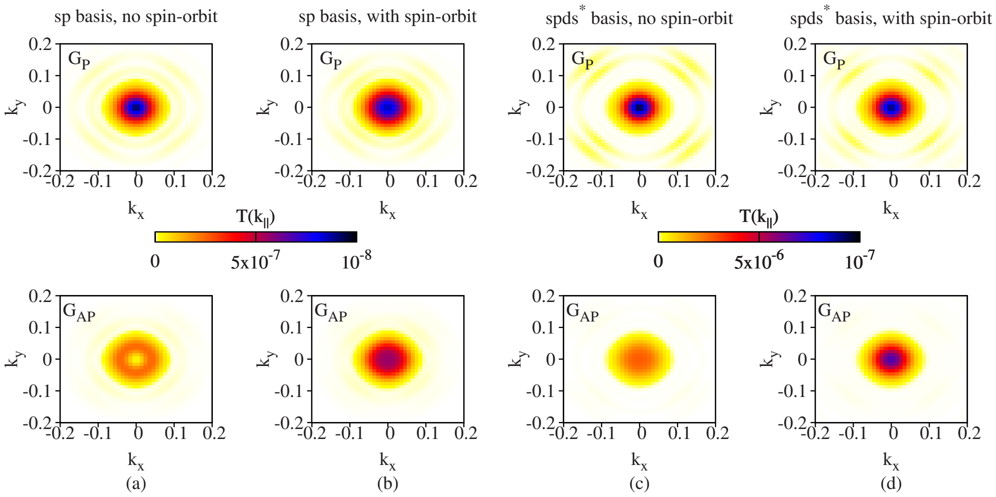


FIG. 4. (Color online) (a) Band structure of Fe and complex band structure of GaAs (b) in the *sp* basis and (c) in the *spds** basis, along the k_z axis.

shows that the conductance in the antiparallel configuration exhibits a hole at $\bar{\Gamma}$, which indicates that the conductance $G_{AP}(\bar{\Gamma})$ is negligible. This all effect is analyzed mathematically in Ref. 24 which shows that the TMR must eventually grow linearly with barrier thickness, as observed in Fig. 3.

The addition of *d* states and of spin-orbit coupling, which are both required to describe the GaAs layer correctly, change this picture completely. First, it can be seen from Fig. 3 that, for a thin layer of GaAs (<20 atomic planes), the TMR is hardly affected by spin-orbit coupling but is strongly modified by the presence of *d* and s^* states in GaAs. This can be explained by the fact that those states open up new tunneling channels that were not allowed in the case of a simple sp^3 orbital basis. The additional *d* channels are mostly located far from the $\bar{\Gamma}$ point in the 2D Brillouin zone and thus their importance decreases with increasing GaAs thickness. For thicker GaAs, the TMR begins to be strongly affected by both spin-orbit coupling and the presence of *d* orbitals. Ultimately these two effects become dominant and cause saturation of TMR with GaAs thickness. Since the saturation due to the presence of *d* orbitals and saturation due to spin-orbit coupling are governed by different physical mechanisms, we shall discuss them separately.

First we explain how the inclusion of *d* states causes a saturation of TMR. In a simple sp^3 basis the most favorable tunneling channel in GaAs is the Δ_1 state at the $\bar{\Gamma}$ point.



(a) (b) (c) (d)

FIG. 5. (Color online) Transmission as a function of $k_{\|}$ near the $\bar{\Gamma}$ point for a Fe/GaAs/Fe trilayer with 25 layers of GaAs. The results are for the two sets of tight-binding parameters with and without spin-orbit coupling in the parallel (G_P) and antiparallel (G_{AP}) configurations: (a) sp^3 basis without spin orbit, (b) sp^3 basis with spin orbit, (c) $sp^3d^5s^*$ basis without spin orbit, and (d) $sp^3d^5s^*$ basis with spin orbit. Note that only the center of the Brillouin zone is shown, the boundaries lie at $k_x,k_y=\pm 1$.

