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Strong Enhancement of the Tunneling Magnetoresistance by Electron Filtering in an Fe/MgO/Fe/GaAs(001) Junction

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Calculations of the tunneling magnetoresistance (TMR) of an epitaxial Fe/MgO/Fe tunneling junction attached to an *n*-type GaAs lead, under positive gate voltage, are presented. It is shown that for realistic GaAs carrier densities the TMR of this composite system can be more than 2 orders of magnitude higher than that of a conventional Fe/MgO/Fe junction. Furthermore, the high TMR is achieved with modest MgO thicknesses and is very robust to disorder at the Fe/GaAs interface and within the GaAs layer itself. The significant practical advantage of this system is that huge TMRs should be attainable for junctions with modest resistances. For a GaAs carrier density of 10^{19} cm^{-3} the system is calculated to have a TMR in excess of 10 000% but its resistance is equivalent to that of a conventional Fe/MgO/Fe junction with only 6–7 at. planes of MgO.

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The spintronics of magnetic tunneling junctions has been revolutionized by the theoretical prediction [1,2] and subsequent observation [3,4] of a very large tunneling magnetoresistance (TMR) in epitaxial junctions with crystalline MgO barrier and Fe/Co electrodes. In particular, it was predicted [1,2] that the TMR should keep increasing with increasing MgO thickness. However, there are at least two problems which prevent arbitrarily large values of TMR in junctions such as Fe/MgO/Fe(001) from being achieved experimentally. First, it is difficult to grow perfect epitaxial junctions with very thick MgO barrier, because the small lattice mismatch eventually spoils the perfect epitaxy. The second problem is that the resistance of a junction with a very thick MgO barrier would be far too large for practical applications.

To improve significantly the highest observed TMR ratio of some 1000% and address the large resistance problem, we need to explore alternative systems that can be realized experimentally. In this context, it is useful to recall the physical mechanism which leads to a very large TMR in junctions with thick MgO barriers. Two ingredients are required. (i) A filter selecting only electrons which tunnel close to the Γ point, i.e., those with parallel wave vector $\mathbf{k}_{\parallel} \approx 0$ (perpendicular tunneling). In a conventional Fe/MgO/Fe junction this is achieved by using a thick MgO barrier. (ii) The special features of the Fe/MgO band structure which ensure that majority-spin electrons in the parallel (P) configuration can tunnel effectively at the Γ point but minority-spin electrons are strongly reflected at the Fe/MgO interface and there is, therefore, a hole in the conductance at the Γ point in the antiparallel (AP) configuration.

To satisfy these two requirements, we propose a composite system in which the filtering toward the Γ point is done separately so that it no longer relies on a thick MgO barrier. The role of the Fe/MgO/Fe junction with a thin barrier, which is incorporated into the system, is solely to provide the band structure mechanism that allows only majority-spin electrons in the P configuration to tunnel effectively at the Γ point. This obviates the need for a thick MgO layer and hence removes both the aforementioned problems.

Our proposal is that the filtering toward the Γ point can be achieved by attaching an Fe/MgO/Fe(001) junction to an *n*-type doped GaAs lead under positive gate voltage. Because the Fermi surface of *n*-type doped GaAs under positive gate voltage is very small, only electrons with $\mathbf{k}_{\parallel}$ very close to the Γ point can tunnel through the whole Fe/MgO/Fe/GaAs(001) structure. We shall show that, for typical electron densities of 10^{17}–10^{19} cm^{-3}, the GaAs Fermi surface filtering toward the Γ point is so efficient that a TMR at least 2 orders of magnitude higher than that currently observed in conventional Fe/MgO/Fe(001) junctions can be achieved in our composite system with MgO thicknesses as small as 2–3 atomic planes.

Before we proceed any further, we wish to clarify two very important points. Large amount of research has been done on spin injection across the Fe/GaAs interface. All of it is quite irrelevant to the operation of the device we propose. Spin filtering at the Fe/GaAs interface is immaterial since the only property of a doped, gated, GaAs we require is that it has a small Fermi surface. This is a property of the bulk GaAs not of the interface.

The second point concerns the bias applied to our junction. We stress that the highest TMR ratios we predict occur for low bias. When a bias is applied, electrons above the Fermi level are injected into the GaAs. This amounts to an effective increase of the projection of the GaAs Fermi surface through which electron can travel. The filtering is therefore reduced. But as long as the filtering toward Γ point in GaAs is stronger than in conventional Fe/MgO/Fe junction, our system gives higher TMR. A simple estimate shows that this condition is satisfied for bias as high as ≈0.5 V.

