PHYSICAL REVIEW B, VOLUME 65, 241306(R)

Ballistic spin injection from Fe(001) into ZnSe and GaAs

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(Received 7 December 2001; published 31 May 2002)

We consider the spin injection from Fe into ZnSe and GaAs in the ballistic limit. By means of the *ab initio* screened Korringa-Kohn-Rostoker method we calculate the ground-state properties of epitaxial Fe|ZnSe(001) and Fe|GaAs(001) heterostructures. Three injection processes are considered: injection of hot electrons and injection of ''thermal'' electrons with and without an interface barrier. The calculation of the conductance by the Landauer formula shows that these interfaces act like a nearly ideal spin filter, with spin polarization as high as 99%. This can be traced back to the symmetry of the band structure of Fe for normal incidence.

DOI: 10.1103/PhysRevB.65.241306 PACS number(s): 72.25.Hg, 72.25.Mk, 73.23.Ad

The controlled injection of a spin polarized current into a semiconductor (SC) is one of the central problems in the field of spin electronics, since it is a prerequisite for the development of spin-dependent devices.[1] Recently some important successes have been achieved. Fiederling *et al.*[2] have demonstrated the injection from the paramagnetic II-VI SC $Be_xMn_yZn_{1-x-y}Se$ into GaAs with a very high spin polarization using an external magnetic field, while Ohno *et al.*[3] were able to show the injection from the ferromagnetic SC $Ga_{1-x}Mn_xAs$ into GaAs with an efficiency of 1%. However both methods have the disadvantage that they require a low temperature. Therefore the injection from a ferromagnet with a large Curie temperature such as Fe would have strong advantages. Such attempts, though, have not been very successful in the past, i.e., the reported spin injection efficiency was low.[4,5] Schmidt *et al.*[6] revealed that a basic obstacle for spin injection from a ferromagnetic metal into a SC exists, being represented by the large conductivity mismatch between both materials. Nevertheless Rashba[7] as well as Fert and Jaffrès[8] have recently pointed out that this obstacle can be overcome by introducing a tunneling barrier. Meanwhile, and independently, Zhu *et al.*[9] were successful in demonstrating the spin injection at room temperature from Fe(001) into GaAs with an efficiency of 2%, which they attributed to tunneling through a Schottky barrier.

Kirczenow[10] has lately pointed out that contrary to the ferromagnet|metal interface the interface between a ferromagnet and a SC could act as an ideal spin filter, if, e.g., the Fermi surface of the majority or minority spin bands has a hole at the Γ point of the two-dimensional Brillouin zone, so that only electrons of the other spin band can scatter into the conduction band states of the SC at the Γ point. However relevant hybrid systems such as Fe|ZnSe(001) and Fe|GaAs(001) for which epitaxial growth has been demonstrated, do not show this simple property.

Recently two ballistic calculations[11,12] for the spin injection process have been published, which basically rely on a free-electron description of the majority and minority spin bands. Grundler[11] could argue in this way that the Fe|SC interface can act as a spin filter with an efficiency of a few percent. Motivated by this work we present here an *ab initio* calculation of the ground-state properties and the ballistic transport through the Fe|ZnSe(001) and Fe|GaAs(001) interfaces. In contrast to the above-mentioned methods our calculations include the whole complexity of the band structures of the ferromagnet and the SC's as well as the even more complex properties of the interface. The important result of our calculation is that the considered Fe|SC interfaces act like nearly ideal spin filters, with spin injection ratios as high as 99%. We can attribute this to the different symmetries of the majority and minority *d* bands of Fe at the Fermi level, a behavior that cannot be described in the free-electron model. Taken together with the results of Zhu *et al.*[9] our calculations give a bright outlook for the spin injection from ferromagnetic Fe into SC's.