When *d* orbitals in GaAs are included, this channel acquires a d_{xy} component due to a twofold symmetry of GaAs (Ref. 8) [see Fig. 4(c)]. In this case, both Δ_1 majority-spin electrons and Δ_2 minority-spin electrons emitted from one of the Fe electrodes travel in the same channel in the barrier and can enter the other Fe electrode whatever the direction of its magnetization. This leads to the opening up of an antiparallel conducting channel G_{AP} at the $\bar{\Gamma}$ point. This is clearly seen in the distribution of partial conductances G_{AP} in Fig. 5(c). Since majority- and minority-spin electrons now tunnel through the same GaAs channel, they have the same decay constant and, since for thick barriers the $\bar{\Gamma}$ point is the only source of tunneling current, the TMR saturates, as seen in Fig. 3.

We now discuss the effect of spin-orbit coupling on the TMR. This discussion is similar to that presented by Popescu *et al.*[10,11] but is only valid when the dominant conductance channel is the majority channel in the parallel configuration. This is not always the case as will be seen in the next section.

In the absence of spin-orbit coupling, the majority- and minority-spin electrons tunneling through GaAs remain independent. So in the antiparallel configuration, a majority-spin electron injected from the left Fe electrode into GaAs is strongly reflected when it reaches the right Fe electrode with opposite magnetization. The spin-orbit interaction changes this picture completely since it mixes up the majority- and minority-spin channels. Now a majority-spin electron injected from the left Fe electrode into GaAs travels through it in a spin state which is an admixture of states with spin parallel and antiparallel to the magnetization of the left electrode. It follows that one of its components can always be transmitted into the right Fe electrode regardless of the direction of its magnetization. The conductance in the antiparallel configuration is thus increased and the TMR reduced. For thick GaAs, the TMR is dominated by the conductances at the $\bar{\Gamma}$ point. Since tunneling at the $\bar{\Gamma}$ point occurs through the same mixed state both in the parallel and antiparallel configurations, the decay constant for parallel and antiparallel conductances are the same, and hence the TMR saturates as a function of GaAs thickness. This interpretation is confirmed by the distribution of partial conductances in Fig. 5(b), which shows an open channel at the $\bar{\Gamma}$ point in the antiparallel configuration.

We conclude this section with some general observations about the effect of spin-orbit coupling. If every electron injected into GaAs completely lost their original polarization due to this effect (i.e., for sufficiently thick GaAs, electrons would have a 50% probability of being either majority- or minority-spin carriers), the parallel and antiparallel configurations would have the same conductances and the TMR would tend to zero as the thickness of the GaAs interlayer increases. This type of behavior is expected for a system with a finite spin-diffusion length. However, the convergence to a nonzero value of TMR seen in Fig. 3 proves that, in the ballistic regime, spin-orbit coupling does not completely destroy the spin polarization of the current no matter how thick the GaAs layer, and we do not have a finite spin-diffusion length. Although spin-orbit coupling can be a source of spin relaxation resulting in a finite spin-diffusion length, this mechanism is not effective in the ballistic limit considered here. As pointed out by Elliott and Yafet,[25,26] spin-orbit coupling needs to be combined with scattering in order to cause spin relaxation. Moreover, whatever the source of spin relaxation, the characteristic length over which such relaxation takes place is hundreds or thousands of atomic planes.[27] Here in the ballistic limit, the spin-orbit coupling only has an afect as soon as electrons pass into GaAs, after that there is no further spin relaxation.

Finally we note that irrespective of whether $s^{*}d$ states are included or not, the TMR in Fig. 3 with spin-orbit coupling included converges to the same value with increasing GaAs thickness. This clearly indicates that the TMR ratio for thick GaAs layers is controlled by the spin-orbit coupling.

IV. DEPENDENCE OF THE TMR ON THE BARRIER HEIGHT IN GaAs

In this section we study the dependence of the TMR on the position of the Fermi level in the GaAs gap (i.e., the barrier height). In order to simplify the discussion we consider only $sp^3d^5s^*$ GaAs parameters with and without spin-orbit coupling. The results are qualitatively similar for the sp^3 parametrization.

