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MgO/FeCo 薄膜垂直磁気異方性の Co 組成比依存性の第一原理計算

Co content dependence on perpendicular magnetic anisotropy of MgO/FeCo film: a first principles study

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The magnetic random access memory is the non-volatile memory, which has lower power consumption and good scalability. For the magnetic tunnel junction (MTJ) used in the memory cell, it is required to have a high tunnel magnetoresistance ratio, a strong perpendicular magnetic anisotropy (PMA), and low critical current of magnetization reversal. MgO/CoFeB-based perpendicular MTJ is realized by using the PMA of the MgO/Fe interface and satisfies the above requirements[1]. To get a more thermal stability, the optimization of CoFeB composition ratio has been attempted. In this work, we investigated the magnetic anisotropy on the MgO/FeCo thin film with the different chemical composition ration of FeCo.

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. We consider multilayer of MgO(9ML)/$Fe_{100-x}Co_x$(9ML) (x=0, 25, 50, 75 and 100). The in-plane lattice constant is taken as a 2.98Å that is bulk MgO lattice constant.

Fig. 1 shows the MAE for each film and the MAE dependence on the number of d electrons for MgO/Fe and MgO/Co film. The large PMA is obtained for MgO/Fe film (1.88mJ/m^2) and the PMA is decreased with increasing Co contents 0 to 50%. When Co contents further increase, PMA is increased with increasing Co contents. The decrease of PMA of the MgO/Fe (MgO/Co) film by increasing (decreasing) Co contents can be explained by the rigid band model. The both of the MgO/Fe and MgO/Co film show large PMA, but the origin of the PMA is quite different in each film. In the MgO/Fe film, almost PMA comes from the first and second Fe layer at the interface. This interfacial PMA is decreased with increasing Co contents. On the other hand, the PMA of the MgO/Co film coms from the anisotropy induced by the tetragonal distortion of the BCC-Co bulk. When in-plane lattice constant is matched with MgO, the PMA of the Co bulk is estimated to be 4.5×10^6J/m^3.

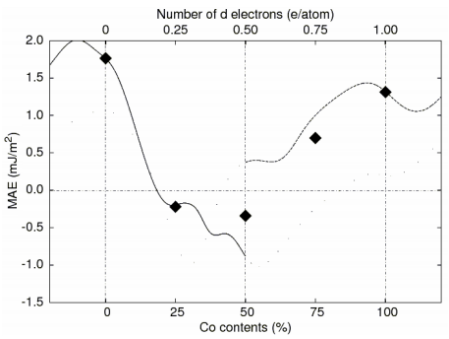

Fig. 1: The MAE of the $MgO/Fe_{100-x}Co_x$ film (diamond points) and the MAE as a function of d-band fillings for the MgO/Fe(solid curve) and MgO/Co film(dashed curve).

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[1] S. Ikeda et al., Nature Mater. 9, 721 (2010).