The effect of Os or Ir layer insertion into MgO/Fe interface on the electric-field modulation of magnetic anisotropy

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

We have carried out first-principles electronic-structure calculations 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 MgO/Os(Ir)/bcc-Fe/Cu(001) films. The MAE was estimated by using the magnetic force theorem.

Figures 1(a) and (b) show the electric-field modulation of MAE for the Os/Fe and Ir/Fe films, respectively, with and without MgO capping layer. The VCMA coefficient is estimated to be -173, 298 fJ/Vm for the MgO/Os/Fe and MgO/Ir/Fe film, respectively, and these values are one order of magnitude larger than that for the MgO/Fe interface. These VCMA coefficients are comparable with that of Os- and Ir-monolayer on the Fe surface. However, perpendicular MAE is drastically decreased in both Os/Fe and Ir/Fe film by MgO capping. In the case of Ir/Fe film, opposite sign of VCMA is obtained for the film with and without MgO. These results indicate that the bonding between 5*d* transition-metal and oxygen plays an important role for the MAE and its electric-field modulation. At the MgO/Os and MgO/Ir interfaces, the density of states (DOS) projected on the majority-spin 5*d*($3z^2$-r^2) orbital, which contributes to the in-plane MAE, is increased near the Fermi level by the hybridization between 5*d*($3z^2$-r2) and O-2*p*(z) orbitals. This is the origin of the reduction of perpendicular MAE by the MgO capping. In particular, MgO/Ir/Fe film shows the huge in-plane MAE, since the DOS of 5*d*($3z^2$-r^2) orbital is located just at the Fermi level. In the presentation, we also discuss the origin of the sign change of VCMA coefficients for the Ir/Fe and MgO/Ir/Fe films.

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Reference

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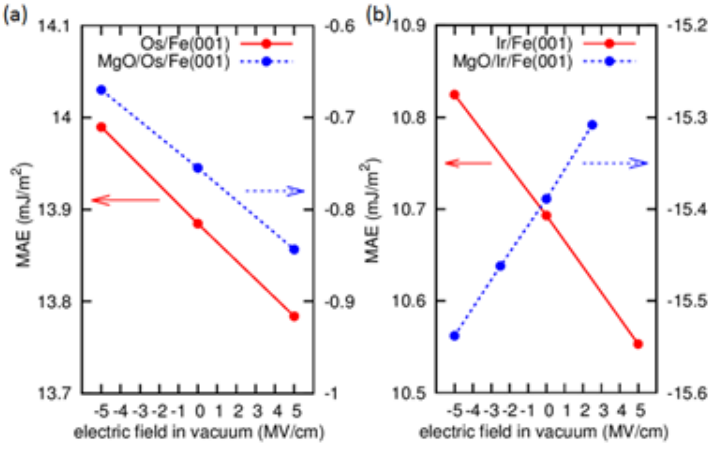

Fig. 1: Magnetic anisotropy energy (MAE) as a function of electric field in vaccum for the Os/Fe (a) and Ir/Fe (b) films with and without MgO capping layer.