Effect of lattice distortion on voltage-controlled magnetic anisotropy at MgO/CoFe interface

RIEC, Tohoku Univ. [1], CSRN, Tohoku Univ. [2], WLRCS, Tohoku Univ.[3],

°Masahito Tujikawa[1,2], Masafumi Shirai[1,2,3]

E-mail: t-masa@riec.tohoku.ac.jp

The voltage-controlled magnetic anisotropy (VCMA) effect is promising technology for realizing the ultra-low energy consumption for magnetization switching. Huge VCMA effect (>1000 fJ/Vm) is required for the voltage-induced magnetization switching in magnetic tunnel junction with 30 nm diameter and enough thermal stablility. Recently, the enhancement of VCMA by the lattice distortion is reported for the Pd/Co and CoFe thin films [1-3]. In this work, we investigated the origin of the enhancement of VCMA by the lattice distrotion.

We have carried out first-principles electronic structure calculations with employing the projector augmented-wave with plane wave basis set by using the Vienna ab initio simulation package [4]. We estimated magnetic anisotropy energy (MAE) and its electric-field modulation for the Al(6ML)/CoFe(8ML)/MgO(5ML) film as a function of in-plane lattice constant *a*.

The VCMA of Al/CoFe/MgO film without distortion (*a* = 2.83Å) is estimated to be 8.0 fJ/Vm. By introducing 2.1% in-plane compressive strain (*a* = 2.77 Å), the VCMA is enhanced to be 14.4 fJ/Vm as shown in Fig. 1. The perpendicular magnetic anisotropy (PMA) energy is also enhanced from 0.6 to 2.0 mJ/m^2 by the 2.1% compressive strain due to enhancement of bulk perpendicular anisotropy. From the analysis of the band filling effect on the MAE, we found that the MAE of the interfacial Fe layer becomes sensitive to the valence electron numbers at the lattice constant *a* near 2.77 Å. By introducing in-plane compressive strain, occupied $d_{x^2-y^2}$ and unoccupied d_{xy} orbital components of the bands close to the Fermi energy contributed to PMA, and thus the MAE becomes sensitive to the valence electron numbers.

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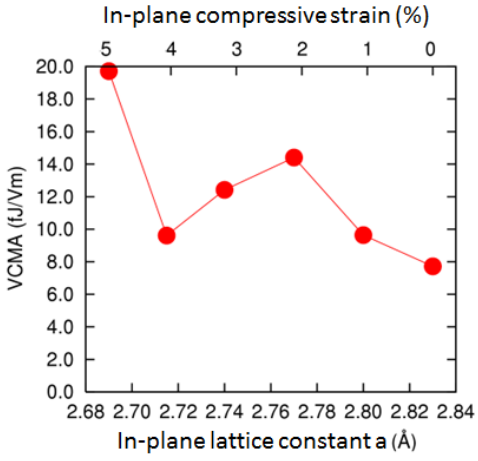

Fig. 1. VCMA as a function of in-plane lattice constant for the Al/CoFe/MgO film.