Theory of ultrahigh magnetoresistance achieved by k-space filtering without a tunnel barrier

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Calculations of the current-perpendicular-to-plane magnetoresistance (CPP GMR) of an epitaxial Fe/Ag/Fe(001) trilayer attached to an n-type InAs lead (collimator) are presented. They show that for realistic InAs carrier densities, the CPP GMR of this k-space selective system can reach peak values of 10⁵%. The very high values of the CPP GMR are achieved because the small Fermi surface of the semiconductor collimator selects only electrons traveling perpendicular to the Fe/Ag interface (Γ point) where the magnetic contrast is as high as that of the Fe/MgO interface. The high calculated CPP GMR is very robust to disorder at the Fe/InAs interface and within the InAs layer itself. It is also much higher than the highest observed tunneling magnetoresistance of MgO-based junctions but the total resistance of the Fe/Ag/Fe trilayer with an InAs collimator is much lower than that of the tunneling junction. Nevertheless, the resistance is high enough to obviate the need for nanopillar geometry necessary for conventional CPP GMR systems.

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The highest magnetoresistance ratio (MR) of the order of 1000% at low temperature has been observed in epitaxial tunneling junctions with a fully crystalline MgO barrier. One might ask whether such record MR ratios can ever be achieved without the MgO tunneling barrier. In particular, can the current-perpendicular-to-plane magnetoresistance (CPP GMR) of fully metallic multilayers be tuned to achieve a CPP GMR higher than the highest observed tunneling magnetoresistance? To answer this question, it is useful to recall the physical mechanism which leads to a very large tunneling magnetoresistance (TMR) in junctions with an MgO barrier. Two ingredients are required: (i) The first is a “collimator” selecting only electrons which travel close to the Γ point, that is, those with parallel wave vector \( k_n \parallel 0 \) (perpendicular tunneling). In a conventional Fe/MgO/Fe junction, such collimation is achieved by using a thick MgO barrier which strongly favors perpendicular tunneling. (ii) The second ingredient is a special feature of the Fe/MgO electronic 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 therefore the conductance vanishes at the Γ point in the antiparallel (AP) configuration. In an earlier publication, we demonstrated that an alternative and more effective way to collimate electrons toward the Γ point is to attach a conventional Fe/MgO/Fe tunneling junction with a thin MgO barrier to a lightly doped n-type semiconductor lead (collimator). Because the Fermi surface of n-type doped semiconductor (e.g., GaAs or InAs) under positive gate voltage is very small, only electrons with \( k_n \parallel 0 \) very close to the Γ point can tunnel through the whole Fe/MgO/Fe semiconductor structure, and therefore the TMR of such a composite system is strongly enhanced. Clearly, the same idea can be used to collimate electrons toward the Γ point in a fully metallic trilayer without any tunneling barrier. It follows that we can engineer the CPP GMR so that it is determined only by electrons with \( k_n \parallel 0 \). To benefit from this collimation, we need to find a combination of ferromagnetic and nonmagnetic metals whose interface has the same spin selectivity as that of Fe/MgO. There are a number of ferromagnet/nonmagnet interfaces that satisfy this condition. One can use bcc Fe, Co, or Py as a magnet and Ag or Au as spacers. Alternatively, one could use the FeCo/Cr interface. On the other hand, the archetypal fcc Co/Cu combination is not suitable since the magnetic contrast at the Γ point is weak (see, e.g., Ref. 3). As an example, we show in Fig. 1 the band structure of Fe and Ag. At the Γ point, there is a good match between Fe and Ag \( \Delta_1 \) bands for majority-spin electrons, but minority-spin electrons are completely reflected at the Fe/Ag interface. This is exactly the same spin-selectivity property at the Γ point as that of the Fe/MgO interface. The complete reflection of minority-spin electrons at the Γ point, which occurs at the Fe/Ag(001) interface, is confirmed by the photoemission experiments of Ortega et al. 4

In this Brief Report, we demonstrate by a fully realistic calculation that the CPP GMR of an Fe/Ag/Fe(001) trilayer attached to n-type InAs collimator is several orders of magnitude higher than the CPP GMR of a conventional Fe/Ag/Fe(001) trilayer without the collimator. We point out that a large amount of research has been done on spin injection across the Fe/semiconductor interface. All of this is quite irrelevant to the operation of the system we propose. This is because the collimation is a property of the bulk semiconductor, not of the interface. We use InAs as a collimator in preference to GaAs since it is known experimentally that an Ohmic contact between Fe and InAs is formed (see, e.g., Refs. 5 and 6).

The CPP GMR system with a semiconductor collimator has also the very useful additional property that its resistance is much higher than that of any metallic lead attached to it. Conventional CPP GMR sensors are being considered for spintronics applications as an alternative to MgO tunneling junctions. However, not only is their CPP GMR much lower than the TMR of an MgO-based junction but the spin-dependent resistance of fully metallic sensors is so low that they have to be fabricated as nanopillars in order that the voltage drop across the sensor be measurable. The advantage of the CPP GMR system with a semiconductor collimator is that it can be designed with a GMR ratio much higher than the...
TMR of an MgO-based tunneling junction but with a resistance that is significantly lower than that of the tunneling junction. Nevertheless, the resistance is high enough to obviate the need for nanopillar fabrication.