We now describe the calculation of the TMR for the Fe/MgO/Fe/GaAs(001) junction. In Fig. 1 we show the geometry of the system and the schematic potentials seen by majority-spin electrons in the parallel configuration. We assume that an Fe/MgO/Fe(001) tunnel junction is attached to an As-terminated n-type doped GaAs(001) lead. The lattice constant of GaAs (5.65 Å) is almost exactly double that of BCC Fe (2.87 Å). Thus it is reasonable to assume a perfect match between the Fe and GaAs lattices. Similarly, there is a very good lattice match between Fe and MgO with the two lattices rotated by 45°. We shall, therefore, assume a perfect lattice match between all three components of our system.

We use a tight-binding approach. The parameters for Fe and MgO were taken from Ref. [5] and the on-site potentials in Fe were adjusted self-consistently to reproduce the correct Fe moment at the interfaces. As in Ref. [1], the Fermi level is assumed to lie in the middle of the MgO gap, leading to a 3.5 eV-high tunnel barrier. The parameters for GaAs, which include d orbitals and spin-orbit coupling, were obtained from Jancu *et al.* [6]. This parametrization of GaAs includes d orbitals and spin-orbit coupling. The hopping parameters between Fe and As atoms at the interface were obtained from Harrison's formula [7]. We consider n-type doped GaAs under positive gate voltage, so that in the bulk of the GaAs layer the Fermi level lies in the conduction band. For a given electron density n in the conduction band, the position of the Fermi level was determined from the parabolic band model formula $n = \frac{2\sqrt{2(m_c E_F)^3}}{3\hbar^3\pi^2}$, where m_c is the effective mass at the bottom of the conduction band.

At the interface between Fe and GaAs, a Schottky barrier is formed. It is modeled by shifting the on-site Hamiltonian elements in each atomic plane of the depletion layer by the potential $V_{\mathrm{SB}}(1 - z/z_{\mathrm{dep}})^{-2}$, where V_{SB} is the Schottky barrier height and z_{dep} is the thickness of the depletion layer [8]. We choose a Schottky barrier height of 0.7 eV, which is a typical value found in experiments [9,10]. The thickness of the depletion layer z_{dep} depends on the Schottky barrier height and the electron density. It was determined for each density considered by solving the one-dimensional Poisson equation [11].

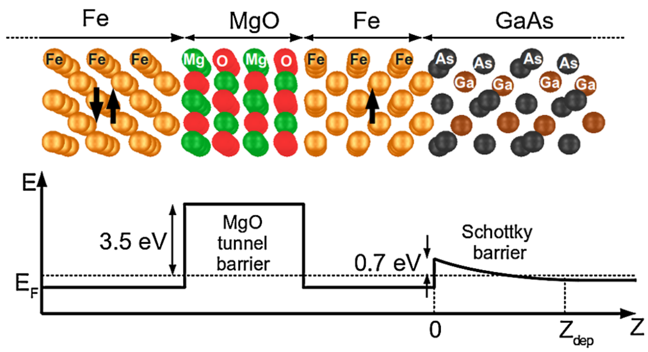

FIG. 1 (color online). Geometry of the system and schematic potentials seen by majority-spin electrons. The scale in z is not respected for the Schottky barrier whose width is of the order of 100 at. planes.

We compute the conductances in the P and AP configurations of the Fe layers using the Kubo-Landauer formula in the linear-response regime. We recall that the tight-binding method combined with the Kubo-Landauer formula gives excellent results for a conventional Fe/MgO/Fe(001) junction studied previously [1].

The total conductance G is obtained by summing the transmission probability $T(E_F, \mathbf{k}_\parallel)$ at the Fermi level (E_F) of electrons with parallel wave vector $\mathbf{k}_\parallel$ over the whole two-dimensional (2D) Brillouin zone (BZ):

$$G = \frac{e^2}{h}\sum_{\mathbf{k}_\parallel} T(E_F, \mathbf{k}_\parallel). \qquad (1)$$

The details of the method are described in Ref. [1]. The optimistic tunneling magnetoresistance ratio (TMR) is defined by TMR $= (G_P - G_{\mathrm{AP}})/(G_{\mathrm{AP}})$, 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).

The TMR ratios of the Fe/MgO/Fe/GaAs(001) structure calculated for a range of electron densities 10^{17}–10^{19} cm^{-3} in GaAs are shown in Fig. 2 as a function of the MgO layer thickness for a fixed thickness of the right Fe interlayer of 20 at. planes (a). The total conductances G_P in the P configuration are also shown (b). The results are compared with the theoretical TMR and conductance of a conventional Fe/MgO/Fe(001) junction [1].

