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Transport properties and electronic structure of epitaxial tunnel junctions

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Abstract

We present ab initio calculations for the electronic ground-state and transport properties of epitaxial Fe/semiconductor/Fe (0 0 1) tunnel junctions. The ground state properties are determined by the ab initio Screened KKR Green's function method and the transport properties by a Green's function formulation of the Landauer–Büttiker formalism. We focus on tunnel junctions with a semiconducting ZnSe barrier and compare them to results for junctions with Si and GaAs barriers. We comment on the presence of metal-induced gap states (MIGS) in the semiconductor, the spin polarization of which strongly depends on the nature of the barrier. We investigate furthermore the influence of one atomic layer at the interface of a non-magnetic metal (Cu, Ag, Al) and of a magnetic 3d transition metal.

Keywords: Electronic structure; Interface magnetism; Tunneling; Transport properties

1. Introduction

Magnetic tunnel junctions are widely studied for their spin-dependent transport properties, namely the tunnel magnetoresistance (TMR) effect [1]. Depending on the relative orientation of the magnetizations of the two metallic leads, the electrical resistance through the junction can vary substantially, up to 40% at room temperature with an insulating Al_2O_3 barrier [2]. An alternative to insulating barriers are semiconductors. Contrary to Al_2O_3 which grows amorphously on 3d transition metals, semiconductors grow epitaxially in an ordered structure, in particular on Fe. In our study we consider Fe/SC/Fe (0 0 1) tunnel junctions with SC corresponding to ZnSe, GaAs and Si barriers. The aim is to shed light on the electronic structure of these systems and correlate it to the transport properties. The tunnel junctions are modelled by two semi-infinite BCC Fe(0 0 1) half-crystals separated by the semiconducting film. We assume a perfect matching of the BCC lattice of Fe with the zinc-blende lattice of the semiconductors: no lattice relaxations are allowed. For the zinc-blende semiconductors ZnSe (or GaAs) the (0 0 1) film consists of a stacking of Zn and Se layers, so that two interfaces with Fe have to be distinguished: a Zn-terminated Fe/ZnSeZn… interface or a Se-terminated Fe/SeZnSe… interface. As we will show in the following, the electronic properties of the junction depend sensitively on the termination. This aspect was not considered in the previous ab initio studies by Butler et al. [3,4].

2. Theoretical method

The electronic ground state properties are determined by means of the ab initio screened KKR method [5]. Combined with the decimation technique [6,7], it enables to study semi-infinite systems with an order N algorithm [8,9], where N is the number of inequivalent layers in the system. Furthermore, we assume spherical atomic sphere approximation (ASA) potentials and a cut-off of the wavefunctions at $lmax = 3$, while the full charge density is included. We use the local density approximation (LDA) of density functional theory in

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the parametrization of Vosko et al. [10]. The conductance G through the junction is calculated by means of a Green's function formulation of the Landauer–Büttiker formalism [11]

$$G = -\frac{e^2\hbar^3}{8\pi m^2}\int_{-\infty}^{+\infty} d\varepsilon\ [-f'(\varepsilon)]\int_S d\vec{S}\int_{S'} d\vec{S}'\ G^+(\vec{r},\vec{r}';\varepsilon) \times \bar{\nabla}\ \bar{\nabla}'\ G^-(\vec{r}',\vec{r};\varepsilon) \quad (1)$$

with $h\bar{\nabla}g = h\nabla g - g\nabla h$ and $f(\varepsilon)$ the Fermi–Dirac function. The conductance is expressed by an integration of the Green's functions over two surfaces S and S' located in each metallic lead of the junction. The Green's functions are directly obtained by the screened-KKR method.

3. Ground-state properties

The magnetic properties in Fe/SC/Fe(0 0 1) junctions show different features according to the barrier considered: the Fe magnetic moments remain close to their bulk values, except in the case of the Fe/Zn and Fe/Ga interfaces for which an enhancement of the Fe interface moments of around $0.3\,\mu_B$ and $0.2\,\mu_B$ is found, respectively. Only very small moments are induced in the semiconductor layers at the interface. While these results were obtained for the experimental lattice constant of Fe, calculations for the 4% smaller LDA lattice constant yield very different magnetization profiles: for the Si barrier, the As-terminated GaAs and the Se-terminated ZnSe barriers, a large drop of the interface magnetic moment of Fe is obtained: almost $1\,\mu_B$ for the As-terminated GaAs barrier. Thus, the moments at the interface do not only depend on the termination but also on the lattice parameter used in the calculations. This suggests that lattice relaxations, not taken into account here, will play an important role.