The saturation of the TMR due to spin-orbit coupling, which was demonstrated in Sec. III, is a universal phenomenon but the precise saturation value of the TMR strongly depends on the height of the tunneling barrier, i.e., the position of the Fermi level E_F in the GaAs gap. In agreement with previous LDA calculations for a perfect Fe/GaAs junction,[9–11,13,14] we placed in Sec. III the Fermi level in the middle of the gap. However, the position of E_F in the GaAs is strongly influenced by factors such as the quality of the Fe/GaAs interfaces. As discussed, for example, by Demchenko and Liu[14] interface-induced gap states play major role in pinning the actual position of the Fermi level in the gap. It follows that interfaces of different quality might lead to different positions of E_F in the gap. Because it is well known[9,13,14] that an interface state for minority-spin electrons, which in an ideal junction lies very close to E_F, leads to a resonant enhancement of the conductance in the minority-spin channel, it is clear that even small deviations of E_F from its position in the middle of the gap should strongly influence the TMR. It is, therefore, important to investigate the TMR as a function of the position of E_F in the gap. It should be noted that the position of E_F in the Fe/GaAs/Fe trilayer is, of course, pinned to the Fermi level of the bulk iron electrodes and hence fixed. Therefore, to study the dependence of the TMR on the position of E_F in the GaAs gap, we need to rigidly shift the band structure of GaAs relative to that of the bulk Fe electrodes. The results of such a calculation are shown in Fig. 6 both in the absence and in the presence of the spin-orbit coupling. We plot in Fig. 6 the dependence of the TMR on the position of E_F relative to the top of the valence band E_V for GaAs thickness of 50 atomic planes. For such a thickness of GaAs the saturation of the TMR due to spin-orbit coupling occurs for all values of E_F in the gap.

There are two interesting features seen in Fig. 6. First, the saturation value of the TMR in the presence of spin-orbit

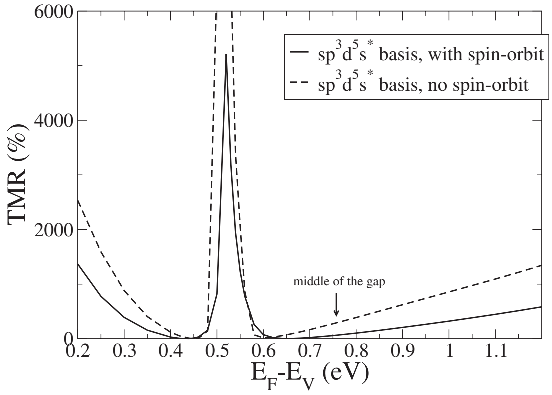


FIG. 6. TMR ratio for a thickness of 50 atomic planes of GaAs as a function of the position of the Fermi level E_F in the gap of GaAs (E_v is the edge of the valence bands) with and without spin orbit. The center of the gap lies at $E_F-E_V=0.76$ eV.

coupling is almost always lower than the corresponding value of the TMR in the absence of the spin-orbit coupling. This reduction in the TMR due to spin-orbit coupling is particularly large for E_F close to its usual position in the middle of the GaAs gap. The second feature is a sharp peak of the TMR which occurs when E_F lies about 0.52 eV above the edge of the valence band. Moreover, the TMR is close to zero on either side of the peak. To understand the origin of the large TMR peak, it is instructive to examine the individual conductances for majority- and minority-spin electrons in the parallel G_{P} and antiparallel G_{AP} configurations. They are shown in Fig. 7.[28] The fact that no peak is observed for majority-spin electrons in the parallel configuration, together with the fact that the conductances are dominated by the $\bar{\Gamma}$ point, strongly indicates that these features are due to a resonance in the minority-spin band structure of the Fe/GaAs/Fe trilayer which is located at the $\bar{\Gamma}$ point. Examination of the local density of states (LDOS) for minority-spin electrons in the vicinity of the Fe/GaAs interface, shown in Fig. 8, confirms the existence of such a resonance which coincides with the Fermi level for a GaAs band shift of 0.52 eV. This minority-spin resonance has a Δ_1 character and thus can easily tunnel through the GaAs barrier. This is in agreement with previous work[9,13,14] where it was shown that for a single Fe/GaAs interface, there is an interfacial resonance at the $\bar{\Gamma}$ point for minority-spin electrons which enhances the transmission in the minority-spin channel. It should be noted that, as the band structure of GaAs is displaced rigidly relative to that of Fe (as shown in Fig. 4), the position of the resonance shifts. In Fig. 8(a) we show the LDOS when the Fermi level coincides with the resonance, i.e., when it lies at 0.52 eV above the valence-band edge and in Fig. 8(b) we show the LDOS when the Fermi level lies in the middle of the gap. Clearly the resonance is not simply pinned to the Fe band structure, but moves with the GaAs barrier height.

