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Spin filtering effects in monocristalline Fe/MgO/Fe magnetic tunnel junctions

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Abstract

Single-crystal magnetic tunnel junctions employing bcc (1 0 0) Fe electrodes and MgO(1 0 0) insulating barrier are elaborated by molecular beam epitaxy. Two extreme regimes have been investigated. First, for extremely thin MgO thickness we show that the equilibrium tunnel transport in Fe/MgO/Fe systems leads to antiferromagnetic interactions, mediated by the tunneling of the minority spin interfacial resonance state. Second, for large MgO barrier thickness, the tunnel transport validates specific spin filtering effect in terms of symmetry of the electronic Bloch function and symmetry-dependent wave function attenuation in the single-crystal barrier. Within this framework, we present giant tunnel magnetoresistive effects at room temperature (125–150%). Moreover, we illustrate that the interfacial chemical and electronic structure plays a crucial role in the filtering. We show that the insertion of carbon impurities at the Fe/MgO interface changes radically the voltage response of the tunnel magnetoresistance. Moreover, we provide experimental evidence for the electronic interfacial resonance states contribution to the spin polarized tunnel transport.

Keywords: Spin electronics; Magnetic tunnel junctions; Epitaxial layers; Spin dependent tunneling; Tunnel magnetoresistance

1. Introduction

The discovery of a tunnel magnetoresistance (TMR) effect at room temperature in amorphous oxide barrier based magnetic tunnel junctions (MTJ) [1] paved the way to intense developments in this field area with many possible application prospects [2]. Recently, this subject has been boosted with the measure at room temperature of TMR values above 200% in MgO crystalline oxide based tunnel barriers [3–5], three times larger than in standard amorphous alumina barriers. These large TMR ratios are determined by the different tunneling mechanisms and symmetry-related decay rates of the Bloch waves for the majority and the minority spin channels.

Roughly, an emitter single-crystalline ferromagnetic (FM) electrode filters in terms of symmetry the electrons subsequently injected across the insulating (*I*) barrier. The filtering effect can be easily understood from Fig. 1, where we illustrate the bulk band structure of bcc Fe, along the $\Gamma - H$ direction, for the majority and minority spins. At the Fermi level for the majority electrons we have the following states: a Δ_1 (spd-like character state), a Δ_5 (pd) and a $\Delta_2^{'}$ (d). Due to the exchange splitting, there is no Δ_1 state for the minority spin. Therefore, one can immediately see that the Fe behaves as a half-metal system in terms of the Δ_1 symmetry. The tunnel transport probes: (i) the differences in spin injection (extraction) efficiency (directly related to the interfacial FM/I matching/coupling), and (ii) the differences in decay rates when tunneling across the barrier. The epitaxial growth of the MgO on Fe, via a rotation by 45° of the MgO lattice with respect to the Fe one, provides the symmetry conservation across the junction stack. One can demonstrate that the Δ_1 state has the smallest decay rate across the MgO, followed by the Δ_5, then the $\Delta_{2,2'}$.

Consequently [6,7], for large MgO thickness, in the asymptotic regime, in the parallel (*P*) configuration, the tunneling is found to be governed by the Δ_1 state. The conductance in the antiparallel (AP) configuration is very low, being only related to the $\Delta_{5,2'}$ state propagation, with a larger decay rate. In the AP configuration, an injected Δ_1 state cannot find equivalent symmetry in the opposite electrode with reversed magnetization. The spin asymmetry is predicted to increase above 1000%. On the other hand, when the thickness of the insulating layer decreases, the contribution of the double degenerate pd character state Δ_5 and even $\Delta_{2,2'}$ becomes significant, the conduc-

