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Ab initio calculations of interface effects in tunnelling through MgO barriers on Fe(100)

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Abstract

The tunnel-magneto-resistance (TMR) effect has been extensively studied in the last couple of years. While some experiments showed a strong dependence on the metal–insulator interface in these systems, most theoretical work gave little emphasis to the complicated interplay between electronic structure, atomic structure and the tunnelling process. We present calculations of the atomic structure of Fe/MgO/Fe(001) interfaces and its influence on the electronic structure. The tunnel current is calculated using the Landauer approach to describe the electron transport.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Spin-polarized tunnelling in a nanostructured tunnel junction is at the heart of the rapidly developing field of spintronics [1]. While setups containing semiconducting materials have been proposed for such magnetic tunnel junctions, most successful experiments have been performed on insulating barriers between metallic contacts. In contrast to the widely used aluminium oxide barriers which are amorphous, MgO as a barrier material offers the possibility to produce epitaxial systems with well defined atomic positions. Recent experiments [2] on the Fe(100)/MgO/Fe tunnel junction have demonstrated high TMR ratios for such epitaxial systems. The same setup has been used in several theoretical studies which focused on the dependence of the TMR value on the thickness of the insulating MgO barrier [3, 4] and on the formation of an FeO interface-layer [5]. In this paper we will concentrate on the effects of the actual interface configuration on the spin-polarized electron transport.

2. Fe/MgO/Fe tunnel junction

We will present three slightly different atomic configurations of the Fe/MgO interface. The basic structure of this interface is shown in figure 1. The MgO layers grow 45° rotated with

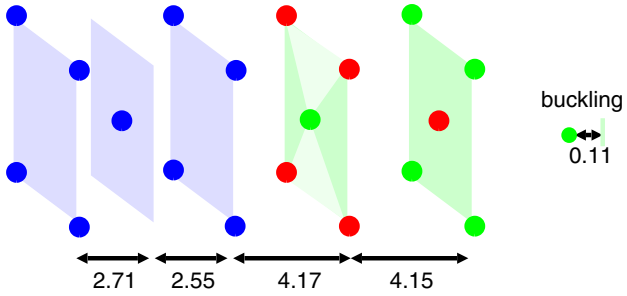

Figure 1. Atomic structure of the Fe(100)/MgO interface. The relaxed interlayer distances and the buckling of the first MgO layer are specified in atomic units (1 au = 0.529 Å).

respect to the Fe layers. An Fe–O bond is formed at the interface with the O atom located on top of the Fe positions, and the Mg is located at the fourfold hollow site of the Fe(100) layer. The first setup we are going to investigate assumes an ideal, unrelaxed structure in which the Fe–O distance equals the interlayer spacing in MgO. For the second setup, we relaxed the structure in a supercell calculation by force calculations and total energy minimization allowing the atoms to move according to their local symmetry. Figure 1 also gives the interlayer distances and the interface buckling obtained in this procedure. One should note that the deviations from the ideal unrelaxed structure are practically confined to within the monolayers forming the actual interface. The most pronounced effect can be seen in the corrugation of the interface MgO layer. The reduced coordination of the small Mg ions results in a movement of these ions towards the Fe layer. As a final, more drastic, modification of the interface we consider a purely hypothetical structure in which the Mg and O atomic positions are interchanged with respect to our first setup. This breaks the Fe–O bonds at the interface and puts the O atoms on top of the hollow sites of the Fe(100) layers. In the present paper we restrict the discussion to a single barrier thickness of three monolayers (ML) of MgO and a ferromagnetic alignment of the two Fe electrodes.

3. Computational details

The computations have been performed within the generalized gradient approximation to the density functional theory using the full-potential augmented plane wave (FLAPW) method as implemented in the FLEUR-code [6]. The conductances were obtained within the embedded Green function method using the Landauer formula as described in [7, 8]. The structural relaxation was carried out using a set of 90 k-points in the irreducible wedge of the Brillouin zone.

4. Results

We will first focus on the transmission rate T (transmission probability summed over all incoming states) of electrons impinging with normal incidence ($\vec{k}_{\parallel} = 0$) on the barrier. Figure 2(a) shows the transmission rate for electrons of the unrelaxed and the relaxed Fe/MgO/Fe interface. Only the majority spin electrons have a significant probability of transmission through the barrier. The corresponding values for the minority spin are about two orders of magnitude smaller. A single band of propagating Bloch states in Fe is responsible

