Half-metallic ferromagnets for magnetic tunnel junctions by *ab initio* calculations

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(Received 23 August 2005; published 29 November 2005)

Using theoretical arguments, we show that, in order to exploit half-metallic ferromagnets in tunneling magnetoresistance (TMR) junctions, it is crucial to eliminate interface states at the Fermi level within the half-metallic gap; contrary to this, no such problem arises in giant magnetoresistance elements. Moreover, based on an *a priori* understanding of the electronic structure, we propose an antiferromagnetically coupled TMR element based on half-metallic zinc-blende chalcogenides, in which interface states are eliminated, as a paradigm of materials design from first principles. Our conclusions are supported by *ab initio* calculations.

DOI: 10.1103/PhysRevB.72.174428 PACS number(s): 75.70.Cn, 73.20.−r, 85.75.−d

I. INTRODUCTION

Half-metallic ferromagnets are ferromagnetic materials showing, in the ideal case, 100% spin polarization at the Fermi level E_F, due to a metallic density of states in one spin direction (usually majority spin) combined with a band gap in the other spin direction (usually minority spin). First discovered via *ab initio* calculations by de Groot *et al.*,[1] these materials have drawn strong attention because of their potential applications in the field of spintronics. In principle, half-metallic ferromagnets are ideal spin injectors and detectors, because under moderate voltage they can carry current in only one spin direction. Therefore, they also constitute ideal components for giant magnetoresistant (GMR) and tunneling magnetoresistant (TMR) devices,[2] with two half-metallic leads sandwiching a nonmagnetic normal metal spacer (in GMR) or a semiconductor or insulator spacer (in TMR). There is, for instance, the experimental result of Bowen and collaborators[3] who obtained a TMR ratio (relative change of resistance upon change of the magnetization alignment of the leads) higher than 1800% in a $La_{2/3}Sr_{1/3}MnO_3/SrTiO_3/La_{2/3}Sr_{1/3}MnO_3$ junction; this extreme value was attributed to the half-metallicity of $La_{2/3}Sr_{1/3}MnO_3$. Motivated by such findings, we set forth to gain theoretical understanding of the conditions under which half-metals can be fully exploited in TMR devices.

The purpose of this article is twofold. First, we demonstrate by theoretical arguments on the electronic structure that it is much easier to exploit the half-metallic property in a GMR element than in a TMR one. We explain the implications caused by interface states in TMR elements and we suggest cases of improved TMR elements without interface states. Then, we propose an antiferromagnetically coupled TMR element (to serve as a magnetic field sensor) based on an *a priori* understanding of the exchange interactions in such systems, as a paradigm of materials design from first principles.

II. HALF-METALS IN TMR JUNCTIONS: THE ROLE OF INTERFACE STATES

The idea of using half-metals in GMR and TMR junctions seems simple. In a parallel (P) alignment of the magnetic moments of the half-metallic leads sandwiching the spacer, *some* current will pass, either by metallic conduction (in GMR) or by tunneling (in TMR) of majority spin electrons. On orienting the moments of the leads in an antiparallel (AP) way, for one spin channel no current can enter the junction (due to the minority-spin gap of the one lead), while in the other spin direction no current can exit the junction (due to the minority-spin gap of the other lead); thus *no* current can pass. Hence this is an ideal spin-controlled switch.

However, in TMR junctions a difficulty arises in the presence of interface states around E_F in the half-metallic gap at the metal-insulator contact. Consider, for instance, the TMR junction in Figs. 1(a) and 1(b), where the bands are shown schematically along the junction. Panel (a) shows the band alignment for both spin directions for a P alignment of the magnetization of the half-metallic leads, while panel (b) shows the same for an AP alignment. At the interfaces, for the minority-spin direction, possible localized interface states are shown. If they exist, it is inevitable that they are coupled to the bulk states of the half-metal, and thus they can be important for the transport properties and for the TMR ratio of the junction, as we will now discuss.