The local density of states (LDOS) of Fe at the interface displays a sharp peak at the Fermi level in the minority band. This state is the analogue to the well-known Fe(0 0 1) surface state. This interface state hybridize weakly with sp-states in the barrier, to form metal-induced gap states (MIGS). MIGS are states from the metal or from the interface with energies in the gap of the semiconductor so that they decay exponentially in the barrier. They play a fundamental role in the TMR effect [12]. In the case of the Zn termination, only weak features are found in the majority band in the barrier, leading to an important spin-polarization of the tunnel current. The features of the MIGS in the barrier depend strongly on the nature of the barrier and its termination. In particular, at the interface of the Se-terminated barrier, stronger features are also found in the majority band, reducing then by a factor 2 the spin-polarization at the Fermi level, defined as the following ratio $P = (N^{\uparrow}(E_F) - N^{\downarrow}(E_F))/(N^{\uparrow}(E_F) + N^{\downarrow}(E_F))$ where $N^{\uparrow}(E_F)$ and $N^{\downarrow}(E_F)$ are the density of states at the Fermi energy for the spin-up and spin-down bands, respectively. This decrease can be related to a local broadening of the d-band due to the strong hybridization with the Se atoms. The same difference as between Zn and Se is found between the Ga and As-terminated barriers. Furthermore, it is expected that the largest TMR effect will occur when the spin polarization in the barrier is the largest too.

A way to monitor the spin polarization in the barrier is to insert a metallic impurity monolayer at the interface. We consider the case of a monolayer of non-magnetic Ag, Cu, and Al atoms, as well as monolayers of 3d transition metals. For all three non-magnetic metals considered, the spin-polarization of ZnSe at the interface with the metallic impurity layer is reduced by about a factor 10 compared to the value (−48%) for the Fe/Zn interface: −4% for Cu, 1% for Ag and −6% for Al. This very likely also leads to the suppression of the TMR effect, as it has been found for Al_2O_3 barriers. On the other hand, the insertion of a 3d transition metal yields more or less a continuous variation of the spin polarization, from large positive values at the beginning of the series to large negative values for Fe, Co and Ni, as can be seen in Fig. 1. The biggest values are actually obtained for Fe and Co, which are already the most commonly used materials for tunnel junctions. One also sees in the figure that the spin polarization in the barrier closely follows the spin polarization of the interface metallic layer, supporting the idea that the electronic structure at the interface plays a fundamental role in the transport properties. For monolayers of V, Cr and Mn, which display an antiferromagnetic alignment to Fe and

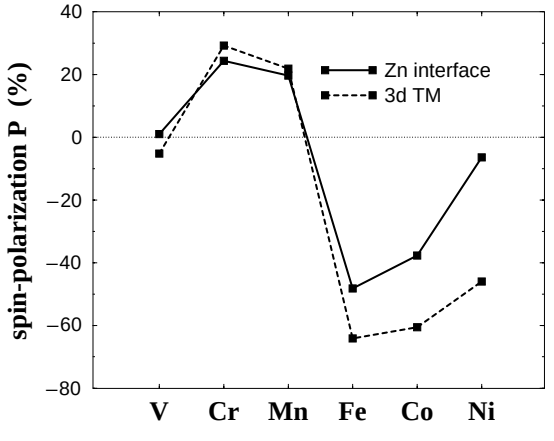

Fig. 1. Spin polarization at the interface in Fe/TM/7 ML ZnSe/Fe(0 0 1) junctions, with TM one monolayer of a 3d transition metal. Dashed line: Spin polarization of the TM monolayer. Solid line: Spin polarization of the Zn monolayer at the interface with TM.

