Ballistic Spin Injection from Fe(001) into ZnSe and GaAs

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We consider the spin injection from Fe into ZnSe and GaAs in the ballistic limit. By means of the ab initio SKKR 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.

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The controlled injection of a spin polarized current into a semiconductor (SC) is one of the central problems in the new field of spin electronics, since it is a prerequisite for the development of new spin dependent devices. Recently some important successes have been achieved. Fiedlering et al. have demonstrated the injection from the paramagnetic II-VI SC Be$_2$Mn$_2$Zn$_{1-x}$Se$_x$ into GaAs with very high spin polarization using an external magnetic field, while Ohno et al. were able to show the injection from the ferromagnetic SC Ga$_{1-x}$Mn$_x$As 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 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. Schmidt et al. 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 as well as Fert and Jaffrès have pointed out, that this obstacle can be overcome by introducing a tunneling barrier. Meanwhile, and independently, Zhu et al. 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 has lately pointed out that contrary to the ferromagnet/SC 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 $\overline{\Gamma}$-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 $\overline{\Gamma}$-point. However relevant hybrid systems like Fe/ZnSe(001) and Fe/GaAs(001) for which epitaxial growth has been demonstrated, do not show this simple property.

Recently two ballistic calculations for the spin injection process have been published, which basically rely on a free-electron description of the majority and minority spin bands. Grundler 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 SCs 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 which cannot be described in the free-electron model. Taken together with the results of Zhu et al. our calculations give a bright outlook for the spin injection from ferromagnetic Fe into SCs.

Our method is based on the local density approximation of density functional theory and apply the screened KKR-method. The heterostructure consists of a Fe halfspace and a SC (either ZnSe or GaAs) halfspace, both oriented in the (001) direction and being epitaxially bonded at the interface, so that the SC lattice constant is double the Fe constant ($a_{Fe} = 5.425$ a.u. is used in the calculation). The two halfspace Green’s functions are determined by the decimation technique. In the interface region the potentials of 4 monolayers (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 cut-off of $\ell_{max} = 2$ for the wavefunctions 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 [12], but adjusted to the asymptotic Bloch character of the wavefunctions and the two-dimensional translation symmetry of the system. The in-plane component $k_\parallel$ of the $k$-vector enumerates then the scattering channels, and we can express the $k_\parallel$-dependent conductance $G(k_\parallel)$ wholly in terms of the Green’s function of the system. Spin-orbit coupling is neglected in the calculation.

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 SCs ZnSe (a) and GaAs (b), for Bloch vectors $k = (0, 0, k_z)$ 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 $k_\parallel \approx 0$. 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 $\Delta_1, \Delta_2, \ldots$ indicating the symmetries of the wavefunctions [13]. On the right side, the SC bands are shown with $E_F$ assumed to be located in the middle of the gap. Most important is here that the lowest conduction states have $\Delta_1^{SC}$-symmetry; they are invariant under all symmetry operations of the zink-blende lattice, that transform the Bloch vector $k = (0, 0, k_z)$ in itself. These operations form the symmetry group $C_4v$, which is at the same time identical with the symmetry of the whole Fe$\text{SC}(001)$ interface. It is now important to single out those Fe states, which are compatible with this $C_4v$ symmetry. In Fe, the $\Delta$-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 $\Delta_1^{Fe}$-states, consisting locally of $s, p_x$ and $d_{z^2}$ orbitals, can couple to the $\Delta_1^{SC}$-band states, but also the $\Delta_2^{Fe}$-states 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 $\Delta_2^{Fe}$-symmetry (with $d_{x^2-y^2}$ character) as well as the Fe states with $\Delta_3^{Fe}$-symmetry (with $p_x$ and $d_{z^2}$ or $p_y$ and $d_{yz}$ character) cannot couple to the $\Delta_1^{SC}$-states, since they do not show the full symmetry $C_4v$ 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 $\Delta_1^{Fe}$-band (below $E_F$ also a $\Delta_2^{Fe}$-band is available) while in the minority band around $E_F$ only a $\Delta_2^{Fe}$-band exists that can couple to the $\Delta_1^{SC}$-states, since the $\Delta_1^{Fe}$-band appears here at about 1.3 eV above $E_F$ (see $\Gamma_{12}$ in Fig. 1).

Not shown in Fig. 1 is the lower $\Delta_1^{Fe}$-band separated from the upper $\Delta_2^{Fe}$-band by the so-called $s$-$d$ hybridization gap. This gap is characteristic for 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 [14].

Firstly we discuss the injection process of hot electrons with Fe states well above $E_F$. Although for hot spin injection states with non-zero $k_\parallel$ 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

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**FIG. 1:** Band structure of Fe (left panel) and the semiconductor (right panel): ZnSe (a) and GaAs (b) around the Fermi energy. The black lines in the Fe band structure are the majority and the gray lines the minority spin bands. The $k$-vector is varied along the (001)-direction $\Delta$. 

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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 $\Delta_{Fe}^{maj.}$-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 $\Delta_{Fe}^{maj.}$-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%.

The strong spin polarization can be understood from the different spatial orientation and extent of the $\Delta_{Fe}^{maj.}$ and $\Delta_{Fe}^{min.}$-states. The $\Delta_{Fe}^{maj.}$-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 $\Delta_{Fe}^{min.}$-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 halfspace 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 3rd, 4th 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 $E_F - E_C$. Fig. 3 shows the resulting conductance at the T-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 [1]. 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.

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 $\sqrt{|E_F - E_C|}$. Since the square-root-like behavior is the same for both the majority and the minority electrons, the spin polarization remains constant for $E \rightarrow E_C$. 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 pic-

**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 $\Gamma$-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 $\Gamma_{12}$ refers to Fig. 1.

**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 T-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.
For a constant potential of height $V_0$ in the right halfspace and a vanishing potential in the left halfspace, the transition probability for an incident electron with energy $E = k'^2$ into a transmitted state with the same energy $E = V_0 + k^2$ is given by $T = \frac{\pi k k'}{(k+k')^2} \approx \frac{4}{\pi} \times \sqrt{E-V_0}$ for $k' \rightarrow 0$.

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 to a value of about 77% for large barrier thicknesses. This effect arises from the existence of minority interface states at the Fe 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 $\Delta_{1}$-symmetry lie within the $\Delta_{Fe}^{F}$-bulk gap and become resonant due to the coupling with the $\Delta_{2r}^{Fe}$-band. In the case of Zn-termination, the interface state at $\Gamma$ lies relatively close to $E_F$, i.e., 0.15eV 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 $\Delta_{2r}^{Fe}$-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 $k_{\parallel}$ conservation and can reduce the spin polarization of the current. Our calculations and the recent successful observation of a 2% spin injection in the Fe|GaAs(001) system suggest, that much larger spin injection efficiencies should be achievable.

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

TABLE I: Spin polarization of the current at the $\Gamma$-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.