If interface states are present, they contribute to the tunneling current j. The current is controlled by two sequential processes: (i) by the tunneling itself, characterized by a rate $1/\tau_{\text{tunn}}$, and (ii) by refilling the interface states after an electron has tunneled out of them, with a characteristic rate of $1/\tau_{\text{fill}}$ (or by emptying these states after an electron has tunneled into them, with a rate of $1/\tau_{\text{empty}}$) (otherwise they are blocked by the Pauli principle or by Coulomb blockade effects). Since these processes take place sequentially, the characteristic times τ_{tunn} and $\tau_{\text{fill(empty)}}$ must be additive. Then, in the AP alignment the current j_{AP} has a nonzero value, and expression for j_{AP} has the form [see also Fig. 1(b)]

$$j_{\text{AP}} \sim \frac{1}{\tau_{\text{fill}} + \tau_{\text{tunn}}^{\uparrow\downarrow}} + \frac{1}{\tau_{\text{tunn}}^{\downarrow\uparrow} + \tau_{\text{empty}}}. \tag{1}$$

The first term refers to filling a spin-down interface state at the left lead in Fig. 1(b) (up) and tunneling to the right lead, while the second term refers to tunneling from the spin-up continuum of the left lead in Fig. 1(b) (down) into the inter-

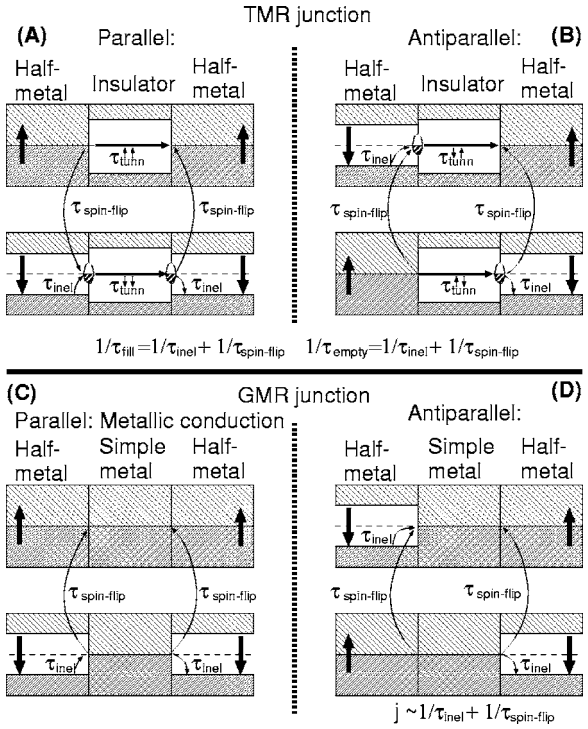

FIG. 1. Schematic band profile in TMR (a), (b) and GMR (c), (d) junctions using half-metallic leads. In the middle of the gaps, E_F is shown as a dashed line. Filled bands are shown as dark shaded regions, empty bands are lightly shaded; unshaded regions correspond to the band gaps. In (a) and (c), the parallel magnetic alignment of the leads is shown for both spin directions; in (b) and (d) the antiparallel one. In the TMR case (a) and (b) there is the possibility of interface states within the half-metallic gap, at E_F. Electrons can enter the interface states on the left at a rate $1/\tau_{\text{fill}}$ and sequentially tunnel at a rate $1/\tau_{\text{tunn}}$ (and similarly exit the interface states on the right). The time τ_{fill} depends on inelastic processes and on the spin-flip rate, which can be much faster than the tunneling rate. Then τ_{tunn} determines the current, and the half-metallic property is irrelevant. In GMR (c) and (d) no such problem appears, since there is metallic conduction in the parallel magnetic alignment.

face state of the right lead, and then emptying it. We distinguish among four different tunneling times, for the four different cases of tunneling between majority and minority states as shown in Figs. 1(a) and 1(b). We name these $\tau_{\text{tunn}}^{\uparrow\uparrow}$, $\tau_{\text{tunn}}^{\downarrow\downarrow}$, $\tau_{\text{tunn}}^{\downarrow\uparrow}$, and $\tau_{\text{tunn}}^{\uparrow\downarrow}$. Evidently the slower of the two processes (i) and (ii) determines the current. If, in comparison to the slow tunneling rate, the states are immediately refilled (or emptied) after a tunneling event (we will argue below that this is expected), then $\tau_{\text{fill(empty)}} \ll \tau_{\text{tunn}}$ and j_{AP} is determined by the tunneling rate alone, irrespective of the half-metallic band gap. Similar considerations hold for the minority-spin current in the P case.

