Interface Design for Concurrent Realization of High Perpendicular Magnetic Anisotropy and Low Magnetic Damping in Fe/MgO

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In spin transfer torque magnetoresistive random-access memory (STT-MRAM) the problem in writing mechanism arises mainly due to the need of large current to switch magnetization direction of the free ferromagnet layer. As the device development of 1x nm cell diameter is preferable, keeping thermal stability to suppress data retention failures while maintaining fast switching mechanism become challenging as trade-off relationship between magnetic anisotropy and damping constant is ongoing. The Fe/MgO system reported as superior structure for magnetic tunnel junctions owing to the high perpendicular magnetic anisotropy (PMA) originated from $\boldsymbol{p-d}$ coupling at interface. Modifying Fe/MgO interface offers prospect of achieving high PMA and low magnetic damping simultaneously. This work focusses in exploring interface modification effect, specifically by using nitride and fluoride compounds, i.e., having one less/more electron than oxide of MgO for high PMA and low magnetic damping from first principles. The result signifies that the LiF/MgO, BN/MgO, and MgN/MgO modifications achieve high PMA enhancement up to 600% while reducing magnetic damping about 75% lower than those in the pristine Fe/MgO model. The origins majorly driven by the band realignment of minority spin from interfacial Fe $\boldsymbol{d}$-orbital at around Fermi level.

***Index Terms*—perpendicular magnetic anisotropy, damping, magnetic tunnel junctions.**

I. Introduction

The current read-write mechanism in spin transfer torque magneto-resistive random-access memory (STT-MRAM) demands advance technologies, specifically for retention failures suppression in small size devices of 1x nm. It remains important to keep a sufficient perpendicular magnetic anisotropy (PMA) for thermal stability of the system while maintaining minimal magnetic damping, i.e., holding the long memory retention without losing switching efficiency. The Fe/MgO system, widely known as one promising magnetic tunnel junction (MTJ) design owing to the high interfacial PMA (iPMA) that majorly accounts to the *p-d* coupling at the interface [1]. Having high PMA and low magnetic damping become critical to achieve a refined MTJ, however the attempts via heavy metal modification, which successfully gives strong iPMA due to strong spin-orbit parameter is also followed by the increase in magnetic damping [2]. This is because the two features share same origin of the spin-orbit coupling. Replacing MgO tunnel barrier with spinel $MgAl_2O_4$ lower a significant magnetic damping due to the small lattice mismatch <1%, however the Fe/$MgAl_2O_4$ model fails to achieve higher iPMA compared to those in Fe/MgO [3]. The exploration of MTJ design with a trade-off relationship between iPMA and magnetic damping is ongoing, e.g., by interface engineering, capping layer modification, and tuning the dielectric constant of the insulator. This work focus is to explore various interface modification in Fe/MgO system, specifically considering the anions with one less/more electron from the MgO oxide, i.e., the nitride and fluoride compounds to achieve MTJ design with high iPMA and low magnetic damping simultaneously.

II. Computational Details and Method

The magnetic tunnel junction is modelled by considering a pristine Fe/MgO system in ten atomic monolayers (ML) of Fe(001) and five ML MgO(001). The interface modification model is constructed by replacing one ML of MgO at the interface with *PX*, i.e., the Fe/*PX*(1 ML)/MgO(4 ML) models. The *PX* is a combination between atomic compounds with a cation site (*P*) and an anion site (*X*). In this work, *PX* modification is divided into two groups, i.e., Group I for nitride anion i.e., BN/MgO, AlN/MgO, GaN/MgO, and MgN/MgO. Group II for fluoride anion i.e., LiF/MgO, and MgF/MgO. In-plane lattice constants are set to the optimized bcc-Fe (2.83 Å). Density-functional theory calculations carried out by full-potential linearized augmented plane wave method [4] within generalized gradient approximation. For anisotropy energy and magnetic damping calculations, a 110×110 $\boldsymbol{k}$-point is implemented. The magnetocrystalline anisotropy energy (E_{MCA}) is determined based on Force theorem, i.e., sum of energy eigenvalue difference between the bands for magnetization oriented along in-plane ($\varepsilon_b^{\rightarrow}(\boldsymbol{k})$) and out-of-plane ($\varepsilon_b^{\uparrow}(\boldsymbol{k})$), with positive E_{MCA} assigned for PMA [5,6], as follows,

