Interface magnetic structures and magnetocrystalline anisotropy of Fe/3*d*-transition-metal-oxide/MgO in external electric field

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Efforts in developing voltage-based magnetic tunnel junction (VMTJ) have been continued for improving energy power consumption of 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 electric-field (MCA modification). Previously, we demonstrated that the MCA modification at an Fe/MgO interface can be enhanced by inserting 5*d* transition-metal and the oxide layers, and interestingly the MCA modification with a double-layer CoO insertion, assuming a ferromagnetic structure, becomes 10 times larger than that with the monolayer insertion [1]. In the present work, we extend our investigation to determine the stability of interface magnetic structures and the MCA of Fe/3*d*-transition-metal-oxides/MgO in an external electric field. Calculations were carried out based on generalized gradient approximation using film full-potential linearized augmented plane-wave method [2] by employing a model of Au/Fe/$(MO)_2$/MgO(001), where $(MO)_2$ is the double-layer 3*d*-oxides of FeO, CoO, and NiO, and is inserted between three-atomic Fe layer and five-atomic MgO layer. 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 difference in total energy for magnetizations oriented along the in-plane and perpendicular directions with respect to the film plane, and then the MCA modification is estimated by difference in E_{MCA} between electric-fields of ±5 V/nm. Several interface magnetic structures of the double-layer 3*d*-oxides are considered; and we find that the antiparallel magnetic configurations between the magnetic moments at the 3*d*-oxide layers is energetically stable among all the magnetic structures. Our calculations for the FeO and NiO insertions give the similar values of E_{MCA}s in zero field and MCA modifications for all magnetic configurations, but for the CoO insertion, they strongly depend on the magnetic configuration. The origin of stability of interface magmatic structures and the MCA will be presented.

[1] T. Nomura, *et al.*, 5p-C18-6, The 78th JSAP Autumn Meeting, Fukuoka, Japan, September 2017.
[2] K. Nakamura, T. Nomura, A.-M. Pradipto, K. Nawa, T. Akiyama, and T. Ito, J. Magn. Magn. Mater. **429**, 214 (2017).