Atomic-layer alignment tuning of Au-Fe multilayer thin-films on MgO(001) for large electric-field-induced modification of magnetocrystalline anisotropy

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Materials informatics has attracted great interest and spurred broad applications for the understanding of structure-property relationships as well as for searching promising materials with desired properties. In the field of spintronics, 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. It is furthermore desired to have a large modification of the MCA energy to an application of external electric field (*E*-field) for improving energy power consumption of the devices. Here, we analyze the relation between atomic-layer alignments and *E*-field-induced modification of MCA energy (MCA modification) in Au-Fe multilayer thin-films. Calculations were carried out by using full-potential linearized augmented plane-wave (FLAPW) method [1] for single slabs with six atomic-layers of Au-Fe thin-films on MgO(001). All possible atomic-layer configurations, i.e. as many as 2^6=64 configurations, were considered in the calculations. The MCA energy is defined as 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 MCA energies between *E*-fields of ±2.5 V/nm. The results predict that the MCA modification depends strongly on the atomic-layer alignments with a variation of 100 fJ/Vm. Thus, one promising way for the design of materials with a large modification of the MCA energy may be achieved by the tuning of atomic-layer alignments in multilayer thin-films. The systematic data analysis for the atomic-layer alignments dependence of the MCA modification will be presented.

[1] K. Nakamura et.al., phys. Rev. B 67, 14405 (2003).