HUGE ELECTRIC-FIELD-INDUCED MAGNETIC ANISOTROPY OF THE 5*d* TRANSITION-METAL MONOLAYERS ON Fe(001) AND Co(0001)

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I. INTRODUCTION

The voltage-torque magnetoresistive random access memory is the ultra-low energy consumption non-volatile memory based on voltage-controlled magnetic anisotropy (VCMA). The variation of the magnetic anisotropy energy (MAE) upon the electric field was reported to be 30-40 fJ/Vm for the MgO/Fe/Au and MgO/CoFeB/Ta films [1, 2]. Recently, large VCMA effect (290 fJ/Vm) was reported for the MgO/Fe/Cr film [3]. However VCMA effect larger than 1000 fJ/Vm is required for realizing voltage-induced magnetization switching in MTJ below 30nm. The purpose of this work is to design the magnetic film exhibiting huge VCMA. We theoretically investigated the electric-field modulation of MAE for Fe(001) and Co(0001) films covered by the 5*d* transition-metal monolayer (ML).

II. METHOD

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 MAE and its electric-field modulation for TM(1ML)/bcc-Fe(4ML)/Cu(001)(5ML) and TM(1ML)/hcp-Co(4ML)/Cu(111)(5ML) films (TM = Hf, Ta, W, Re, Os, Ir, Pt, Au). The MAE was estimated by using the magnetic force theorem. To discuss the origin of the MAE and its electric-field modulation, we also evaluated the contribution of the MAE from the second-order perturbation of the spin-orbit coupling [5].

III. RESULT

Figures 1(a) and (b) show the MAE and its electric-field modulation, respectively, for the TM/Fe/Cu and TM/Co/Cu films. The modulation lager than 100 fJ/Vm was obtained for the Ta/Fe, W/Fe, Ir/Fe, Hf/Co and Ir/Co films. In particular, the Ir/Fe film has the largest value, 263 fJ/Vm, which is about 8 times larger than that for the Fe surface (-32 fJ/Vm). The Ir/Fe, Os/Fe and Ir/Co films have huge perpendicular magnetic anisotropy (PMA) energy greater than 10 mJ/m^2 and thus films are promising for the voltage-controlled MRAM application. We also evaluated the electric-filed modulation of MAE for the MgO/TM/Fe films. Huge electric- field modulation is obtained for the MgO/Os/Fe (176 fJ/Vm) and MgO/Ir/Fe (-298 fJ/Vm) films.

IV. DISCUSSION

We discuss the origin of huge PMA and its electric-field modulation of the Ir/Fe film. Figures 2(a) and (b) show the contribution arising from the second-order perturbation of spin-orbit coupling to the MAE and its electric-field modulation, respectively, for the Ir and Fe atoms in the Ir/Fe film. We found that the PMA and tis electric-field modulation are predominantly originated from the Ir layer. The contribution from the Fe layers is smaller by several orders of magnitude compared to that from the Ir layer. As shown in Fig. 2(a), the spin-flip term between occupied majority-spin and unoccupied minority-spin states ($E_{\uparrow\downarrow}$) mainly contributes to the PMA of the Ir layer. We cannot ignore the spin-flip term for the 5d-transition-metal atoms, since both the majority- and minority-spin states exist near the

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Fermi level due to the small exchange splitting. Especially, the matrix element $\langle d_{yz,\uparrow}|\hat{\ell}_x|d_{3z^2-r^2,\downarrow}\rangle$ of the Ir atom plays an important role in the huge PMA, since the density of states projected on the minority-spin d_{yz} and the majority-spin $d_{3z^2-r^2}$ orbital exhibits prominent peak structure below and above the Fermi level, respectively. On the other hand, spin-conservation term between occupied and unoccupied majority-spin states ($E_{\uparrow\uparrow}$) and the spin-flip term between occupied minority- and unoccupied majority-spin states ($E_{\downarrow\uparrow}$) contribute to the electric-field modulation of MAE (see. Fig. 2(b)).

V. SUMMARY

We investigated the MAE and its electric-field modulation of the Fe and Co films covered by the 5*d* transition-metal ML. The huge MAE and its electric-field effect are expected for the Of/Fe, Ir/Fe, Ir/Co films. The enhancement of MAE and electric-field modulation can be attributed to strong spin-orbit coupling as well as large induce spin moment of 5*d* transition-metals.

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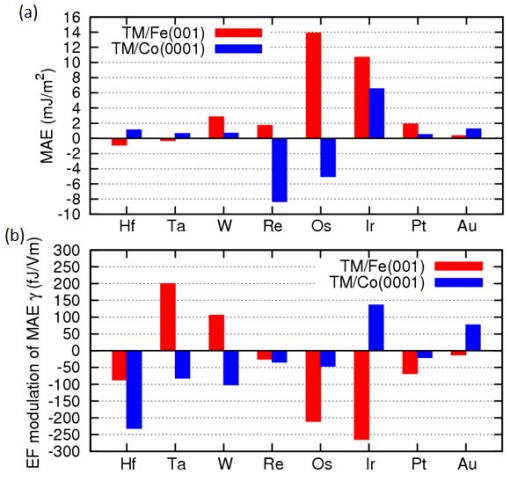

Fig. 1 Magnetic anisotropy energy (MAE) (a) and its electric field modulation γ (b) for the 5*d*-TM/Fe(001) and 5*d*-TM/Co(0001) surface.

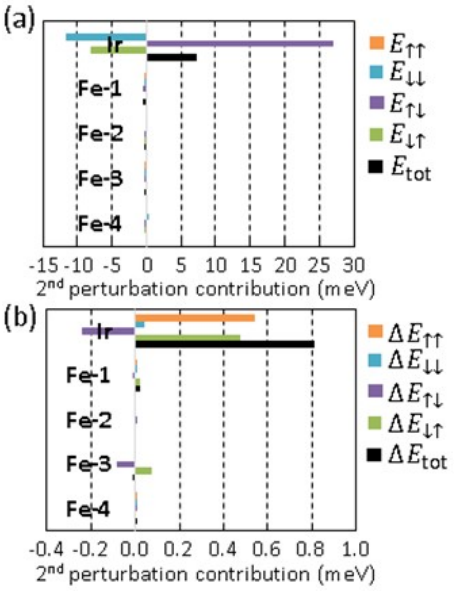

Fig. 2 The contribution arising from the second-order perturbation of spin-orbit coupling to the MAE (a) and its variation ΔE at the electric field of -0.5 GV/m (b) for the Ir/Fe film.