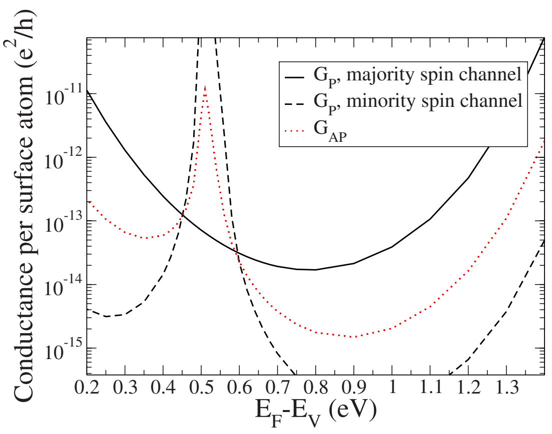


FIG. 7. (Color online) Conductance for 50 atomic planes of GaAs, of majority and minority spin electrons in the parallel (G_{P}) and antiparallel (G_{AP}) configurations, as a function of the position of the Fermi level E_F in the gap of GaAs (*spds** parameters without spin orbit). The center of the gap lies at $E_F-E_V=0.76$ eV.

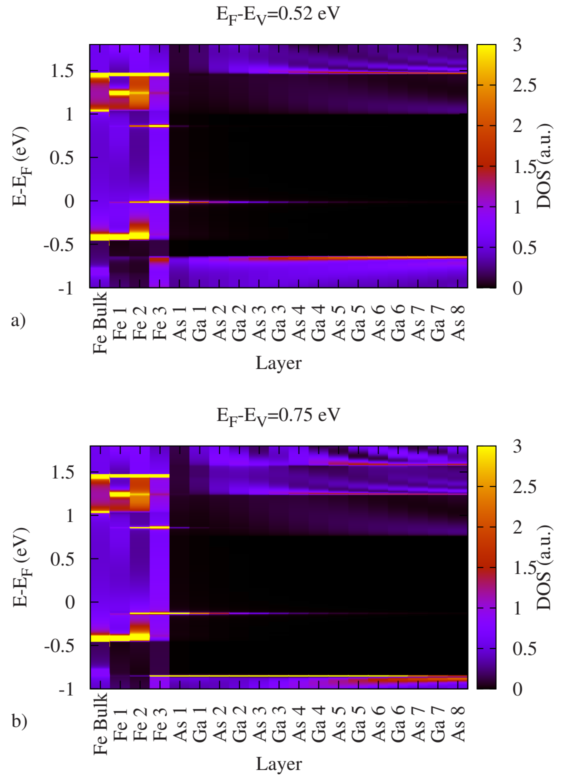


FIG. 8. (Color online) Local density of states in several layers of an Fe/GaAs interface, for minority spin electrons at the $\bar{\Gamma}$ point in the 2D Brillouin zone, (a) when the Fermi level lies 0.52 eV above the valence bands edge and (b) when the Fermi level lies in the middle of the gap. The peaks in Fe bulk LDOS, at $E-E_F\approx -0.5$ eV correspond to the band edge of Δ_2' and Δ_5 states while those at $E-E_F\approx 1$ eV correspond to the band edge of Δ_1 and Δ_2 states [see Fig. 4(a)].