What determines the coupling of the interface states with the bulk and thus the characteristic times τ_{fill} and τ_{empty}? On one hand, there are inelastic processes contributing with a rate $1/\tau_{\text{inel}}$. These can be of thermal nature or quantum fluctuations (scattering of electrons with phonons, magnons, other electrons, etc.). Usually inelastic processes are slow at low temperatures, but if the Fermi level is in the proximity of the band edges, rather than in midgap, they can be of significance. More importantly, there is always some spin-orbit coupling present. Therefore even in the bulk of the half-metal the polarization at E_F, $P(E_F)$, is always lower than the ideal 100%; e.g., $P(E_F) \simeq 99\%$ for NiMnSb,[4] and the value decreases when the material is composed by heavier elements or when E_F is touching the band edges [e.g., $P(E_F) \simeq 67\%$ for PtMnSb].[4] Spin-orbit coupling will contribute to filling or emptying the interface states with a rate of $1/\tau_{\text{spin flip}}$. This acts in parallel with the inelastic processes, and thus

$$1/\tau_{\text{fill(empty)}} = 1/\tau_{\text{inel}} + 1/\tau_{\text{spin flip}}. \tag{2}$$

Additional factors can come into this equation in the presence of defects or impurities which reduce $P(E_F)$ by introducing gap states. For majority electrons we do not discuss the interface states separately from the bulk states, since they are irrelevant for the half-metallic property; their effect is included in τ_{tunn}.

Although the rate $1/\tau_{\text{fill(empty)}}$ in Eq. (2) is low, we recall that tunneling can be a very slow process (τ_{tunn} is long, growing exponentially with insulator thickness and barrier height). Therefore, for thick or high insulating barriers the interface states are immediately refilled (or reemptied) after each tunneling event, and they act as a reservoir of electrons. The fact that they are much weaker coupled to the bulk than the majority-spin states does not help, since everything is determined by the much slower tunneling rate. Assuming then that all tunneling times τ_{tunn} are long, Eqs. (1) and (2) lead to

$$j_{\text{AP}} \sim \frac{1}{\tau_{\text{tunn}}^{\downarrow\uparrow}} + \frac{1}{\tau_{\text{tunn}}^{\uparrow\downarrow}} \quad \text{and} \quad j_{\text{P}} \sim \frac{1}{\tau_{\text{tunn}}^{\uparrow\uparrow}} + \frac{1}{\tau_{\text{tunn}}^{\downarrow\downarrow}}. \tag{3}$$

This means that the current depends only on the tunneling rates for the two spin directions and not at all on the half-metallic property of the lead.

The tunneling rates themselves depend on numerous factors: the insulating barrier thickness, electronic, and complex band structure,[5–7] the details of the interface structure, the presence of interface disorder, the symmetry character of the interface states (see below), the presence of defects in the insulating spacer,[8] etc. Particularly important is the spin polarization $P(E_F)$ at the interface.[9,10] This, in the absence of interface states, is approximately the same as in the bulk of the half-metal, but in their presence it can have a completely different value and can even be reversed.[11] The influence of these factors is in general different on each of the four tunneling times $\tau_{\text{tunn}}^{\downarrow\uparrow}$, $\tau_{\text{tunn}}^{\uparrow\downarrow}$, $\tau_{\text{tunn}}^{\uparrow\uparrow}$, and $\tau_{\text{tunn}}^{\downarrow\downarrow}$, since the nature of the states involved is different. Thus *some* TMR ratio can appear, but no extraordinary effect can be guaranteed by the half-metallic property, unless one can eliminate the interface states. We note that if these are eliminated, there is still a low rate of incoming minority-spin states from the bulk to the interface, because of the spin-orbit coupling.[4] This rate, however, is very low [determined by the high polarization $P(E_F)$].

In GMR junctions, on the other hand, the interface states play no significant role in this context, as demonstrated sche-

matically in Figs. 1(c) and 1(d). In the P case the conduction is metallic, while in the AP case it is confined at most to the value of the spin polarization at E_F in the bulk of the half-metallic leads (plus inelastic effects); if this is determined by the spin-orbit coupling, it should lead to an effect of the order of 1%. This means that the half-metallic property is fully exploited in the case of GMR, in contrast to TMR.