Our method is based on the local-density approximation of the density-functional theory and apply the screened Korringa-Kohn-Rostoker method.[13] The heterostructure consists of a Fe half-space and a SC (either ZnSe or GaAs) half-space, both oriented in the (001) direction and being epitaxially bonded at the interface, so that the SC lattice constant is double the Fe constant ($a_{Fe}^{exp}=5.425$ a.u. is used in the calculation). The two half-space Green's functions are determined by the decimation technique.[14] In the interface region the potentials of 4 ML of Fe and 2 ML of SC are determined selfconsistently. The potentials of all other ML are identified with the asymptotic bulk values. In all calculations we use a cutoff of $l_{max}=2$ for the wave functions and an atomic-sphere approximation for the potentials, but include the full charge density. The ballistic conductance G is calculated by the Landauer-Büttiker formalism for $T=0$. Here we use an expression similar to the one derived by Baranger and Stone,[15] but adjusted to the asymptotic Bloch character of the wave functions and the two-dimensional translation symmetry of the system. The in-plane component $\mathbf{k}_\parallel$ of the $\mathbf{k}$ vector enumerates then the scattering channels, and we can express the $\mathbf{k}_\parallel$-dependent conductance $G(\mathbf{k}_\parallel)$ wholly in terms of the Green's function of the system. Spin-orbit coupling is neglected in the calculation.

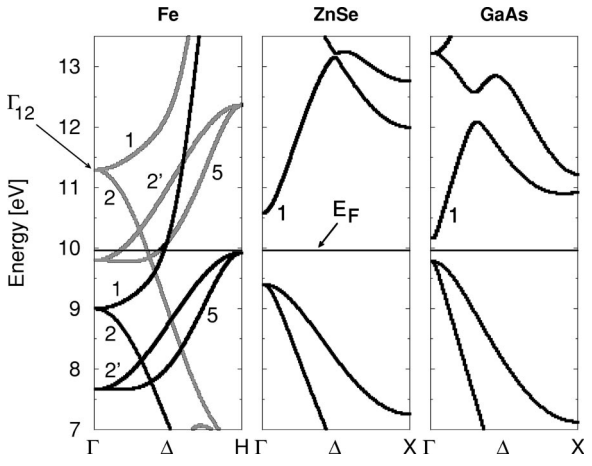

FIG. 1. Band structure of Fe (left panel) and the semiconductor: ZnSe (middle panel) and GaAs (right panel) around the Fermi energy. The black lines in the Fe band structure are the majority and the gray lines the minority spin bands. The numbers denote the corresponding symmetries of the (001)-direction Δ.

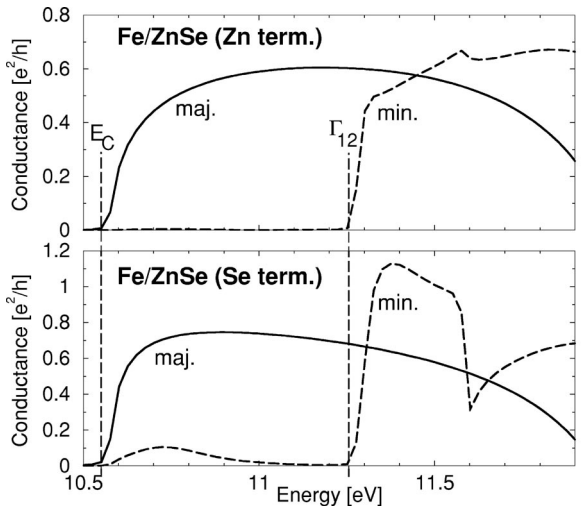

FIG. 2. Injection of hot electrons from Fe into ZnSe with a Zn termination (a) and a Se termination (b). For simplicity the conductance is calculated only at the Γ point. The solid line shows the conductance in the majority and the dashed line in the minority band. The energy E_C marks the bottom of the SC conduction band and Γ_{12} refers to Fig. 1.