We now describe the calculation of the CPP GMR for the Fe/Ag/Fe trilayer system. The geometry of the system is shown in Fig. 2. We took a fixed thickness of eight atomic planes for the second Fe layer. The schematic potentials seen by majority- and minority-spin electrons in the parallel configuration of the ferromagnetic layers are also shown in Fig. 2. We assume that an Fe/Ag/Fe(001) trilayer is attached to an As-terminated $n$-type doped InAs(001) lead. The lattice constant of InAs (6.05 Å) is close to double the lattice constant of BCC Fe (2.87 Å). Thus, it is reasonable to assume a good match between the Fe and InAs lattices. Similarly, there is a very good lattice match between Fe and Ag with the two lattices rotated by $45^\circ$. We therefore assume a perfect lattice match throughout our system.

We use a tight-binding approach to calculate the CPP GMR. The tight-binding parameters for Fe and Ag were taken from Ref. 7, and the onsite potentials in Fe were adjusted self-consistently to reproduce the correct Fe moment at the interfaces. The parameters for InAs were obtained from Jancu et al. This parametrization of InAs includes $d$ orbitals and spin-orbit coupling. The hopping parameters between Fe and As atoms at the interface were obtained from Harrison’s formula. We consider $n$-type doped InAs under positive gate voltage, so that in the bulk of the InAs layer the Fermi level lies in the conduction band. For a given electron density $n$ in the conduction band of bulk InAs, the position of the Fermi level was determined from the parabolic band model formula $n = 2\sqrt{2(m^*_F)}^{3/2}/\hbar^2\pi^2$, where $m^*_F$ is the effective mass at the bottom of the conduction band.

For the calculation of the conductance from the Kubo-Landauer formula, we require the onsite tight-binding potentials for every atomic plane of the Fe/InAs interface which extends over large number of planes. They were determined from the known alignment of the Fe and InAs bands across the interface combined with the solution of a one-dimensional Poisson’s equation. This method allows us to determine the potential profile across the whole extended Fe/InAs interface. We find that, in agreement with experiments, no Schottky barrier is formed at the Fe/InAs interface.

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): $G = \frac{1}{\pi} \sum_k T(E_F, k)$. The details of the method are described in Ref. 12. The optimistic magnetoresistance ratio (CPP GMR) is defined by $\text{GMR} = (G_P - G_AP)/(G_AP)$, where $G_P$ is the conductance when the magnetizations of the Fe electrodes are parallel (P) and $G_AP$ is the conductance when the magnetizations of the electrodes are antiparallel (AP).

The CPP GMR of the Fe/Ag/Fe/InAs(001) system is plotted in Fig. 3 as a function of the Ag spacer thickness for different doping levels of InAs. For comparison, the CPP GMR of a conventional Fe/Ag/Fe trilayer is also shown. Our calculated CPP GMR for the Fe/Ag/Fe trilayer is in good agreement with experimental values of the CPP GMR which are also of the order of 100%.

Figure 3 shows that the CPP GMR of Fe/Ag/Fe trilayers with an InAs collimator reaches peak values of $10^5\%$, which
is three orders of magnitude higher than the CPP GMR of a conventional Fe/Ag/Fe trilayer. Since the CPP GMR oscillates with a large amplitude, it is clearly necessary to control the Ag thickness accurately to achieve such record values of the GMR. However, this should not be too difficult experimentally since the oscillation period is long, \( \approx 5 \) monolayers. In fact, it is known from previous work on interlayer exchange coupling that Fe/Ag/Fe trilayers can be grown with interfaces of such a high quality that even the short interlayer coupling period of 2.37 monolayers is observable.\(^{14}\)

Given that large oscillations of the CPP GMR are clearly an important feature of the collimation toward the \( \Gamma \) point, we need to clarify their origin. Oscillations of the conventional CPP GMR are expected because the nonmagnetic spacer represents a quantum well or step, resulting in quantum interference.\(^{15}\) However, as seen in Fig. 3, the amplitude of such oscillations for a conventional Fe/Ag/Fe trilayer is very small. It is small because the total conductance (GMR) is the sum of partial conductances over the whole 2D BZ. Each partial conductance oscillates with a different period determined by the spacer perpendicular wave vector \( k_\perp \), and there is a strong cancellation of such oscillations in the 2D BZ sum. As discussed by Itoh et al.,\(^{15}\) only an extremal period with a small decaying amplitude survives. However, in our system with a semiconductor collimator, the 2D BZ sum is restricted to a very small circle around the \( \Gamma \) point determined by the size of the semiconductor Fermi surface. It follows that all oscillations have approximately the same period determined by the spanning vector of the Ag Fermi surface belly. They thus add up coherently, which results in nondecaying large-amplitude oscillations of the conductance. There is also another factor which contributes to the large amplitude of the CPP GMR. An examination of the partial conductances of predominantly majority- and minority-spin electrons in the P and AP configurations shows that the CPP GMR is almost entirely determined by the majority-spin electrons in the P configuration and by the transmission of minority-spin electrons to the majority-spin band in the AP configuration.

