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Effect of oxidation on interlayer exchange coupling in Fe|MgO|Fe tunnel junctions H.-X. YANG, M. CHSHIEV, A. KALITSOV, A. SCHUHL, SPINTEC, CEA/CNRS/UJF, Grenoble, France, W.H. BUTLER, MINT Center, University of Alabama, Tuscaloosa, AL, USA — The interlayer exchange coupling (IEC) in MgO-based magnetic tunnel junctions (MTJ) is a subject of major interest for spintronics community [1,2]. Recent experiments demonstrated that oxydation conditions strongly affect the character of the IEC in Fe/MgO/Fe(001) MTJs [3]. In order to elucidate the effect of over- and under-oxidation on the nature of the IEC in Fe|MgO|Fe MTJs, we performed systematic studies of the influence of O impurities and vacancies on the IEC using ab-initio and tight-binding approaches. We found that the O vacancies cause strong AF IEC in agreement with previous studies [2-4]. Furthermore, an additional O atom at the Fe|MgO interface makes the IEC ferromagnetic in for 3ML and above MgO thicknesses in agreement with experiment [3]. We demonstrate also that the full structural relaxation of ideal Fe|MgO|Fe MTJs may lead to the antiferromagnetic IEC. Tight-binding calculations of the IEC in the framework of the Keldysh formalism were also performed. The results obtained support our first principles calculations. [1] J. Faure-Vincent et al, Phys. Rev. Lett. 89, 107206 (2002); [2] T. Katayama et al., Appl. Phys. Lett. 89, 112503 (2006); [3] Y.F. Chiang et al, Phys. Rev. B 79, 184410 (2009); [4] M.Y. Zhuravlev et al, Phys. Rev. Lett. 94, 026806 (2005).

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