Mechanisms of Perpendicular Magnetic Anisotropy at Fe(001)|MgO(001) Interfaces

H. X. Yang[1], J. H. Lee[1,2], **M. Chshiev[1],** A. Manchon[1,3], K. H. Shin[2] and B. Dieny[1]

[1]SPINTEC, UMR-8191 CEA/CNRS/UJF Grenoble 1, 38054 Grenoble, France
[2]Korea Institute of Science and Technology, Seoul 136-791, Korea
[3]King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia
mair.chshiev@cea.fr

Perpendicular magnetic anisotropy (PMA) at the interface between ferromagnetic (FM) and non-magnetic layers has become of major interest in a view of next generations of magnetic tunnel junction (MTJ) based spintronic devices with increased density and thermal stability. The presence of a heavy non-magnetic layer (Pt, Pd, Au, W, Mo) at the interfaces was believed to be essential to trigger the PMA due to strong spin orbit interaction (SOI) [1] but this yield low spin polarisation and increased Gilbert damping which detrimental for spin transfer torque based devices. However, the PMA with surprisingly large values up to 1 to 2 erg/cm^2 have been first observed at Co(Fe)|MOx interfaces (M=Ta, Mg, Al, Ru etc) [2] despite the weak SOI. Furthermore, large PMA values have been reported for Co|MgO [3] and CoFeB|MgO magnetic tunnel junctions MTJs [4]. The latter have been extensively studied because of Bloch state symmetry based spin filtering phenomenon leading to high tunnel magnetoresistance (TMR) values [5] making them ideally suitable for implementation in hard disk reading heads or as bit cells in magnetic random access memories (MRAM).

Here we investigate the effect of interfacial oxidation conditions on the PMA in Fe(001)|MgO(001) MTJs and elucidate mechanisms responsible for the PMA from first-principles [6]. Two structures have been chosen to model the ideal and overoxidized interfaces as shown in Fig. 1(a) and (b), respectively. These structures be viewed as a model system for FM|MOx interfaces comprising bcc electrodes including $Co_xFe_{(1-x)}$ alloys. Full structural relaxation in shape and volume has been performed. We found very large PMA values up to 2.96erg/cm^2 [7] for MTJs with pure interfaces in agreement with recent experiment [4]. Furthermore, the PMA weakens in case of overoxidized interfaces (see below) indicating that PMA correlates with TMR) in agreement with experiment [8]. In order to understand the correlation between PMA and TMR, in Fig. 1(c) we plot the wave function character of Δ_1 Bloch state as a function of the position across the supercells used for PMA calculations. One can clearly see that the Δ_1 decay rate is strongly enhanced in the case of overoxidized interface compared to the ideal one.

To elucidate the PMA origin at Fe|MgO interfaces, we performed detailed analysis of the impact of SOI on electronic band structure with out-of-plane (d_{z2}, d_{xz}, d_{yz}) and in-plane (d_{x2-y2}, d_{xy}) Fe-3d and O-p_z orbital character. When no SOI is included (middle subcolumns in Fig. 2a), the band level resulting from hybridization between Fe-d_{z2} and O-p_z orbitals is present. The double degenerated bands with Δ_5 symmetry related to minority Fe are also present close to the Fermi level. When spin-orbit interaction is switched on, the degeneracy is lifted and majority Δ_1 and minority Δ_5 are mixed up producing bands with both symmetry characters. As a result, band levels with d_{z2}, d_{xz}, d_{yz} and p_z character split around the Fermi level and this splitting is larger and the lowest band deeper for out-of-plane magnetization orientation as clearly seen in left and right subcolumns in Fig.2(a), respectively. Thus, the lift of degeneracy of d_{xz} and d_{yz} orbitals along with their mixing with Fe-d_{z2} and O-p_z orbitals is at origin of perpendicular magnetic anisotropy for pure Fe|MgO interfaces.

Next, we proceed with the same analysis for overoxidized Fe|MgO interfaces. In this case (Fig.2b), SOI lifts again the degeneracy for states with $d_{xz,yz}$ causing stronger splitting and deeper level position in case of out-of-plane orientation of magnetization compared to the in-plane one. However, these states are not mixed anymore with Fe-d_{z2} and O-p_z orbitals due to local charge redistribution induced by additional oxygen atoms [9]. Since d_{z2} and p_z orbital hybridization which is mainly responsible for PMA is not splitted, the anisotropy is significantly reduced (0.98 erg/cm^2).

In conclusion, we clarified the mechanisms responsible for large PMA at Fe|MgO MTJs as well as mechanisms of PMA degradation in the case of overoxidized interfaces. This work was supported by Chair of Excellence Program of the Nanosciences Foundation in Grenoble, France, ERC Advanced Grant Hymagine and the KRCF DRC program.