The presence of such a resonance in the minority-spin channel can explain both the peak in TMR and the two minima located on either side of the peak. In the antiparallel configuration, we have two independent Fe/GaAs interfacial resonances which strongly enhance the conductance G_{AP}. In the parallel configuration, we have two interacting resonant states, one on each interface, which give rise to an even stronger enhancement (see, e.g., Ref. 29) of the minority-spin channel conductance. This effect results in a G_{P} which

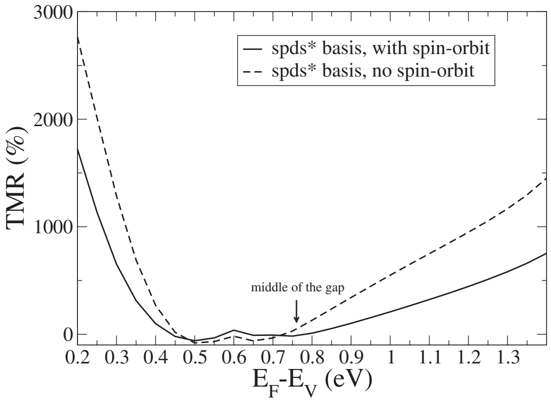


FIG. 9. TMR ratio for a thickness of 50 atomic planes of GaAs, as a function of the position of the Fermi level E_F in the gap of GaAs for an asymmetric junction. The center of the gap lies at $E_F - E_V = 0.76$ eV.

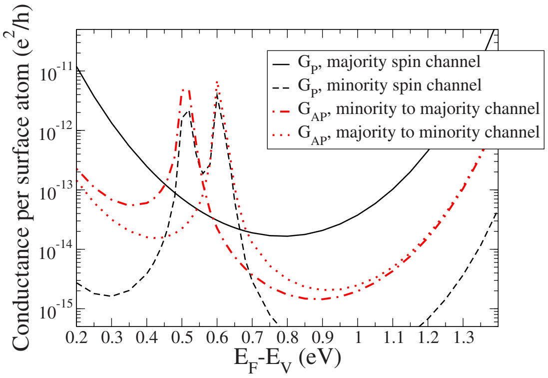


FIG. 10. (Color online) Conductance for 50 atomic planes of GaAs of majority and minority spin electrons in the parallel (G_P) and antiparallel (G_{AP}) configurations of an asymmetric junction as a function of the position of the Fermi level E_F in the gap of GaAs (*spds** parameters without spin orbit). The center of the gap lies at $E_F - E_V = 0.76$ eV.

is much higher than G_{AP}, as seen in Fig. 5. This explains the large peak in the TMR. The minima on either side of the peak must occur because at the $\bar{\Gamma}$ point, away from the resonant energy, we expect $G_P(\text{majority}) \gg G_P(\text{minority})$. On the other hand, in the vicinity of the resonant energy we expect $G_P(\text{minority}) \gg G_P(\text{majority})$. This explains the shape of the G_P(majority) and G_P(minority) curves in Fig. 7 and the fact that they cross on either side of the peak. Furthermore, we also expect G_{AP} to lie between G_P(majority) and G_P(minority) so that all three curves must cross near the same point and hence there must be a minimum in TMR on either side of the peak.

It should be noted that E_F in the middle of the gap for a perfect junction lies very close to one of the minima in Fig. 4 and, therefore, the corresponding small value of TMR is due to the existence of the resonance. It is now pertinent to ask whether the large resonant enhancement of the TMR, which occurs for a perfect junction when E_F lies about 0.52 eV above the edge of the valence band, can be observable in real tunneling junctions. As discussed in Ref. 29, the large enhancement of the conductance G_P relies on the fact that the interfacial states on either side of the barrier are strictly identical and lie at exactly the same energy. Only if these conditions are satisfied, perfect transmission mediated by the interfacial states can occur. However, it is well known that for real junctions the two Fe/GaAs interfaces are never identical and the above conditions almost certainly cannot be satisfied for experimentally prepared junctions. Similarly, an applied bias would break the perfect symmetry. To investigate the effect of small deviations from perfect symmetry of the junction on the TMR, we shifted the on-site potentials in one of the Fe electrodes by a small amount of 0.1 eV and recalculated the dependence of the TMR on the position of E_F in the gap. The results are shown in Fig. 9. It can be seen that a small deviation from a perfect symmetry of the junction almost completely removes the large TMR peak and the TMR is very small for quite a wide range of barrier heights, including the case when E_F is close to the middle of the gap.

