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 5d 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 5d 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 5d(3z^2-r^2) orbital, which contributes to the in-plane MAE, is increased near the Fermi level by the hybridization between 5d(3z^2-r^2) and O-2p(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 5d(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

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