Moreover, these two dominant partial conductances oscillate almost perfectly in antiphase, which results in a very large amplitude of the CPP GMR oscillations. The reasons for this behavior are discussed in detail in Ref. 16.

Although the Fe/Ag/Fe/InAs system has many advantages, there is a potential penalty to pay. One now has a more complicated system that may be more difficult to grow experimentally with good interfaces. We therefore have investigated the effect of interfacial roughness using the lateral supercell method, averaged over configurations, as described in Ref. 17. We have determined the effect of 10\% intermixing at the Fe/Ag and Fe/InAs interfaces. The results are shown in Fig. 4 as a function of Ag thickness and compared with the CPP GMR of a perfectly epitaxial conventional Fe/Ag/Fe junction. As expected, intermixing at the Fe/Ag interface has the strongest effect on the GMR. This is because minority-spin electrons can be scattered from the \( \Gamma \) point to other regions of the Fe 2D BZ and then can travel in these states in the Fe electrode. This mechanism opens up new conduction channels in the AP configuration which reduces the GMR. However, since high quality of the Fe/Ag interfaces has been demonstrated in previous work,\(^{14}\) poor quality of Fe/Ag interfaces is unlikely to be a serious problem. More relevant is the effect of roughness at the new Fe/InAs interface. Figure 4 demonstrates that roughness at the Fe/InAs interface has only a small effect on the GMR. This can be easily understood because the role of InAs is simply to act as a collimator selecting small values of \( k_\parallel \), and this collimation action depends only on the size of the InAs Fermi surface which is a bulk, not interface, property. Whether the Fe/InAs interface and InAs layer itself is well ordered is therefore largely immaterial.

In many applications, not only the magnitude of the magnetoresistance but also the total resistance of the structure is important.\(^{18}\) Therefore, we show in Fig. 5 the magnetoresistance ratio plotted against the total resistance of Fe/Ag/Fe junctions with different thicknesses of the Ag spacer and different doping levels of the InAs collimator. For comparison, we also show the corresponding results for a conventional Fe/Ag/Fe trilayer, conventional Fe/MgO/Fe tunneling junction, and

**FIG. 4.** (Color online) CPP GMR ratio of an Fe/Ag/Fe trilayer attached to an n-type InAs lead for different values of the electron density \( n \) in InAs. The CPP GMR of a conventional Fe/Ag/Fe trilayer is also shown.

**FIG. 5.** (Color online) Magnetoresistance plotted against resistance-area product for a variety of spacer thickness.
Fe/MgO/Fe tunneling junctions with an InAs collimator (see Ref. 2). The calculated TMR of the Fe/MgO/Fe junction includes small amount of interfacial roughness to make the theoretical results\textsuperscript{17} agree with experimental results.\textsuperscript{19} The results for a Fe/Ag/Fe system with a collimator are for perfect interfaces since the effect of interfacial roughness is relatively small (see Fig. 4). It can be seen that MR ratios much higher than those for either conventional CPP GMR or conventional TMR can be achieved by adding a semiconductor collimator to the system. Moreover, the total resistance of Fe/Ag/Fe trilayers with an InAs collimator is much lower than that of the conventional Fe/MgO/Fe tunneling junction. Although InAs makes an Ohmic contact with Fe, the resistance of the Fe/InAs interface is relatively high because of the small size of the InAs Fermi surface. It is important that the interfacial resistance is sufficiently high so that the CPP GMR can be measured even for a planar system and there is thus no need for nanopillar geometry.

In conclusion, our calculations demonstrate that forcing electrons by means of an \textit{n}-type InAs collimator to travel perpendicular to the Fe/Ag interface the CPP GMR of the Fe/Ag/Fe(001) trilayer can be greatly enhanced. This occurs because the magnetic contrast of the Fe/Ag interface at the $\bar{\Gamma}$ point (perpendicular incidence) is as high as that of the Fe/MgO interface. What we propose is a very general recipe since a number of ferromagnet/nonmagnet interfaces (some of them are listed above) exhibit a very high magnetic contrast at the $\bar{\Gamma}$ point. Similarly, any \textit{n}-type suitably doped semiconductor can be employed as a collimator. Although we used for simplicity a semi-infinite collimator in our calculations, in practice, a semiconductor layer of only a few nanometers thick is sufficient to collimate electrons toward the $\bar{\Gamma}$ point. This means that the resistance of the collimator is always much lower than the resistance of the magnet/nonmagnet interface and our results obtained in the ballistic limit remain valid even in the presence of impurities in the collimator.

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