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Tunneling magnetoresistance of Fe/ZnSe (0 0 1) single- and double-barrier junctions as a function of interface structure

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Abstract

In this contribution, we calculate the spin-dependent ballistic and coherent transport through epitaxial Fe/ZnSe (0 0 1) simple and double magnetic tunnel junctions with two different interface terminations: Zn-terminated and Se-terminated. The electronic structure of the junctions is modeled by a second-nearest neighbors spd tight-binding Hamiltonian parametrized to *ab initio* calculated band structures, while the conductances and the tunneling magnetoresistance are calculated within Landauer's formalism. The calculations are done at zero bias voltage and as a function of energy. We show and discuss the influence of the interface structure on the spin-dependent transport through simple and double tunnel junctions.

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1. Introduction

Mixed ferromagnetic/semiconductor nanostructures are gaining an increasing interest due to their potentialities for spintronic applications, such as magnetic random access memories and magnetic field sensors (see, for example, Ref. [1]). It is known that the magnetic and electronic properties of these heterostructures depend on the nature of the metal/semiconductor interface, which affects their magnetotransport properties in a significant way [2].

For example, Eddrief et al. [3] have recently shown in photoemission experiments that the Fe Δ_1 spin-up band along the (0 0 1) direction, which is the band that couples most efficiently to the ZnSe complex bands in Fe/ZnSe (0 0 1) magnetic tunnel junctions (MTJs) [4], is strongly modified due to Zn interdiffusion into the Fe electrodes, and that these modifications may be the origin of the very low tunneling magnetoresistance (TMR) measured in these systems. On the theoretical side, Freyss et al. [5] have shown that the spin polarization $P_S = (N_{up} - N_{dn})/\ (N_{up} + N_{dn})$ (being $N_{up/dn}$ the density of states of the majority/minority electrons) at the Fermi level of Fe/ZnSe (0 0 1) interfaces is more negative for the Zn-terminated interface than for the Se-terminated interface, and the transport calculations on Fe/ZnSe (0 0 1) single-barrier junctions done by Herper et al. [6] clearly indicate that the TMR is higher for Se-terminated interfaces than for Zn-terminated ones. These examples concerning Fe/ZnSe hybrid nanostructures, together with those of Ref. [2] for other hybrid junctions, demonstrate that the metal/barrier interfaces play a major role in determining the magnetotransport properties of MTJs.

In this contribution, we analyze the transport properties of some examples of Fe/ZnSe (0 0 1) double-barrier tunnel junctions (DMTJs) as compared to MTJs, as a function of interface termination. To do this, we calculate the conductances and the TMR of epitaxial Fe/ZnSe (0 0 1) tunnel junctions with two different interface structures: (a) Zn-terminated (both interfaces contain Fe and Zn atoms), and (b) Se-terminated (both interfaces contain Fe and Se atoms). The results obtained could be relevant for the practical use of MTJs and of DMTJs in spintronic devices.

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2. Systems under study and calculation methods

Our single-barrier MTJs consist of n layers of zincblende ZnSe (0 0 1) sandwiched by two BCC Fe (0 0 1) semi-infinite electrodes. We form DMTJs by inserting m layers of BCC Fe (0 0 1) in between the $2n$ layers of ZnSe, so that the Fe midlayers are sandwiched by n identical ZnSe layers at each side. In what follows, we will call the *active region* (AR) to whatever is sandwiched by the left and right semi-infinite Fe electrodes. Each ZnSe layer and Fe midlayer has a width of 0.567 and 0.287 nm, respectively. The junctions are periodic in the x–y plane, being z the transport direction. Fig. 1 shows, as an example, the interface structure of a Zn-terminated MTJ with $n = 1$. The Se-terminated junctions are formed by interchanging the Zn and the Se atoms. We note that the junctions are epitaxial and that interface relaxation is not taken into account.

In the parallel configuration (P), the magnetizations of all the magnetic regions are parallel to each other. In the antiparallel configuration (AP), in MTJs the electrodes' magnetizations are antiparallel to each other, while in DMTJs they remain parallel to each other and the Fe midlayer's magnetization is antiparallel. We note that, since the coercive fields of the electrodes and of the midlayer are different, these magnetic configurations are experimentally achievable [7].

The electronic structure of the junctions is modeled by a second nearest neighbors spd tight-binding Hamiltonian fitted to *ab initio* band structure calculations for bulk Fe and bulk ZnSe [8]. When forming the junctions, the ZnSe tight-binding on-site energies are rigidly shifted to make the Fe Fermi level fall 1.1 eV below its conduction band minimum, as indicated in photoemission experiments performed on Fe/ZnSe junctions [9]. Further details can be found in Ref. [10].

