Effect of transition-metal oxide insertions in magnetocrystalline anisotropy at Fe/MgO interface

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Magnetocrystalline anisotropy (MCA) by an application of electric field (E-field) has received much attention as a potential approach for providing a pathway to improve energy power consumption in magnetic recording/memory devices. In practice, however, it is still desired to search ferromagnetic thin-films with high magnetization-switching in response to an external E-field (MCA modification). Previously, we demonstrated that the MCA modification at Fe/MgO interface can be enhanced by inserting heavy metals such as 4d or 5d transition-metals [1]. Here, we extend first principles calculations to investigate the MCA modification at Fe/MgO interface with insertions of oxides of 3*d* (Fe, Co, Ni), 4*d* (Ru, Rh, Ir), 5*d* (Ni, Pd, Pt). Calculations were carried out based on generalized gradient approximation by using full potential linearized augmented method [1]. A model of Au/Fe/MO/MgO (001) was employed, where the 3d, 4d and 5d oxide monolayers (MO) are inserted between three-atomic Fe layer and six-atomic MgO layer, and a nonmagnetic overlayer of three-atomic Au layer is capped at the opposite surface of the Fe layer. The MCA energy (E_{MCA}) is defined as the difference in total energy for magnetizations oriented along the in-plane and perpendicular directions with respect to the film plane, and the MCA modification is estimated by the difference in E_{MCA} between E-fields of ±5 V/nm. For the insertions of 3*d* or 4*d* oxides, the E_{MCA}s in zero field and MCA modifications are almost same with those of their pure metal insertions [1]. For the insertions of 5d oxides, however, we find that the E_{MCA}s in zero field are 44.6, 27.7, and 1.98 mJ/m^2 and MCA modifications are -490, -497, and -48.1 fJ/Vm for OsO, IrO, and PtO, respectively; the magnitudes of the MCA modifications are roughly twice larger than those of the pure metal insertions. With the band-filling analysis, we also find that the large enhancement of the MCA modification can be attributed to the change in hybridization between O 2p-M 3d orbitals at the MO/MgO interface caused by E-field-induced atomic displacements.

[1] K. Nakamura, T. Nomura, A.-M. Pradipto, K. Nawa, T. Akiyama, and T. Ito, J. Magn. Magn. Mater. **429**, 214 (2017).