$$E_{MCA} = \frac{1}{a^2}\sum_k\left\{\sum_b \varepsilon_b^{\rightarrow}(k) - \sum_b \varepsilon_b^{\uparrow}(k)\right\}, \qquad (1)$$

where a is the lattice constant. Magnetic damping constant, α is estimated following the Landau-Lifshitz-Gilbert equation by Kamberský torque correlation model [7,8], as in,

$$\alpha = \frac{\pi}{M}\sum_{\boldsymbol{k}}\sum_{b,b'}|\Gamma^{-}{}_{bb'}(\boldsymbol{k})^{-}|^2 W_{bb'}(\delta). \qquad (2)$$

where M is the magnetization, b and b' are band indices, $\Gamma^{-}{}_{bb'}(\boldsymbol{k})$ is the matrix element of the spin–orbit torque operator, and $W_{bb'}(\delta)$ is the energy factor with two Lorentz functions scattered at energies ε_b and $\varepsilon_{b'}$ with a scattering rate δ.

III. RESULT AND DISCUSSION

The calculated result for PMA and magnetic damping constant for all models are shown in Fig. 1(a). The red cross shows result for the pristine Fe/MgO model, and the blue dots for the Fe/*PX*/MgO models with the legends indicate insulating barrier interface modification. The pristine Fe/MgO model exhibits PMA of 0.3 mJ/m^2 and α is 0.02. The magnitude agrees with previous experimental and first-principles studies [9,10]. The offset may arise due to different lattice constants and/or number of Fe layers. The MgN/MgO and BN/MgO modifications from Group I, also the LiF/MgO modification from Group II, show significant improvement in both PMA and α, i.e., achieving a high PMA with low α simultaneously. Meanwhile, the other modifications, i.e., GaN/MgO, AlN/MgO, and MgF/MgO, alters PMA and α within a close range as of those in the pristine Fe/MgO model.

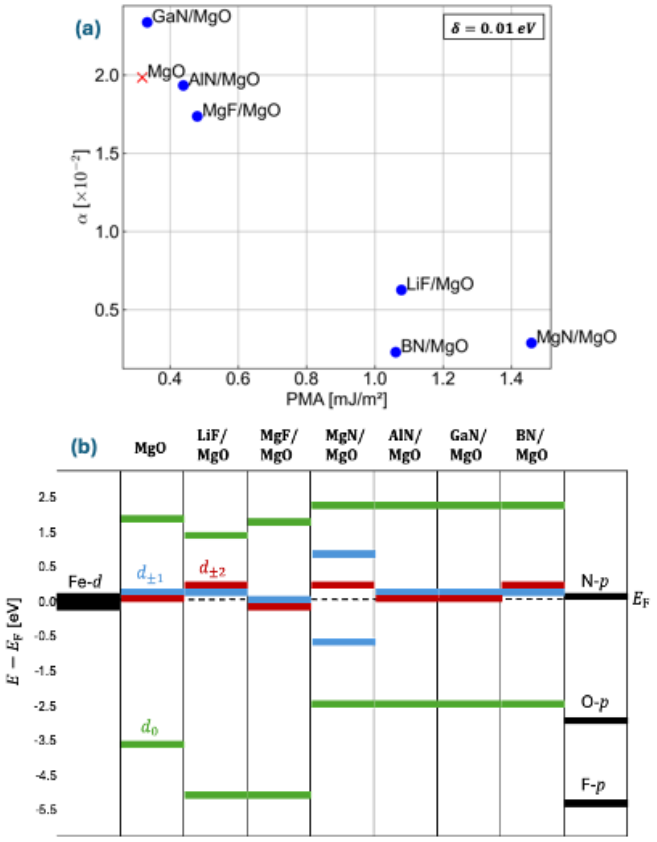

Fig. 1.(a). Relationship between PMA and α for the pristine Fe/MgO and the interface modified model, Fe/MX/MgO. (b). Minority-spin *d*-orbital configuration by *p-d* hybridization between the interfacial Fe and the adjacent anion (N, O, and F), for all models. Green, blue, and red represent d_0 (d_{z^2}), $d_{\pm1}$ ($d_{xz,yz}$), and $d_{\pm2}$(d_{xy,x^2-y^2}), respectively.