The ballistic conductances Γ are calculated using Landauer's formalism expressed in terms of Green's functions (see Ref. [10,11]). The self-energies describing the influence of the electrodes on the AR are calculated from the electrodes' surface Green's functions (SGFs) in the usual way [11], while the SGFs are obtained using the semi-analytical method described in Ref. [12]. The TMR coefficient is defined as $\mathrm{TMR} = 100 \times (\Gamma_{\mathrm{P}} - \Gamma_{\mathrm{AP}})/\Gamma_{\mathrm{P}}$, where Γ_{P} and Γ_{AP} are the conductances in the P and in the AP magnetic configurations, respectively. With this definition, the TMR ranges from $-\infty$ to 100%. By calculating Γ using different numbers of parallel-to-the-interface wavevectors $\mathbf{k}_{//} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}}$ (see Fig. 1), we find that 5000 is enough to reach convergence. More details on the method used to calculate conductances can be found in Ref. [10].

In this work, we restrict ourselves to zero temperature, to infinitesimal bias voltage and to the coherent regime (see Ref. [11]). We assume that the electron's $\mathbf{k}_{//}$ and spin are conserved during tunneling, since the junctions are epitaxial and the Fe midlayer is thin (<1.8 nm) and ordered.

3. Results and discussion

Fig. 2 shows the TMR of Se- and of Zn-terminated MTJs with $n = 2$ (1.13 nm), and of DMTJs with $n = 2$ and $m = 6$ (1.72 nm), as a function of energy (referred to the Fermi level E_F). For single-barrier junctions, it is seen that the Se-terminated MTJ has a large TMR, near 80% on the average, while the Zn-terminated MTJ has a much lower one of 40%, in qualitative agreement with the results of Herper et al. [6]. For both terminations, the dependence of the TMR on energy is rather smooth.

For double-barrier junctions, it is seen that the DMTJs' TMR versus energy behaviors are quite different for each termination. The Se-terminated double junction shows an almost *constant* TMR enhancement of 20% with respect to the MTJ, except for certain energies at which the TMR

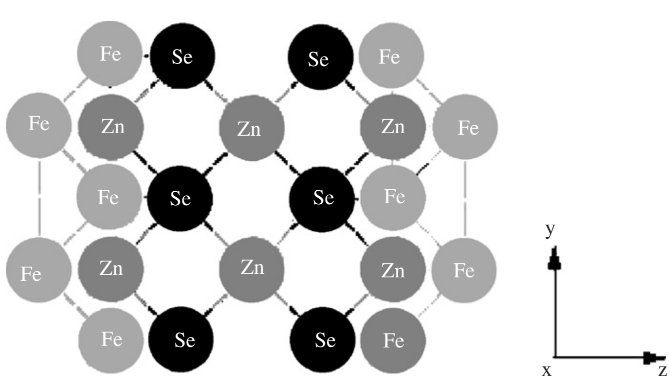

Fig. 1. Interface structure along the z direction of a Zn-terminated Fe/ZnSe (0 0 1) single-barrier junction with a ZnSe thickness of 0.567 nm ($n = 1$). The junction is periodic in the x–y plane and the Fe electrodes are semi-infinite.

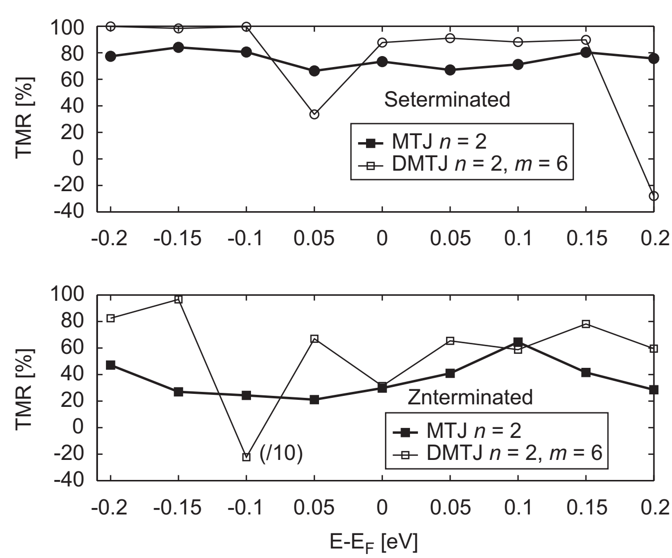

Fig. 2. Tunneling magnetoresistance as a function of energy of MTJs with $n = 2$ (1.13 nm) and of DMTJs with $n = 2$ and $m = 6$ (1.72 nm), for two different terminations. *Upper panel*: Se-terminated. *Lower panel*: Zn-terminated.