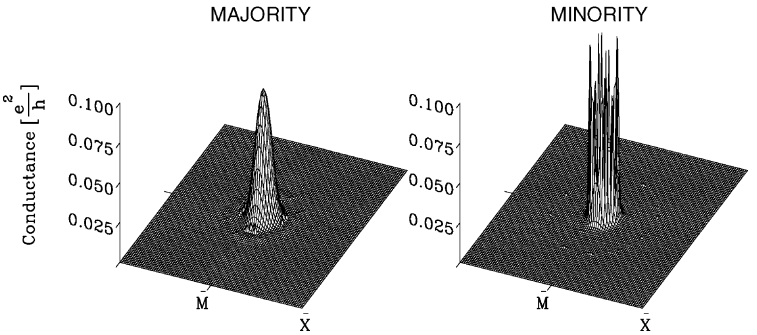

Fig. 2. $q_\parallel$-resolved conductance through a Zn-terminated Fe/15 ML ZnSe/Fe (0 0 1) junctions with parallel orientation of the magnetization.

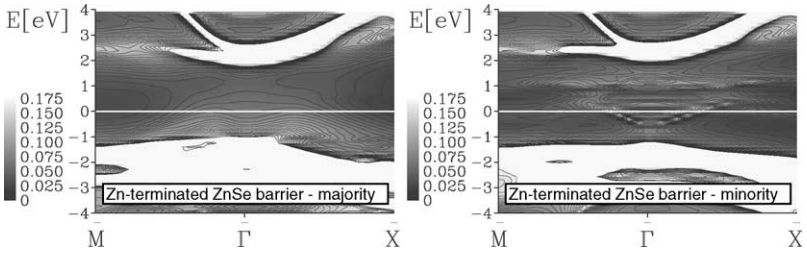

Fig. 3. $q_\parallel$-DOS along high symmetry lines of the 2D BZ for the center layer of the Zn-terminated ZnSe semiconducting barrier in the Fe/7-ML ZnSe/Fe(0 0 1) junction. The color scale denotes the number of states (from black: no states, to white: maximum number of states). The horizontal line corresponds to the Fermi level being located within the 1.23 eV-wide band gap obtained within the LDA.

a positive spin polarization, an inverse TMR effect is to be expected.

4. Conductance

The ballistic conductance was calculated in a Zn-terminated Fe/15 ML ZnSe/Fe (0 0 1) junction with parallel orientation of the Fe magnetizations. Such a thick barrier, constructed with frozen potentials in the middle, is considered in order to get rid of the contribution of surface states resonances to the current [13]. The resulting conductance through such a junction is plotted in Fig. 2 for $q_\parallel$-values in the 2-dimensional Brillouin zone (2D BZ) for both majority and minority electrons. A very different behavior of the conductance is obtained for each spin channel. In the majority band, the conductance is free-electron-like, with a maximum transmission at the $\bar{\Gamma}$ point, i.e. for electrons with a perpendicular incidence to the interface. On the other hand, for the minority channel, almost no transmission occurs for states at the $\bar{\Gamma}$ point. The states contributing to the conductance form a sharp ring around the $\bar{\Gamma}$ point. These features are in very good agreement with the results obtained by Butler et al. [3,4].

One can understand these features by correlating them to the $q_\parallel$-resolved density of states ($q_\parallel$-DOS) in the barrier, as shown in Fig. 3, along the $\bar{\Gamma}$–$\bar{X}$ and the $\bar{\Gamma}$–$\bar{M}$ directions. The $q_\parallel$-DOS is plotted for the central layer of the barrier, and for both majority (left panel) and minority (right panel) bands. In the minority band, the MIGS originating from the Fe interface state at E_F are located around the $\bar{\Gamma}$ point, and yield the ring in the $q_\parallel$-resolved minority conductance (Fig. 2). In the majority band, on the other hand, no such sharp features can be seen at E_F and only very few states remain around the $\bar{\Gamma}$ point.

5. Conclusion

We have calculated the electronic ground state properties and conductance in some Fe/semiconductor/Fe (0 0 1) tunnel junctions with ZnSe, GaAs, or Si barriers. We have shown that the magnetic properties of the junctions strongly depend on the lattice parameter and might thus be very sensitive to relaxations. We find that the spin polarization in the barrier is closely related to properties of the interface and could be controlled by inserting a monolayer of an metallic impurity at the interface. We have also shown the different features of

the conductance for minority and majority electrons through a Fe/ZnSe/Fe (0 0 1) junctions. These properties can be closely linked to the features of the metal-induced gap states which decay in the barrier. In the near future, TMR ratios will be explicitly calculated in the different junctions as well as the influence on the TMR of metallic layers at the interface.

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