

# COMBINATION OF COMPUTATIONAL AND EXPERIMENTAL MATERIAL SEARCH FOR EFFICIENT MAGNETIZATION MANIPULATION AND INFORMATION STORAGE

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Development of emerging magnetic random access memory (MRAM) elements requires a search for new materials with the goal to achieve efficient manipulation of magnetization and thermal stability at small dimensions. Magnetization manipulation can be achieved through several phenomena such as spin transfer torque (STT), spin orbit torque (SOT) and voltage controlled magnetic anisotropy (VCMA). Scalability of MRAM devices based on interfacial perpendicular magnetic anisotropy (PMA) crucially depends upon the ability of obtaining significantly high PMA required for thermal stability and therefore for reliable information retention. Optimal combination of materials is necessary to achieve high interfacial PMA while maintaining high spin torque efficiency and spin polarization as well as low damping for energy efficient magnetization switching. Computational atomistic modeling approaches allow to provide an insight for experimental research narrowing down search for materials with optimal performance.

An atomistic approach based on the non-equilibrium Green's function formalism within the tight binding Hamiltonian model was developed for STT calculations [1-4]. The model predicts that the in-plane and out-of-plane components of STT in magnetic tunnel junctions (MTJ) can be expressed through longitudinal spin current and spin-dependent reflection coefficients respectively, greatly simplifying analyses of this phenomenon [1]. The bias dependence of STT in various systems was revealed included ferroelectric [2], ferrimagnetic [3] and antiferromagnetic [4] tunnel junctions. Finally a systematic study of STT dependence of material specific parameters such as the band width, exchange splitting, band filling as well as the influence of disorder and quality of interfaces on STT efficiency was performed. Recently the aforementioned tight binding model was extended for the geometry with in-plane charge current to simulate SOT induced by interfacial Rashba spin-orbit coupling (SOC) [5]. This atomistic SOT description provides insight into the physical picture of this phenomenon suggesting an optimal choice of material specific parameters to improve SOT efficiency.

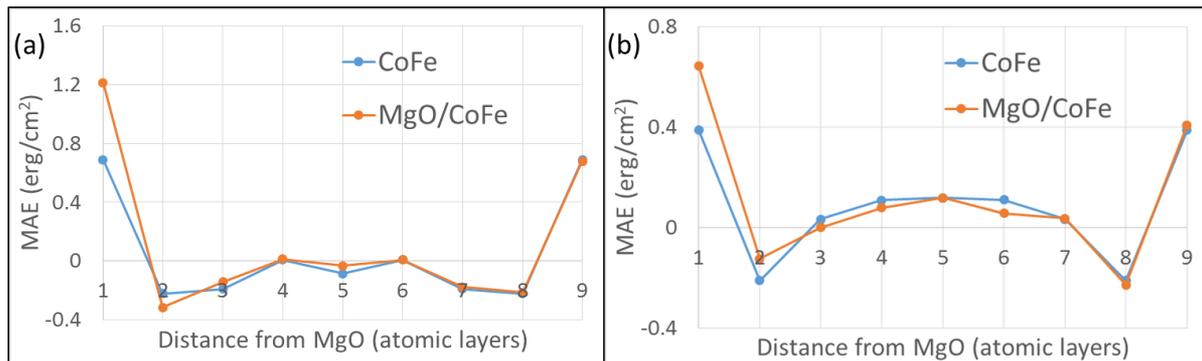


Fig. 1. Layer resolved contribution to MAE in ordered CoFe and MgO/CoFe thin layers: (a) Fe-terminated and (b) Co-terminated CoFe and MgO/CoFe layers.

One of most promising candidates for STT-MRAM devices is CoFeB/MgO-based MTJ due to its high spin polarization and low damping. PMA in CoFeB/MgO MTJ arises from its surface anisotropy which is considerably smaller compare to bulk magnetic anisotropy in materials containing heavy elements with large intrinsic SOC. Therefore interface engineering of CoFeB based alloys is essential to achieve high

PMA. Density functional theory (DFT) electronic structure calculations were used to explore PMA in CoFe and CoFeB based structures. On Fig. 1 atomic layer resolved contribution into magnetic anisotropy energy (MAE) in ordered Fe-terminated and Co-terminated CoFe and CoFe/MgO layers is shown. The calculations indicates that the largest contribution to PMA arises at MgO/Fe interface and therefore PMA in CoFe/MgO structure can be enhanced by using Fe-rich CoFeB alloys. Influence of different metallic layers (M) on PMA in MgO/CoFe/M structures was also studied.

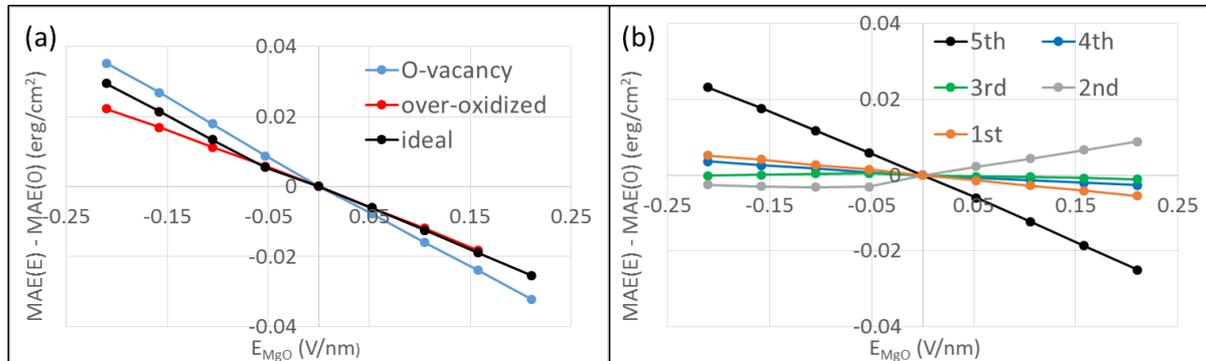


Fig. 2 (a) VCMA in MgO/Fe bilayer with ideal interface and in MgO/Fe bilayers with over-oxidized interface and with O-vacancy at the interface between Fe and MgO. (b) Contribution to VCMA in ideal Fe/MgO structure from different atomic monolayers of Fe away from their interface with MgO.

Magnetization manipulation by STT and SOT requires high current density that may result in significant limitations for spin torque MRAM applications. VCMA is an alternative, energy efficient way for magnetization switching. Restricted by the constraint of maintaining high PMA required for thermal stability, VCMA effect needs to be large enough to overcome high PMA to switch magnetization. DFT calculations were used to obtain VCMA coefficient through the difference between MAE at applied electric fields and MAE at zero electric field. Calculated data shown in Fig 2 (a) indicates that VCMA coefficient in MgO/Fe structures is not too sensitive to the quality of the interface between Fe and MgO. For instance calculated VCMA coefficient is -140 fJ/Vm in Fe/MgO bilayers with ideal interface, -105 fJ/Vm for over-oxidized interface and -160 fJ/Vm in the presence of O-vacancies at MgO/Fe interface. Layer resolved contribution to VCMA shown in Fig. 2 (b) explains these findings and in agreement with [6] points out that in contrast with magnetic anisotropy where interfacial atoms of 3d transition elements determine the magnitude of PMA, the contribution from Fe/MgO interface to VCMA is relatively small. In this talk a comparison between measured and calculated values of PMA and VCMA coefficients will be presented. Such a combination of experimental and theoretical analyses allows to understand the underlying physics and to determine dominant mechanism of the aforementioned phenomena.

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