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Overview**First-principles studies of perpendicular magnetic anisotropy and interlayer exchange coupling in MgO-based tunnel junctions****Research activities**

Magnetic tunnel junctions (MTJ) comprising ferromagnetic (FM) electrodes with MgO insulating spacer have been an object of a high interest for spintronics due to prediction of Bloch states symmetry based spin filtering giving rise to high tunnel magnetoresistance (TMR) ratios [1]. In addition, these structures have been attracting a major attention of scientific community due to observation of antiferromagnetic (AF) coupling between FM electrodes across MgO spacer [2]. Recently, there is a huge interest in MTJs with perpendicularly to the FM/insulator interface magnetized electrodes (p-MTJs). The latter originates from interfacial perpendicular magnetic anisotropy (PMA) which may reach surprisingly large values up to 1 to 2 erg/cm² observed at Co(Fe)/MO_x interfaces (M=Ta, Mg, Al, Ru etc) [3] and in Co|MgO [4] and CoFeB|MgO MTJs [5].

Scientific productions**Partnership****People****Practical links****Job opportunities****Scientific journals**

The first part of the presentation will be devoted to ab-initio investigations of perpendicular magnetic anisotropy (PMA) at Fe(001)|MgO(001) and Co(001)|MgO(001) interfaces along with mechanisms responsible for the PMA. In particular, in case of Fe|MgO interfaces very large PMA values up to 2.96erg/cm² are found for MTJs with pure interfaces in agreement with recent experiment [5]. Furthermore, it will be demonstrated that the oxidation conditions strongly affect the PMA and it strongly correlates with tunnel magnetoresistance (TMR) in agreement with experiments [6,7].

The second part of the presentation will be devoted to phenomenon of interlayer exchange coupling (IEC). In particular, using ab-initio and tight-binding approaches, we will address the impact of structural relaxation and interfacial oxidation conditions on amplitude of IEC in MTJs [8] as well as the importance of occupation numbers (Fermi level) on period of IEC oscillations as a function of ferromagnetic electrode thickness [9] and dynamics of exchange coupled magnetic moments [10].

[1] W. H. Butler et al, Phys. Rev. B, 63, 054416 (2001); S. Ikeda et al, Appl. Phys. Lett. 93, 082508 (2008). [2] J. Faure-Vincent et al, Phys. Rev. Lett. 89, 107206 (2002); T. Katayama et al., Appl. Phys. Lett. 89, 112503 (2006); Y.F. Chiang et al, Phys. Rev. B 79, 184410 (2009). [3] S. Monso et al, Appl. Phys. Lett. 80 (2002) 4157; B. Rodmacq et al, J. Appl. Phys. 93 (2003) 7513. [4] L. E. Nistor et al, Phys. Rev. B 81 (2010) 220407. [5] S. Ikeda et al, Nature Mater. 9 (2010) 271. [6] H. X. Yang et al, arXiv:1011.5667. [7] L. E. Nistor et al, IEEE Trans. Magn. 46 (2010) 1412. [8] H. X. Yang et al, Appl. Phys. Lett. 96, 262509 (2010). [9] L. E. Nistor et al, Phys. Rev B 81, 220407 (2010). [10] D. Terrade et al, in preparation.