The principal results are as follows.

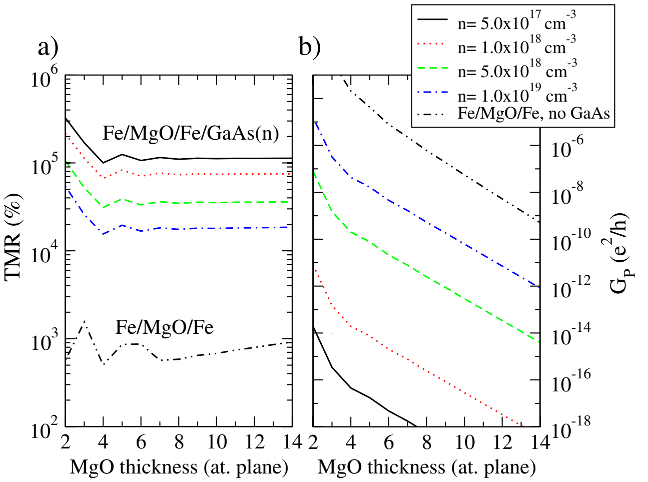

FIG. 2 (color online). TMR ratio (a) and the conductance G_P (b) of an Fe/MgO/Fe junction attached to an n-type GaAs lead for different values of the electron density n in GaAs. The TMR and conductance of a conventional Fe/MgO/Fe junction are also shown.

The TMR ratios for the Fe/MgO/Fe/GaAs system are at least 2 orders of magnitude higher than the TMR of a conventional Fe/MgO/Fe junction.

The TMR is highest for GaAs with the lowest electron density, i.e., smallest Fermi wave vector k_F. However, the dependence of the TMR on the electron density is quite weak and a TMR in excess of 10 000% is predicted even for the highest electron density considered of 10^{19} cm^{-3}.

In contrast to a conventional Fe/MgO/Fe junction, high TMR values are obtained even for very thin MgO layers, as thin as 2–3 at. planes. It can be also seen that after a few small oscillations the TMR becomes almost independent of MgO thickness.

Finally, while the TMR ratio is rather insensitive to the electron density, the conductance of the Fe/MgO/Fe/GaAs(001) junction increases by more than 8 orders of magnitude when the electron density in GaAs is varied from 10^{17} to 10^{19} cm^{-3}.

The above features of the TMR of an Fe/MgO/Fe/GaAs system can be explained by the behavior of the partial conductances $G_P(\mathbf{k}_\parallel)$ and $G_{\mathrm{AP}}(\mathbf{k}_\parallel)$ in the P and AP configurations. The distribution of these partial conductances in the two-dimensional Brillouin zone (2D BZ) is shown in Fig. 3 for a junction with 4 atomic planes of MgO and electron density in GaAs of 10^{18} cm^{-3}. Note that only a small central region ($1/5 \times 1/5$) of the 2D BZ is shown in Fig. 3.

A much higher TMR for the Fe/MgO/Fe/GaAs system is obtained because electrons can now only tunnel through the GaAs Fermi surface projection on the 2D BZ [small circle centered at the gamma point, Figs. 3(a) and 3(b)]. This is much smaller than the corresponding effective tunneling region for a conventional Fe/MgO/Fe junction with the same thickness of MgO [Fig. 3(c) and 3(d)].

The result that the TMR is highest for GaAs with the lowest electron density simply reflects the fact that the diameter of the tunneling region in the 2D BZ decreases with decreasing electron density and tunneling electrons are, therefore, progressively restricted to channels which become ever closer to the Γ point. However, since the electron density $n \propto k_F^3$, the radius of the tunneling region changes only very slowly with n, which explains why the TMR is rather insensitive to the electron density.

The result that the conductance changes with electron density by many orders of magnitude follows because the dependence of the conductance on electron density is determined by tunneling through the Schottky barrier. This is very strongly dependent on the thickness of the Schottky barrier, which in turn is governed by the electron density in GaAs. It should be noted that the presence or absence of a Schottky barrier is irrelevant to the TMR of our device. The Schottky barrier's main effect is only to increases the total resistance of the device.

Our calculated results demonstrate that the Fe/MgO/Fe/GaAs system we propose has many advantages over the traditional Fe/MgO/Fe junction. However, there is a potential penalty to pay for these advantages. One now has a more complicated system that may be more difficult to grow experimentally while preserving good interfaces.