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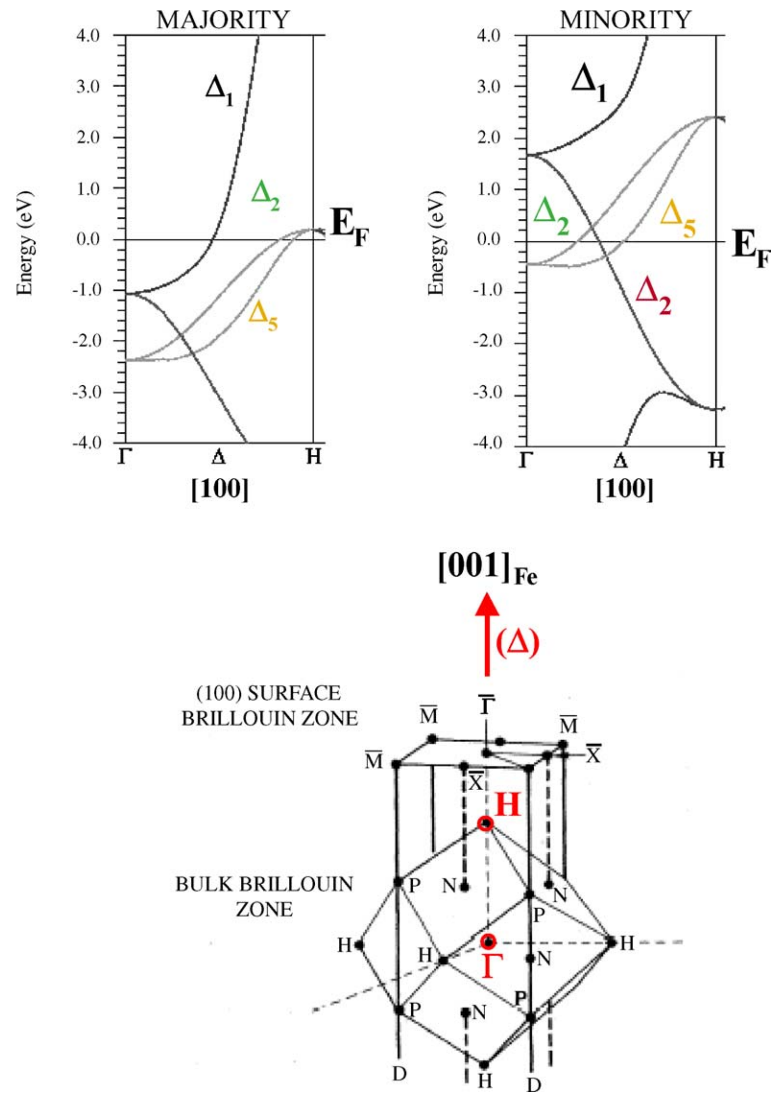

Fig. 1. Top: Bulk energy bands for the majority and minority spins in bcc Fe. Bottom: Representation of the bulk and the (0 0 1) surface Brillouin zone for the bcc Fe.

tivity in the AP state increases and therefore the TMR ratio decreases.

In the thin MgO barrier thickness regime, the tunnel transmission becomes strongly affected by resonant effects at the interfaces [8,6,7,10]. Indeed, for the Fe(0 0 1)/MgO interface, an interfacial minority density of states (DOS) is found above the Fermi energy. The interfacial resonance states from both sides of the barrier may couple to each other leading to a resonant tunneling mechanism [8] which manifests itself as spikes in the conductivity distribution in particular $K_{\|}$ points in the two-dimensional Brillouin zone. The width of these spikes is determined by the strength of the coupling in the barrier, which decreases exponentially with the barrier thickness. Consequently, the conductance from an interfacial resonance state is particularly important for thin barriers. The contribution of the resonant assisted tunneling is major in the equilibrium regime and determines the antiferromagnetic coupling interactions observed in our Fe/MgO/Fe system [11]. Alternatively, the contribution to the tunneling of an interfacial state may be activated by biasing the junction at finite bias voltage, even at large MgO thickness regime.

2. Sample elaboration

The MTJ multilayer stacks subjected to our studies have been elaborated by molecular beam epitaxy (MBE), in a chamber with a base pressure of 5×10^{-11} Torr. Two set of samples have been grown on (1 0 0) MgO substrates, previously annealed at 600 °C for 20 min. For the sample type A, a 50 nm thick bottom Fe layer was deposited at room temperature directly on the MgO substrate. For the sample type B, a 10 nm thick seed MgO under-layer was grown at 450 °C on the substrate before the deposition of the 50 nm thick Fe layer. This MgO under-layer acts as an antidiffusion barrier which traps the residual carbon impurities and prevents their diffusion within the layers during subsequent annealing stages. Indeed, to improve its surface quality, the bottom Fe layer was annealed at 450 °C for 20 min. The surface RMS roughness after annealing, estimated from atomic force microscope analysis, was about 0.3 nm. However, the Fe top surfaces post-annealing are not equivalent for sample types A and B, as highlighted in Fig. 2a containing reflecting high energy electron diffraction (RHEED) patterns. For both sets of samples, the