As we will demonstrate in this paper, the spin injection process is to a large extent determined by the symmetries of the bulk band structures. For this reason we show in Fig. 1 the band structure of Fe and of the SC's ZnSe and GaAs, for Bloch vectors $\mathbf{k}=(0,0,k_z)$ normal to the interface. These are the states relevant for the injection process, since in the SC only states close to the conduction band minimum E_C will be populated, having $\mathbf{k}_\parallel \approx 0$. The left panel shows the spin split majority and minority bands of Fe in the region of the Fermi level E_F. As usual the different bands in (001) direction are indexed by Δ_1, Δ_2, etc. indicating the symmetries of the wave functions.[16] In the middle and right panel, the SC bands are shown with E_F assumed to be located in the middle of the gap. Most important here is that the lowest conduction states have Δ_1^{SC} symmetry; they are invariant under all symmetry operations of the zink-blende lattice, which transform the Bloch vector $\mathbf{k}=(0,0,k_z)$ in itself. These operations form the symmetry group C_{2v}, which is at the same time identical with the symmetry of the whole Fe|SC(001) interface. It is now important to single out those Fe states which are compatible with this C_{2v} symmetry. In Fe, the Δ nomenclature refers to the C_{4v} symmetry group, since, contrary to the zink-blende lattice, in the bcc lattice the (001) direction is a fourfold axis. Thus, not only the Δ_1^{Fe} states, consisting locally of s, p_z, and d_{z^2} orbitals, can couple to the Δ_1^{SC} band states, but also the $\Delta_{2'}^{\mathrm{Fe}}$ states consisting locally of in-plane d_{xy} orbitals. Here we assume that the x and y directions point along the cubic axes. On the other hand the Fe states of Δ_2^{Fe} symmetry (with $d_{x^2-y^2}$ character) as well as the Fe states with Δ_5^{Fe} symmetry (with p_x and d_{xz} or p_y and d_{yz} character) cannot couple to the Δ_1^{SC} states, since they do not show the full symmetry C_{2v} of the heterostructure. For the spin injection it is now important that in the majority band at E_F and above there exists only a Δ_1^{Fe} band (below E_F also a $\Delta_{2'}$ band is available) while in the minority band around E_F only a $\Delta_{2'}^{\mathrm{Fe}}$ band exists that can couple to the Δ_1^{SC} states, since the Δ_1^{Fe} band appears here at about 1.3 eV above E_F (see Γ_{12} in Fig. 1).

Not shown in Fig. 1 is the lower Δ_1^{Fe} band separated from the upper Δ_1^{Fe} band by the so-called *s-d* hybridization gap. This gap is characteristic of the transition metals and arises from the hybridization of the *s* with the d_{z^2} orbitals. For the (001) orientation this gap is so large that for the minority band E_F lies in the gap, giving rise to the spin filtering effect discussed in this paper. This effect is also important in magnetic tunnel junctions.[17]

First we discuss the injection process of hot electrons with Fe states well above E_F. Although for hot spin injection states with nonzero $\mathbf{k}_\parallel$ values also play a role, we consider here for simplicity only states with normal incidence. The calculated transmission probabilities for injection into ZnSe are shown in Fig. 2 for both spin directions, with Fig. 2(a) referring to a Zn-terminated interface and Fig. 2(b) to a Se-terminated one. The transmission starts at the energy E_C of the SC conduction band minimum. In the majority band the conductance strongly increases to values of around 0.6 or 0.7 (in units of e^2/h), while the conductance in the minority band is much smaller. As a result, the spin polarization of the injected current is very large; for Zn termination always larger than 97%, for Se termination larger than 75%. However, the situation completely changes, if the energy of the injected Fe electrons exceeds the value $E_{\Gamma_{12}}$ of the minimum of the minority Δ_1^{Fe} band. There the transmission in the minority band increases very sharply and even overcomes the majority transmission, so that the spin polarization changes sign. This clearly illustrates that the absence of the Δ_1^{Fe} state in the minority band leads for lower energies to the very large spin polarization of the current. Similar results are also obtained for the hot spin injection into GaAs(001), resulting, for lower energies, even in polarizations extremely close to 100%.