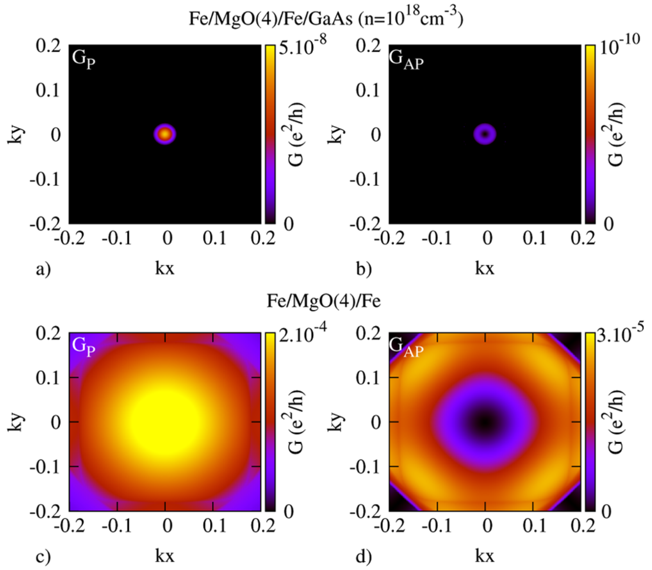

FIG. 3 (color online). $G_P(\mathbf{k}_\parallel)$ and $G_{\mathrm{AP}}(\mathbf{k}_\parallel)$ near the center of the 2D Brillouin zone for an Fe/MgO/Fe junction deposited on top of n-type GaAs (a) and (b) and for a conventional Fe/MgO/Fe junction (c) and (d). k_x and k_y are given in unit of the size of the 2D BZ (π/a, where $a = 5.65$ Å is the lattice constant of GaAs).

We have, therefore, investigated the effect of interfacial roughness using the lateral supercell method, averaged over configurations, as described in Ref. [12]. There are three different interfaces in Fe/MgO/Fe/GaAs and we have determined the effect of 10% intermixing at each of them. The results are shown in Fig. 4 as a function of MgO thickness and compared with the effect of intermixing of the same magnitude in a conventional Fe/MgO/Fe junction. The results for a perfectly epitaxial Fe/MgO/Fe/GaAs junction are also included.

As expected, intermixing at the left Fe/MgO interface has the strongest effect on the TMR. This is because minority-spin electrons can be scattered from the Γ point to other regions of the iron 2D BZ and can then travel in these states in the left Fe electrode. This mechanism opens up new conduction channels in the AP configuration which reduces the TMR. The above mechanism is exactly the same as for a conventional Fe/MgO/Fe junction with a disordered interface and is discussed in detail in Ref. [12]. Scattering from the Γ point to other regions of the iron 2D BZ has no strong effect at the right MgO/Fe interface because electrons scattered to Fe states far from the Γ point are subsequently filtered out of transport by the small GaAs Fermi surface. However, it should be noted that very effective methods have been developed to grow almost perfect interfaces in conventional Fe/MgO/Fe junctions as demonstrated by the very high TMRs measured [13]. It follows that a poor quality of the Fe/MgO interfaces is

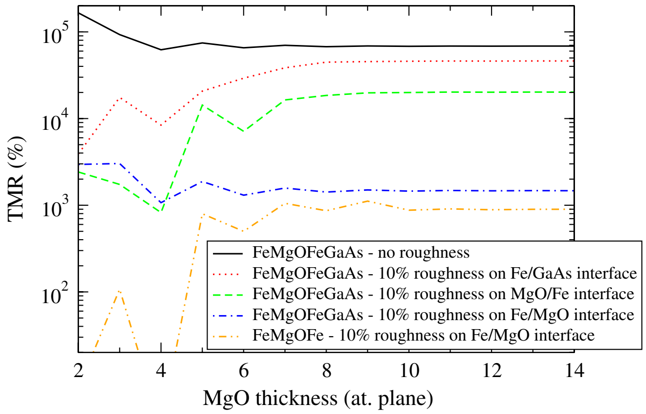

FIG. 4 (color online). TMR ratios of an Fe/MgO/Fe/GaAs junction with interfacial roughness. The GaAs electron density is $n = 10^{18}$ cm^{-3}. The TMR of a conventional Fe/MgO/Fe junction with the same roughness at one interface is also shown.

unlikely to be a serious problem. More relevant is the effect of roughness at the new Fe/GaAs interface we are adding to the well-investigated Fe/MgO/Fe junction. Figure 4 demonstrates that roughness at the Fe/GaAs interface has only a very small effect on the TMR. This can be easily understood because the role of GaAs is simply to act as a filter selecting small values of $\mathbf{k}_{\|}$, and this filtering action depends only on the size of the GaAs Fermi surface which is a bulk not interface property. Whether the Fe/GaAs interface and, indeed, GaAs layer itself is well ordered or not is, therefore, largely immaterial.