The reason for this very low TMR can be seen in Fig. 10 which shows the individual conductances for majority- and minority-spin electrons in the parallel G_P and antiparallel G_{AP} configurations for an asymmetric junction in the absence of spin-orbit coupling. Note that there are two peaks here because the potentials of the Fe electrodes are shifted by 0.1 eV with respect to each other. We observe that G_P(minority) and G_{AP} curves both still have resonances when E_F lies about 0.52 eV above the valence-band edge. However, they are now of similar magnitude, and it is this feature which causes the very low TMR. The reason for this is as follows. We recall that for a symmetric junction in the parallel configuration, the two minority-spin resonant states on each Fe/GaAs interface combine to give a strongly enhanced conduction channel, much larger than in the antiparallel configuration where the interface resonances are independent. When the symmetry of the junction is broken, these combined resonant states decouple and become independent. The enhancement in minority-spin conduction in the parallel configuration is then of similar magnitude to that of the antiparallel configuration. This feature is seen explicitly in Fig. 10 and gives rise to very small TMR when E_F lies in this region.

We now discuss the effect of spin-orbit coupling on the TMR near the resonance in Fig. 9. Generally speaking spin-orbit coupling opens up new channels of conductance. When the Fermi level is far from the resonance, the effect of spin orbit is mainly to increase the antiparallel conductance. The parallel conductance which is dominated by the majority-spin channel is less affected. This always results in a decrease in the TMR. Near the resonance, the parallel conductance is dominated by the minority channel which is strongly affected by spin-orbit coupling. Thus both parallel and antiparallel conductances are increased by the spin-orbit coupling. The effect on the very small TMR ratio in this region is then less predictable and it could lead either to a small increase (Fig. 9) or a decrease (Fig. 6) of the TMR.

V. CONCLUSIONS

Although the band structure of GaAs is similar to that of MgO, which gives rise to a very large tunneling magnetoresistance in excess of 1000%, our calculations of the tunneling magnetoresistance of Fe/GaAs/Fe(001) junction show that the TMR ratio of such a junction is remarkably low, on the order of 30% when the Fermi level E_F lies close to its usual position in the middle of the GaAs gap. There are several reasons for this large difference between MgO and GaAs barriers. We shall now summarize the fundamental physical differences between the two systems which cause such a very different behavior.

First of all, we find that, in contrast to MgO for which TMR increases indefinitely with MgO thickness (in the absence of spin-flip scattering), TMR of a tunneling junction with GaAs barrier always saturates with increasing GaAs thickness to a finite value. There are two different mechanisms which cause the saturation. The first one is due to the twofold symmetry of GaAs(001). For a thick GaAs barrier, perpendicular tunneling at the $\bar{\Gamma}$ point is favored ($k_{\parallel} \approx 0$) because of the exponential decay of tunneling wave functions. The twofold symmetry of GaAs opens up a new tunneling channel for d-like states at the $\bar{\Gamma}$ point in the antiparallel configuration and that inevitably leads to a saturation of TMR with GaAs thickness because both majority- and minority-spin electrons tunnel via the same dominant channel at the $\bar{\Gamma}$ point. The inclusion of d states in the parametrization of GaAs is necessary to describe this effect correctly. This saturation mechanism has already been discussed by Mavropoulos *et al.*[8] in the case when the Fermi level lies close to the bottom of the conduction band of GaAs.

