Spintronic Phenomena in MgO-based Magnetic Tunnel Junctions: First principles and Tight-Binding insight

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Magnetic tunnel junctions (MTJ) comprising ferromagnetic (FM) electrodes with MgO spacer have been an object of high interest for spintronics due to Bloch states symmetry spin filtering leading to high tunnel magnetoresistance (TMR) [1], and due to observation of antiferromagnetic interlayer exchange coupling (IEC) between FM electrodes across MgO [2]. This attention has been strongly reinforced and refocused on MTJs with out-of-plane magnetized magnetic layers (pMTJ) [3] which owe their creation to phenomenon of perpendicular magnetic anisotropy (PMA) at transition metal/oxide interfaces [4], and can be used as bit cells in spin transfer torque switching based magnetic random access memories (STT-MRAM) since they offer much better down-size scalability than their in-plane counterparts [3].

We present theoretical studies of spintronic phenomena in MTJs using first-principles and tight-binding approaches. First, a theory of spin transfer torques (STT) in MTJs with both symmetric and asymmetric electrode composition will be presented which in particular allowed prediction of STT voltage dependences and provided solutions for STT-MRAM [5,6]. This part will also include our latest results on voltage dependences of both STT and TMR in MTJs with asymmetric barriers [7]. Next part of the talk will be devoted to studies of IEC in MgO-based MTJs. In particular, we will address the impact of structural relaxation and interfacial oxidation conditions on amplitude of IEC in Fe|MgO MTJs [8], as well as the importance of the Fermi level position on period of IEC oscillations as a function of ferromagnetic electrode thickness observed in Co|MgO pMTJs [9]. In the final part of the talk we will present ab-initio theory of perpendicular magnetic anisotropy (PMA) at Fe|MgO and Co|MgO interfaces [10]. It will be demonstrated that the oxidation conditions strongly affect the PMA and it strongly correlates with tunnel magnetoresistance (TMR) in agreement with experiments [10,11]. Finally, we unveil and elucidate microscopic mechanisms of PMA by evaluating the orbital and layer resolved contributions to magnetic anisotropy in Fe|MgO interfaces and MTJs with different interfacial conditions [12].

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