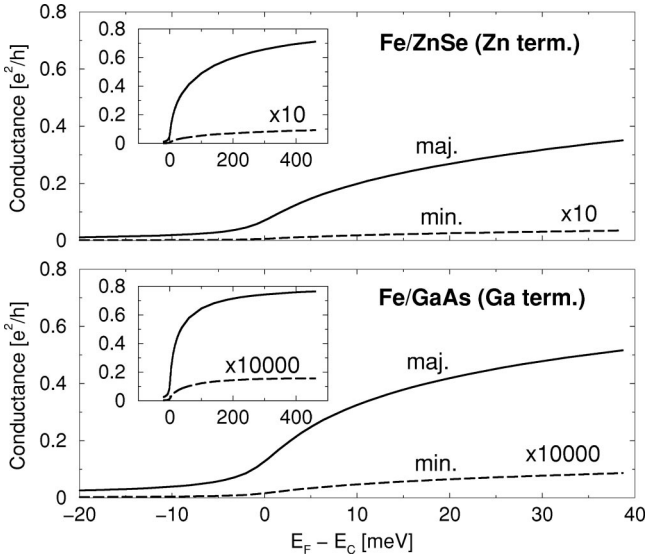

FIG. 3. Energy dependence of the barrier-free injection of electrons at E_F for a Fe|ZnSe junction with Zn termination (a) and a Fe|GaAs junction with Ga termination (b) at the $\bar{\Gamma}$ point. The solid lines show the conductance in the majority and the dashed lines in the minority band. In (a) the minority conductance is enlarged by a factor of 10 and in (b) by a factor of 10^4. The insets show the conductance in a wider energy range.

The strong spin polarization can be understood from the different spatial orientation and extent of the Δ_1^{Fe} and $\Delta_{2'}^{\mathrm{Fe}}$ states. The Δ_1^{Fe} states have s, p_z, and d_{z^2} admixtures. In particular, the s and p_z components have large spatial extent and a strong overlap with the SC states. Moreover the d_{z^2} and, in particular, the p_z orbitals point directly into the SC, so that a large transmission is possible. In contrast to this the minority $\Delta_{2'}^{\mathrm{Fe}}$ states consist of in-plane d_{xy} orbitals, which are much less extended and point in the wrong direction.

To model the injection of electrons at E_F we lower the potential in the SC half-space such that the Fermi level falls slightly above the conduction band energy E_C. Here we consider two situations by simulating the injection process both without and with a tunneling barrier. In the first case, we lower the potentials of the third, fourth and all further away SC ML by the same constant value, so that $E_F - E_C$ becomes positive. We do not change the potentials of the two SC ML closest to the interface, since they are important for the interface characteristics. By continuously varying the potential step, we calculate then the conductance as a function of $E_F - E_C$. Figure 3 shows the resulting conductance at the $\bar{\Gamma}$ point for an Fe|ZnSe(001) junction with Zn interface termination [Fig. 3(a)] and for an Fe|GaAs(001) junction with Ga termination [Fig. 3(b)]. The energy scale in the order of 10 meV refers to typical carrier concentrations in a two-dimensional electron gas.[11] The insets show the results over a larger energy region. The minority intensities are enhanced by a factor of 10 for ZnSe and by a factor of 10^4 for GaAs. Thus the spin polarizations are larger than 97% for ZnSe and practically 100% for GaAs. Very similar results are also obtained for the other terminations not shown here, i.e., the Se termination of ZnSe and the As termination of GaAs.

TABLE I. Spin polarization of the current at the $\bar{\Gamma}$ point for Fe|ZnSe and Fe|GaAs systems with different tunneling barrier thicknesses N. All four terminations are shown: Zn and Se for a Fe|ZnSe junction and Ga and As for a Fe|GaAs junction. In the last row also the polarization is given for a 32-ML-thick tunneling barrier when integrating over the whole two-dimensional Brillouin zone.

