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 \(\Gamma\) point, i.e., those with parallel wave vector \(k_\| = 0\) (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 \(\Gamma\) point but minority-spin electrons are strongly reflected at the Fe/MgO interface and there is, therefore, a hole in the conductance at the \(\Gamma\) point in the antiparallel (AP) configuration.

To satisfy these two requirements, we propose a composite system in which the filtering toward the \(\Gamma\) 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 \(\Gamma\) 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 \(\Gamma\) 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 \(k_\|\) very close to the \(\Gamma\) 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 \(\Gamma\) 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 \(\Gamma\) point in GaAs is stronger than in conventional Fe/MgO/Fe junction, our system gives higher TMR. A simple esti-
mate 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 \(n = \frac{2\sqrt{2m_0 EF}}{3h^2 \pi^2}\), where \(m_0\) 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 \(V_{SB}(1 - z/z_{dep})^{-2}\), 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].

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 \(T(E_F, k_{||})\) at the Fermi level \((E_F)\) of electrons with parallel wave vector \(k_{||}\) over the whole two-dimensional (2D) Brillouin zone (BZ):

\[
G = \frac{e^2}{h} \sum_{k_{||}} T(E_F, k_{||}).
\]

The details of the method are described in Ref. [1]. The optimistic tunneling magnetoresistance ratio (TMR) is defined by TMR = \((G_P - G_{AP})/G_{AP}\), 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 \(10^{17} - 10^{19} \text{ cm}^{-3}\) 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. 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.](image)

![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.](image)
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 atomic 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 $G_P(k)$ and $G_{AP}(k)$ 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 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 $\Gamma$ point. However, since the electron density $n \propto k_F^2$, 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 po-

![FIG. 3 (color online). $G_P(k)$ and $G_{AP}(k)$ 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 ($\pi/a$, where $a = 5.65$ Å is the lattice constant of GaAs).](image-url)
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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