The presence of interface states can affect the TMR also in usual magnetic tunnel junctions. This has been discussed in the literature in the past.[2,12,13] In particular, interface states can couple to the bulk Bloch states via a lowering of symmetry at the interface, caused, for example, by interface roughness or a change of crystal structure. Then interface resonances are formed, which can even lead to resonant tunneling[12] and "hot spots" of the tunneling conductance. Even if they remain orthogonal to the bulk states, interface states can become resonant via inelastic electron-electron or electron-phonon scattering and they can contribute to the tunneling at already low temperatures.[13] The strong influence of the interface states on the TMR effect has also been verified experimentally, for example in Fe/MgO/Fe junctions,[14] where even a reversal of the TMR sign was observed due to a bias-induced "activation" of interface resonances. In junctions based on half-metals, a lowering of symmetry at the interface cannot lead to a coupling of minority-spin interface states to corresponding bulk states, since the latter are absent in the gap region. Symmetry plays a role, in the sense that the spin-orbit Hamiltonian conserves the translational symmetry (the Bloch vector $\mathbf{k}_\parallel$ parallel to the interface is conserved during spin-orbit scattering for an ordered interface), so that the spin-flip processes can be intensified in the presence of interface disorder, when $\mathbf{k}_\parallel$ is not conserved. The inelastic events are of course always present.

At this point we conclude that, in order to exploit the half-metallic property in TMR junctions, we must find half-metal/insulator interfaces without interface states; and to this we now turn.

In the discussion above we referred to half-metallic leads. We note, however, that the same effects (extreme TMR ratio without minority-spin interface states, but strong reduction in their presence) are expected even if the half-metals are not used as infinite leads, but as thin films in a multilayered half-metal-semiconductor (HM/SC) structure, e.g., of the form (lead)/HM/SC/HM/(lead) or (lead)/SC/HM/SC/HM/SC(lead). Here, the leads can be simple metals, thus avoiding growth of half-metallic leads over hundreds of angstroms, while the half-metallic films serve as spin filters. If, in addition, the HMs are coupled antiferromagnetically via the SC, the pinning of the magnetic moment via exchange bias with an antiferromagnet can be avoided (for use of the junction as a magnetic sensor). In what follows, we demonstrate by theoretical considerations and first-principles calculations that such a system is possible.

III. AP COUPLED HALF-METALLIC ELEMENTS

The most studied half-metallic ferromagnets are probably Heusler alloys. The bulk band structure and the origin of the gap are well understood,[15] and so are their surface[16] and interface[11] properties. Unfortunately, calculations of Heusler alloy/semiconductor interfaces are conclusive on the appearance of interface states at E_F in almost all cases. Thus, our previous analysis rules out Heusler alloys as good candidates for TMR junctions.

On the other hand, the class of half-metallic zinc-blende pnictides and chalcogenides shows no interface states at E_F when brought in contact with zinc-blende (ZB) semiconductors.[17] The reason is that, here, the gap originates from a hybridization and repulsion of the transition-metal *d* states with the *p* states of the *sp* anion. This continues coherently at the interface between the *sp* anion and the cation of the semiconductor. No unsaturated bonds are left to produce spurious interface states. Such compounds [in particular CrAs,[18] CrSb,[19] and small islands of MnAs (Refs. 20 and 21)] have already been experimentally realized by molecular beam epitaxy, and show Curie points well above room temperature. Also multilayers of CrAs and CrSb with GaAs have been made.[22,23] Therefore, we consider this class of compounds well suited for TMR junctions.

In magnetic field sensor applications of GMR and TMR, it is desirable that the leads of the junction are coupled magnetically AP in the ground state; then, with the application of a magnetic field, the leads are reoriented in a P fashion, and the conductance changes. Moreover, the energy difference ΔE between AP and P should be small enough that the switching occurs at moderate fields. In GMR, both the property of AP coupling and the coupling energy can be tuned by changing the spacer thickness d, since $\Delta E(d)$ follows a decaying, oscillating pattern.[24] In the case of TMR, the interlayer exchange coupling weakens exponentially with increasing d.[25] Therefore, we seek TMR systems where the AP coupling is dictated by *a priori* known physical properties, while $|\Delta E|$ can be tuned *a posteriori* by changing the insulator spacer thickness. Again this can be achieved by using half-metallic ZB compounds.

The magnetic coupling in such ZB compounds is well understood.[26,27] The origin of ferromagnetism is mainly the broadening of the majority *p-d* hybrid band, whenever it is partly occupied (the double-exchange mechanism). This is the case, e.g., for CrAs, MnAs, and CrTe. On the contrary, FeAs and MnTe have one electron too many: the majority *p-d* band is fully occupied, so that no energy is gained by its broadening, and the antiferromagnetic susceptibility prevails.