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Figures

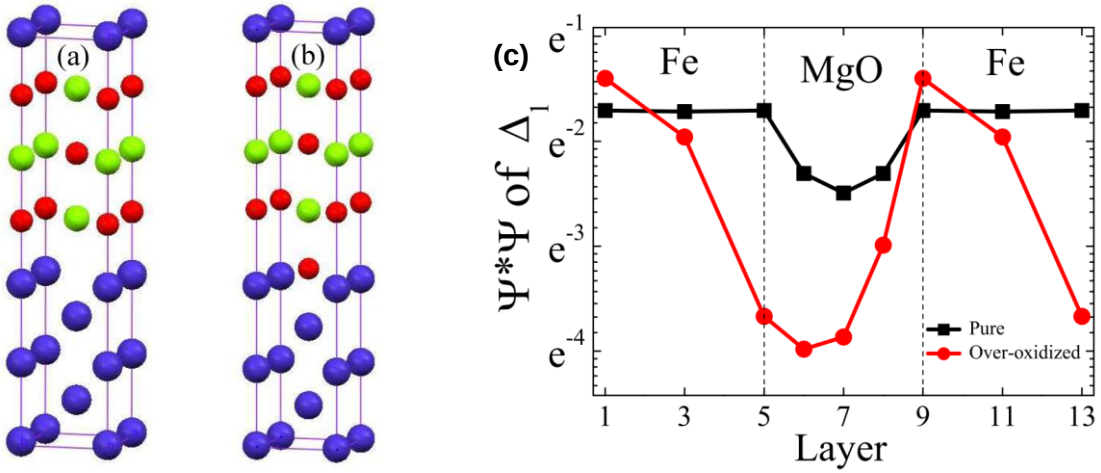

Figure 1. Schematics of the calculated crystalline structures for (a) pure, and (b) over-oxidized Fe(001)| MgO(001) (Fe, Mg and O are represented by blue, green and red balls respectively); (c) Δ_1 Bloch state character at Γ-point around the Fermi level as a function of layer number in pure and over-oxidized interfaces shown in (a) and (b), respectively.

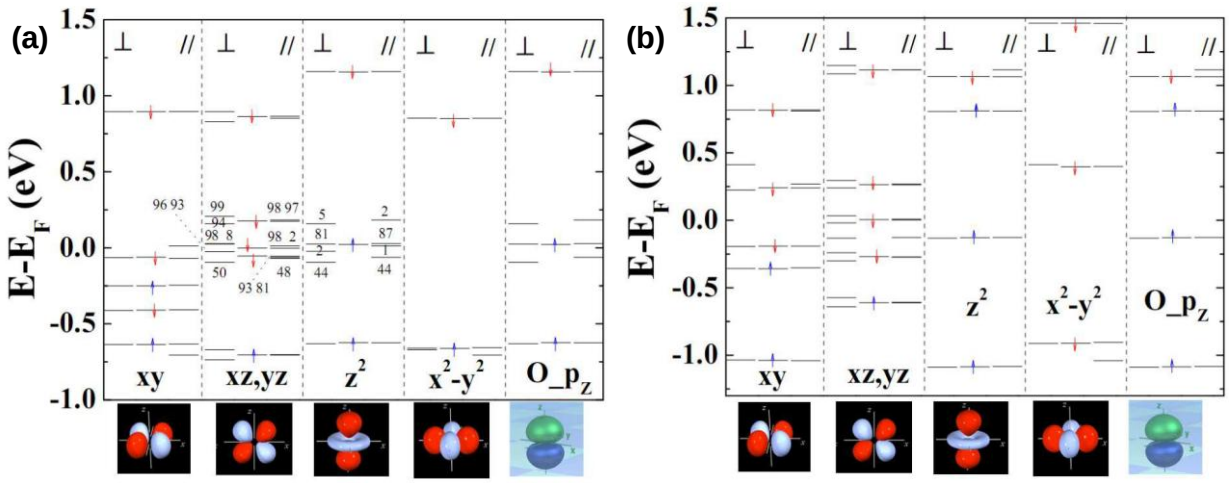

Figure 2. Spin-orbit coupling effects on wave function character at Γ point of interfacial Fe-d and neighbor oxygen p_z orbital for (a) pure and (b) over-oxidized Fe|MgO interfaces. Three subcolumns in each column show the band levels for out-of-plane (left) and in-plane (right) orientation of magnetization as well as for the case with no spin-orbit interaction included(middle), respectively. Numbers are the percentage of the orbital character components within Wigner-Seitz spheres around interfacial atoms.