One potential problem that needs to be addressed is the well-known resonance in the minority-spin density of states which lies close to the middle of the GaAs gap (see, e.g., [14]). If the Fermi level coincided with the resonance at the Γ point the minority-spin conductance would be enhanced and TMR reduced. For the typical height of the Schottky barrier we used (0.7 eV) and the electron densities we considered the resonance does not lie at the Fermi level and thus has no effect on the TMR. When we varied the height of the Schottky barrier to make the resonance coincide with the Fermi level, we find that the TMR is reduced but only by a factor of 2 or 3; i.e., it remains some 2 orders of magnitude higher than for a conventional Fe/MgO/Fe barrier.

Finally, we discuss briefly the choice of the thickness of the right Fe layer which separates MgO from GaAs. All our results are for a typical thickness of 20 at. planes. We find that varying the thickness of the Fe layer between 5 and 40 at. planes has negligible effect on the TMR except for two isolated thicknesses of 16 and 32 at. planes for which a quantum well resonance strongly reduces the TMR. However, these very special thicknesses can be easily avoided and our supercell calculations show that a small interfacial roughness or steps at one of the Fe interfaces remove the resonances.

In conclusion, the Fe/MgO/Fe/GaAs system we propose has a number of advantages over a conventional Fe/MgO/Fe junction. First of all, the TMR ratio is predicted to be more than 2 orders of magnitude higher than that of Fe/MgO/Fe. The second great advantage is that these very high TMR ratios are essentially independent of MgO thickness and occur for MgO layers as thin as 2–3 at. planes. Third, the very high TMR we calculate is very robust to disorder at the Fe/GaAs interface and in the GaAs layer itself. We also expect it to be insensitive to details of the interface such as the Ga or As termination. Finally, by varying the degree of doping and applied gate voltage of the GaAs layer, one can tune the resistance of the whole structure by many orders of magnitude without spoiling the very high TMR. In particular, the resistance of our Fe/MgO/Fe/GaAs junction with the highest electron density of 10^{19} cm^{-3} is equivalent to that of a conventional Fe/MgO/Fe junction with only 6–7 at. planes of MgO. Yet the TMR is predicted to be in excess of 10 000%, which is equivalent to that calculated for an MgO thickness of about 100 at. planes in a conventional Fe/MgO/Fe junction.

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[1] J. Mathon and A. Umerski, Phys. Rev. B **63**, 220403(R) (2001).
[2] W. H. Butler, X. G. Zhang, T. C. Schulthess, and J. M. MacLaren, Phys. Rev. B **63**, 054416 (2001).
[3] S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki, and K. Ando, Nature Mater. **3**, 868 (2004).
[4] S. S. P. Parkin, Ch. Kaiser, A. Panchula, P. M. Rice, B. Hugues, M. Samant, and See-Hun Yang, Nature Mater. **3**, 862 (2004).
[5] D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).
[6] J-M. Jancu, R. Scholz, F. Beltram, and F. Bassano, Phys. Rev. B **57**, 6493 (1998).
[7] W. A. Harrison, *Electronic Structure and the Properties of Solids* (Dover Publications, New York, 1989).
[8] W. Mönch, *Electronic Properties of Semiconductors Interfaces* (Springer, New York, 2003).
[9] J. Waldrop, J. Vac. Sci. Technol. B **2**, 445 (1984).
[10] A. B. McLean and R. H. Williams, J. Phys. C **21**, 783 (1988).
[11] I.-H. Tan, G. L. Snider, and E. L. Hu, J. Appl. Phys. **68**, 4071 (1990).
[12] J. Mathon and A. Umerski, Phys. Rev. B **74**, 140404(R) (2006).
[13] S. Ikeda, J. Hayakawa, Y. Ashizawa, Y. M. Lee, K. Miura, H. Hasegawa, M. Tsunoda, F. Matsukura, and H. Ohno, Appl. Phys. Lett. **93**, 082508 (2008).
[14] A. N. Chantis, K. D. Belashchenko, D. L. Smith, E. Y. Tsymbal, M. van Schilfgaarde, and R. C. Albers, Phys. Rev. Lett. **99**, 196603 (2007).