The zinc-blende structure, along the $\langle 001 \rangle$ direction, can be viewed as an epitaxial structure of chemically alternating atomic layers. For example, CrTe has alternating layers of Cr and Te in the form $\cdots$CrTeCrTe$\cdots$. We interrupt this succession by introducing semiconducting CdTe layers which decouple two CrTe leads. The structure will have the form $\cdots$CrTeCrTeCdTeCrTeCrTe$\cdots$. This structure is still ferromagnetic and half-metallic with no interface states at E_F (we verified this by *ab initio* calculations). But now we introduce one layer of Mn at the CrTe/CdTe interface to cause an AP coupling of the leads. The layer-by-layer structure will be $\cdots$CrTeCrTeMnTeCdTeMnTeCrTeCr$\cdots$. The AP coupling is expected because of the Mn-Mn interaction, by the same mechanism which brings MnTe to an antiferromagnetic[28] state. The idea of this interface engineering is to introduce an element with higher number of valence electrons at the in-

TABLE I. The proposed half-metallic TMR element. The arrows indicate the calculated magnetic moment direction in each layer. The ground state is AP with the P state 15 meV higher. More CdTe layers will provide further decoupling.

⋯	Cr	Te	Cr	Te	Mn	TeCdTe	Mn	Te	Cr	Te	Cr	⋯	
⋯	↑		↑		↓		↑		↓		↓	⋯	(AP)
⋯	↑		↑		↓		↓		↑		↑	⋯	(P)

terface (here Mn in the place of Cr), so that the double-exchange mechanism is not any more present, because the bands are filled.

We verified these predictions by first-principles calculations. We employed the full-potential linearized augmented plane-wave method as implemented in the FLEUR code,[29] within the generalized gradient approximation of density-functional theory, using the CdTe lattice constant $a_{\mathrm{CdTe}}=6.48$ Å. The calculated $a_{\mathrm{CrTe}}=6.26$ Å is 3.5% smaller, while $a_{\mathrm{MnTe}}=6.34$ Å lies in between. Half-metallic zinc-blende compounds are grown only in thicknesses of a few monolayers;[18,22,23] theoretical investigations indicate that thicker structures can become unstable.[30] As we see below, two CrTe layers suffice to create a spin filter, while more than two CdTe layers are needed. Thus we consider our choice of the common lattice constant well suited. Nevertheless, we checked that our conclusions are also valid in the calculated CrTe equilibrium lattice constant (see below). Note that moderate tetragonal distortions do not destroy the half-metallic property.[17]

In Table I we present the calculated geometry in more detail. A supercell was used in the calculation, consisting of two half-metallic parts, each having two Cr and two Mn layers (and corresponding Te layers), separated by a CdTe for decoupling. Various possible magnetic configurations were examined. In the ground state (AP in Table I), the leads are AP coupled, as expected. In addition, the Mn atoms are antiferromagnetically coupled to the Cr atoms. The nice feature is that, in the ground state, each lead is by itself half-metallic, so that the whole system is nonconducting. This is evident also from Fig. 2, where the layer-resolved density of states at E_F is shown over the whole supercell. Spin-down electrons are blocked in the first half of the junction, whereas spin-up electrons are blocked in the second part. By applying an external magnetic field the system switches to the P configuration with an energy cost of 15 meV (per CdTe slab). The P state is half-metallic throughout the junction and conducting by tunneling of spin-up electrons, as can be seen in Fig. 2 (bottom). Figure 3 shows in more detail the spin-dependent density of states of the multilayer (containing one CdTe bilayer) in the P state. In the spin-down DOS, the half-metallic gap is evident, starting just below E_F and ending at 1.2 eV. From the partial DOS at the Cr atoms (full lines) and at the Mn atoms (dashed lines) one recognizes that the Mn atoms are antiferromagnetically aligned to the Cr atoms: the occupied Mn d states are of spin-down character (between −4 and −2 eV), while the occupied Cr d states are of spin-up character (between −1.5 eV and E_F).