The majority-spin of interfacial Fe d-orbital, being fully occupied and located at energy range between 1.0 to 4.0 eV, gives the major role to drive anisotropy and magnetic damping only arises from the minority-spin. Fig. 1(b) illustrates the energy diagram of minority-spin d-orbital by $p-d$ orbitals hybridization between the interfacial Fe and the adjacent anion, (N, O, and F) in all models. For all models, p_0-d_0 coupling is observed, creating bonding and anti-bonding states at energy around 2.0 eV and -2.5 to -5.0 eV, respectively. While $d_{\pm1}$ and $d_{\pm2}$ orbitals are degenerated at around E_F. A special exception observed in the MgN/MgO modification as the coupling between $p_{\pm1}-d_{\pm1}$ orbitals creating additional bonding and anti-bonding states around 1.0 eV and -1.0 eV, respectively.

Anisotropy energy calculated by perturbative theory considering that the spin conserving terms from minority spin at around E_F gives main contribution to E_{MCA} is as follows,

$$E_{\mathrm{MCA}}^{\downarrow\downarrow}=\xi^2 \sum_{\boldsymbol{k}} \sum_{m,m'} \frac{\left|\langle m,\boldsymbol{k}|L_z|m',\boldsymbol{k}\rangle\right|^2-\left|\langle m,\boldsymbol{k}|L_x|m',\boldsymbol{k}\rangle\right|^2}{\varepsilon_{m'}-\varepsilon_m}, \quad (3)$$

where ζ is SOC strength and $\varepsilon_m(|m,\boldsymbol{k}\rangle)$ is the energy eigenvalue (eigenfunction) for m, i.e., m and m' are for occupied and unoccupied state, respectively. The angular momentum L_a has weight depending to the pair of m, i.e., $m=m'$ gives positive contribution to E_{MCA} while it is the opposite for $m\neq m'$. In the LiF/MgO and BN/MgO modifications, $d_{\pm2}$ state is pushed above E_F while the rest of d-states are at E_F, reducing the second term of Eq. (3), resulting a 400% PMA enhancement from pristine Fe/MgO model. For the MgN/MgO modification, $d_{\pm1}$ state completely removed from E_F leaves only $d_{\pm2}$ states at E_F, consequently the first term in Eq. (3) is raised while the second term become insignificant [11], and E_{MCA} is 600% higher than the pristine Fe/MgO model.

In Eq. (2), Lorentz function of energy attributes to the states closest to E_F, and the non-zero matrix element of $\Gamma^{-}{}_{bb'}(\boldsymbol{k})$ governs only by d −orbitals from minority spin at E_F since the spin-lowering operator may vanishes due to the large exchange splitting, consequently a clean E_F gives lower α. Here, δ is set empirically to 0.01 eV for a typical bulk Fe [12] in all models as α mainly accounts for the interfacial Fe. This is true for the LiF/MgO, BN/MgO, and MgN/MgO modifications, as the d-states which are pushed above and/or below E_F, gives significant reduced α, around 75% lower than those of the pristine Fe/MgO model.

In summary, achieving high PMA and low α simultaneously in Fe/MgO system by interface engineering is observed from first principles. The result signifies that the interfacial Fe d-orbitals configuration at around E_F plays an important role for the generation of high PMA and low α simultaneously. Specifically, the LiF/MgO, BN/MgO, and MgN/MgO [11] modifications exhibit nearly a 600% enhancement in PMA and a 75% reduction in α compared to those in the pristine Fe/MgO model.

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