Thickness N (ML)	P (Zn)	P (Se)	P (Ga)	P (As)
8	96%	99.3%	99.99%	99.8%
32	86%	99.3%	99.99%	99.6%
80	80%	99.3%	99.98%	98.6%
144	77%	99.3%	99.97%	97.6%
32 (integr.)	84%	96.9%	99.52%	99.4%

All the calculated results in Fig. 2 and Fig. 3 suggest that near the energy E_C of the SC conduction band minimum the transmission probability varies for both spin directions as $\sqrt{E_F - E_C}$.[18] Since the square-root-like behavior is the same for both the majority and the minority electrons, the spin polarization remains constant for $E \to E_C$. Moreover, in the interesting energy region of about 10 meV, the reduction of the conductance is rather modest. The square-root-like behavior of the transition probability can be understood from a simple picture where a potential step in one dimension is assumed. For a constant potential of height V_B in the right half-space and a vanishing potential in the left half-space, the transition probability for an incident electron with energy $E = k^2$ into a transmitted state with the same energy $E = V_B + k'^2$ is given by $T = 4kk'/(k+k')^2 \cong 4k'/k \propto \sqrt{E - V_B}$ for $k' \to 0$.

To simulate the effect of a Schottky barrier, we modify the above model by smearing out the potential step, i.e., by lowering the external potential continuously over a distance of N SC ML. Within this barrier of N ML thickness effectively the Fermi level slowly increases with respect to the local potential from the ground-state value deep in the gap to an energy value slightly above E_C. Assuming for this final position of E_F a typical energy value $E_F - E_C = 10$ meV, we list in Table I the resulting spin polarizations P at the $\bar{\Gamma}$ point obtained for Fe|ZnSe(001) and Fe|GaAs(001) junctions with four different barrier thicknesses of $N = 8$, 32, 80, and 144 ML. As an example for the polarization obtained by integrating over the two-dimensional Brillouin zone, in the last row the polarization is given for a 32-ML-thick barrier. Since the integration affects both spin channels approximately equally, the polarization is changed only slightly. While in the case of Se, Ga, and As termination the spin polarization of the current is equally high ($\geqslant 97\%$) as in the barrier-free case, we see a gradual lowering of the spin polarization for the Zn termination, which however levels off at a value of about 77% for large barrier thicknesses. This effect arises from the existence of minority interface states at the Fe|SC(001) interface. These states of Δ_1 symmetry lie within the Δ_1^{Fe} bulk gap and become resonant due to the coupling with the $\Delta_{2'}^{\mathrm{Fe}}$ band. In the case of Zn termination, the interface state at $\bar{\Gamma}$ lies relatively close to E_F, i.e., 0.15 eV below. Its effect is

to reduce the (positive) spin injection ratio. If this state would coincide with E_F, its effect would be much bigger and could even lead to a strong negative polarization.

In summary, we have performed *ab initio* calculations to investigate the ballistic spin injection from a Fe half-crystal into ZnSe and GaAs SCs. Three processes of injection have been considered: the injection of hot electrons as well as the injection of electrons at the Fermi level with and without an interface tunneling barrier. The calculations demonstrate that the Fe|ZnSe and Fe|GaAs(001) interfaces act as highly spin-polarizing filters yielding polarizations as high as 99%. This behavior can be traced back to some simple properties of the band structure of Fe for normal incidence: the majority states at the Fermi level have Δ_1^{Fe} symmetry and a strong s and p_z admixture, so that they can couple well to the conduction band states of the SC, while the Fe minority states at E_F have a different symmetry and can either couple only weakly or not at all to the SC states. This picture becomes clearer the more ordered the interface is, since interface disorder breaks the $\mathbf{k}_\parallel$ conservation and can reduce the spin polarization of the current. Our results provide the spin-polarization parameters of the tunneling barrier, which are required in the treatment of Refs. 7 and 8. Our calculations and the recent successful observation of a 2% spin injection in the Fe|GaAs(001) system[9] suggest that much larger spin injection efficiencies should be achievable.

Note added in proof. During the proofreading we became aware of an article about the ballistic spin injection in Fe/InAs(001) (Ref. 19). Also some of us have written an article about the ballistic spin injection and detection in Fe/SC/Fe(001) where SC stands for ZnSe and GaAs (Ref. 20).

ACKNOWLEDGMENTS

The authors thank G. Schmidt for helpful discussions. This work was supported by the RT Network *Computational Magnetoelectronics* (Contract No. RTN1-1999-00145) of the European Commission.

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