The switching energy from the AP to the P state can be tuned by introducing more CdTe layers. To show this, we

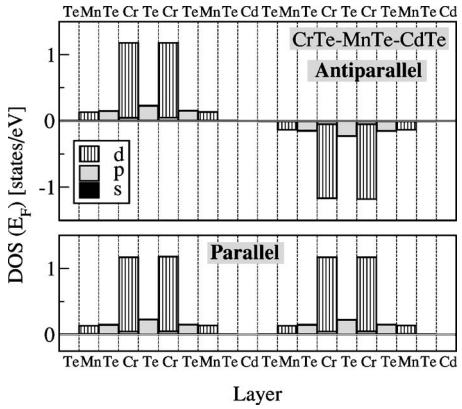

FIG. 2. Layer-resolved density of states (DOS) at E_F for the junction shown in Table I in the ground state (top) (AP alignment) and also in the P alignment (bottom). (The symmetry resolution of the DOS is also given.) Each lead by itself is half-metallic, and there are no minority-spin interface states at E_F. Thus, in the antiparallel case no current can pass. In the parallel case there can be tunneling of spin-up electrons, while no spin-down states are present at E_F.

compare the case without a CdTe layer (the interface is then of the form Mn-Te-Mn), where $\Delta E=124$ meV, to the case of Mn-CdTe-Mn ($\Delta E=15$ meV), and then to the case of Mn-CdTeCdTe-Mn ($\Delta E=3.6$ meV). Each additional CdTe layer lowers the energy difference by an order of magnitude. One or two more CdTe layers should decouple the layers sufficiently.

Calculations in the CrTe equilibrium lattice constant lead to the same conclusions. In the P configuration, E_F slightly enters the valence band (by about 30 meV) for a CdTe thickness of one layer, and is found again in the gap for four CdTe layers. In the AP configuration each CrTe part remains always half-metallic (irrespective of the CdTe thickness),

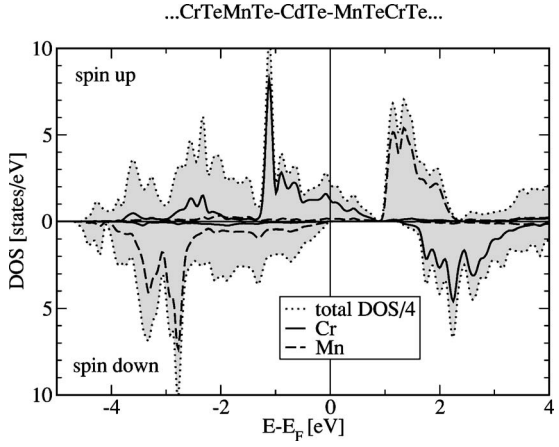

FIG. 3. Spin-resolved density of states for the P configuration of the proposed TMR element. The half-metallic property is evident. The Mn atoms (dashed lines) are antiferromagnetically aligned to the Cr atoms (solid lines); the occupied Mn d states are of spin-down character (between −4 and −2 eV), while the occupied Cr d states are of spin-up character (between −1.5 eV and E_F). The DOS of the AP configuration is similar, but alternating in spin character between successive half-metallic regions (see Fig. 2).

blocking current. The coupling energy changes by a factor of about 1.5, always favoring the AP coupling (194 meV in the case Mn-Te-Mn and 25 meV in the case Mn-CdTe-Mn). Thus the switching properties are still there.

IV. SUMMARY

In summary, we have discussed the use of half-metallic ferromagnets in TMR and GMR junctions. We concluded that, while in GMR junctions the half-metallic property can be exploited fully, in TMR junctions the same property does not help if there are interface states present at E_F within the half-metallic gap of the half-metal/insulator interface (as is typical for Heusler alloys). The reason is that the tunneling rate is slow compared to the spin-flip rate, hence minority-spin interface states are efficiently coupled to the metallic reservoir of the majority-spin states.

Moreover, we have proposed that such TMR elements can be made by using half-metallic zinc-blende pnictides and chalcogenides in contact with II-VI semiconductors, which show no interface states at E_F. We showed that, under certain conditions, an antiparallel magnetic coupling of the leads is possible, avoiding the difficulty of pinning one of the leads in these systems. Due to the complete blocking of the electric current, such a device will show an ideal magnetoresistance ratio and can serve as an ideal magnetic field sensor.

ACKNOWLEDGMENTS

We are grateful to Professor H. Akinaga, Professor P. H. Dederichs, and Dr. G. Bihlmayer for fruitful discussions.

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