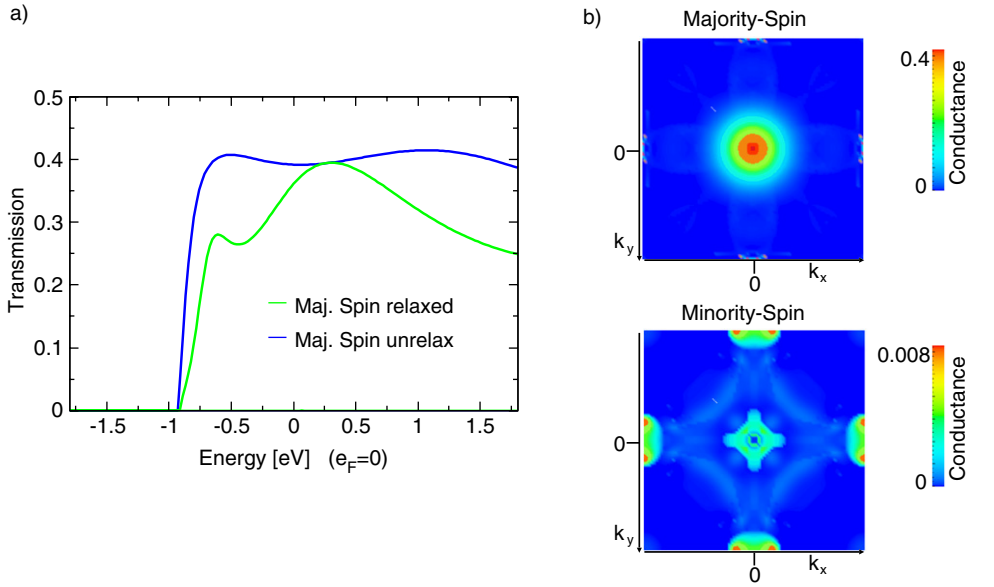

Figure 2. Ferromagnetic Fe/MgO(3 ML)/Fe junction. (a) Transmission rate (in units of e^2/h). Only electrons with normal incidence are considered. The plot shows the values for the majority spin in the relaxed and the unrelaxed structure. The transmission rate of minority electrons is invisible on this scale. The Fermi energy e_F is the origin of the energy scale. (b) Zero-bias Landauer conductance (in units of e^2/h) for the relaxed tunnel junction as a function of $\vec{k}_\parallel$. $\vec{k}_\parallel = 0$ corresponds to the centre of the square Brillouin zone. Note the difference in the scaling between the plot exhibiting the majority and minority states.

for the finite transmission in the majority spin channel starting at -0.8 eV. Even though the second setup is only slightly modified by including the atomic relaxations, the small atomic displacements modify the transmission considerably.

Accidentally, at the Fermi level e_F both setups show nearly identical transmission rates $T(e_F)$, and hence the zero-bias limit of the conductance Γ given by the Landauer equation

$$\Gamma(\vec{k}_\parallel = 0) = \frac{e^2}{h} T(\vec{k}_\parallel = 0; e_F)$$

is about the same. So far, this discussion included only states of normal incidence. Figure 2(b) shows the zero-bias conductance for all $k_\parallel$ values. Only the data for the relaxed interface are shown; the unrelaxed setup shows a very similar behaviour. The total integrated conductance is clearly dominated by the majority spin by two orders of magnitude and the most significant contribution is due to the peak around $\vec{k}_\parallel \sim 0$.

In the hypothetical setup, in which the Mg and O atoms are interchanged, a much more drastic effect can be seen. Figure 3(a) depicts the transmission for $\vec{k}_\parallel = 0$ for this setup. At first glance the overall shape of the transmission curve looks similar to those in figure 2(a). However, one should note that the values are significantly lower. This sharp decrease in the transmission probability is probably due to the decrease in coupling as a consequence of the breaking of the Fe–O bonds. However, as seen in the zero-bias conductance for the complete Brillouin zone (figure 2(b)), at other $\vec{k}_\parallel$ values a large contribution to the minority-spin conductance can now be found. Hence, the spin-polarization of the total conductance is strongly reduced and even changes sign in this setup.

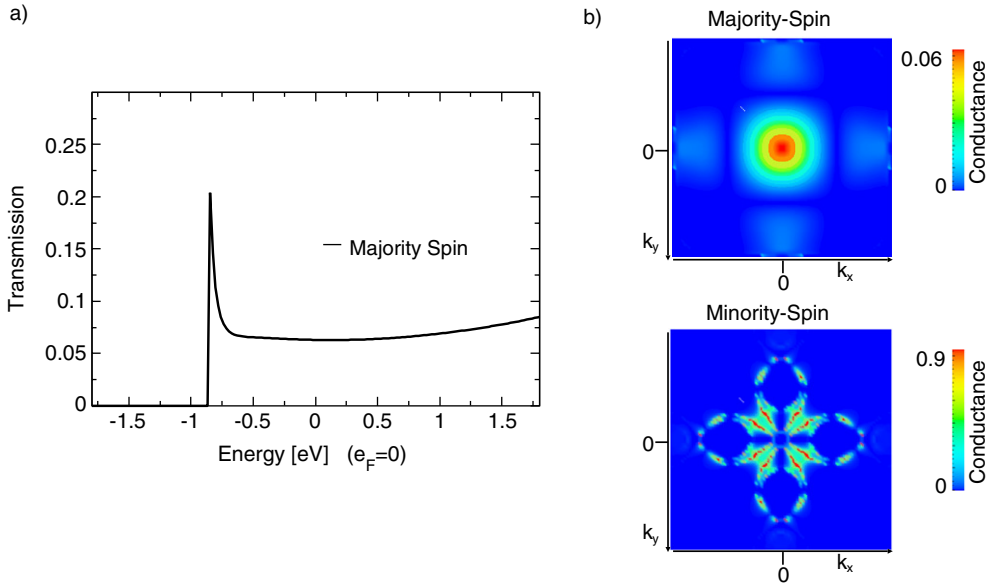

Figure 3. Ferromagnetic Fe/MgO(3ML)/Fe junction in which the Mg and O atoms have been interchanged. For further details, see the caption of figure 2.

5. Summary

By investigating different atomic modifications of the Fe/MgO/Fe tunnel junctions we demonstrated that the details of the interface have in general a large effect on the conductance of the junction. This clearly demonstrates that the popular interpretation of the tunnelling conductance in terms of pure bulk properties like the spin-polarization at the Fermi-level is insufficient for a profound understanding, and detailed calculations are required.

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