The second, even more important, saturation mechanism is due to the presence of spin-orbit interaction which is very strong in GaAs. Our calculations including the spin-orbit interaction show that this mechanism leads to a much faster saturation of the TMR with GaAs thickness than the presence of d-like states in GaAs. Moreover, we find that the TMR with spin-orbit interaction included almost always saturates to a smaller value than that calculated in the absence of the spin-orbit interaction. This effect has already been discussed by Popescu *et al.*[10,11] for the special case when the Fermi level lies in the middle of the GaAs gap. We thus conclude that the spin-orbit interaction limits ultimately the magnitude of the TMR in a junction with GaAs barrier. The saturation occurs because, in the presence of spin-orbit interaction, a majority-spin electron injected from the left Fe electrode into GaAs travels through it in a spin state which is an admixture of states with spin parallel and antiparallel to the magnetization of the left electrode. When it arrives at the interface with the right Fe electrode having the opposite magnetization, it can be partially transmitted through it. It follows that majority- and minority-spin electrons can tunnel through the same dominant conductance channel at the $\bar{\Gamma}$ point and the TMR ratio thus saturates when this channel becomes the only source of the tunneling current, which occurs for large thickness of GaAs. We stress that the saturation of the TMR due to spin-orbit interaction occurs despite the fact that the spin-diffusion length remains infinite. It is infinite because spin-orbit interaction does not cause any spin-flip scattering in the ballistic limit.

Although the spin-orbit interaction reduces the TMR by a large factor and causes saturation of TMR with GaAs thickness (see Fig. 3), this mechanism alone cannot explain why our calculated tunneling magnetoresistance, with the Fermi level E_F in the middle of the GaAs gap, is so small ($\approx 30\%$). The underlying reason for this is the presence of a resonance in the minority-spin band structure of the Fe/GaAs/Fe trilayer which is located at the $\bar{\Gamma}$ point at an energy of about 0.52 eV above the edge of the valence band. In the vicinity of the resonance the minority-spin carriers dominate the conductance and the magnitude of the TMR is now qualitatively and quantitatively different from the situation when the Fermi level lies far from the resonance. For an ideal perfectly symmetric junction, the TMR has a very large peak when E_F is close to the resonance but becomes very small on either side of the resonance peak and that includes the region in the vicinity of the middle of the gap where E_F is usually expected to lie. The precise reason for the reduction in the TMR on either side of the resonance are discussed in detail in Sec. IV. In this somewhat idealistic case of a perfectly symmetric junction a very small shift of the GaAs band structure or Fermi level can lead to a variation of 4 orders of magnitude in the TMR. We believe that this explains the discrepancy in the magnitude of our TMR in comparison to that of Popescu *et al.*[10,11]

However, real junctions are most unlikely to be perfectly symmetric and our calculations with symmetry broken show that even a small asymmetry of the junction removes the TMR peak and reduces the TMR to small values. The underlying reason for this is again the resonance in the minority-spin band structure of the Fe/GaAs/Fe trilayer. The precise mechanism is discussed in Sec. IV, and the general arguments given there are valid regardless of the precise position of the resonance in the gap. We thus conclude that for realistic junctions the TMR should be always small, of the order of 50%, for a rather large interval of values of E_F in the vicinity of the middle of the GaAs gap. This is supported by experimentally measured values.[6,7] However, we stress that even with the spin-orbit interaction included the TMR can be large (of the order of 1000%) when E_F is close to the conduction- or valence-band edges (see Fig. 9). Manipulation of the height of the barrier (position of E_F in the gap) thus offers scope for achieving a high TMR ratio in a junction with GaAs barrier.

Finally, we would like to mention that the effects discussed here are also relevant for an Fe/GaAs interface with a Schottky barrier since electrons must first tunnel through the Schottky barrier before they can reach the conduction band of a doped GaAs.

Note added. Recently, we were made aware of a publication by Honda *et al.*[30] discussing the affect of interface states on conduction through across a Fe/GaAs interface, and through a Fe/GaAs/Fe junction under large finite bias.

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