Atomic-layer alignment dependence of the electric-field-induced modification of magnetocrystalline anisotropy

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For the next-generation memory devices like Magnetoresistive Random Access Memory, ferromagnetic 3*d* transition-metal thin-films with large perpendicular magnetocrystalline anisotropy (MCA) are required.[1] It is furthermore desired to have an easy control of the MCA by using an external field such as external electric field (*E*-field) for improving energy power consumption of devices. In this regard, for the design of materials with such properties, materials informatics has been largely regarded as a powerful computational tool as well as for the understanding of structure-property relationships. Here, we analyze the relation between atomic-layer alignments and *E*-field-induced modification of MCA energy (MCA modification) in Co-Fe and Au-Fe multilayer thin-films. Calculations were carried out by using full-potential linearized augmented plane-wave method for single slabs with six atomic-layers of Co-Fe or Au-Fe thin-films on MgO(001). All possible atomic-layer configurations, which in total consist of 2^6=64 configurations, were considered in the calculations. The MCA energy is defined as the difference in total energy for magnetizations oriented along the in-plane and perpendicular directions with respect to the film plane. *E*-field effects have been considered by applying the homogenous fields of ±2.5 V/nm at vacuum region, and the MCA modification is estimated by the difference in MCA energies between these applied *E*-fields. The results predict that the MCA modification depends strongly on the atomic-layer alignments of Au-Fe with a variation of 100 fJ/Vm while in the Co-Fe binary systems, the MCA modifications are less than 50 fJ/Vm. Details of the MCA modification dependence on the atomic later alignments will be discussed in the presentation.

[1] K. Hotta et al., Phys. Rev. Lett. **110**, 267206 (2013).