$Fe/MgAl_2O_4$ 界面の垂直磁気異方性に関する第一原理解析

First-principles study on perpendicular magnetic anisotropy at $Fe/MgAl_2O_4$ interface

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Perpendicular magnetic anisotropy (PMA) is required in ferromagnetic electrodes in magnetic tunnel junctions (MTJs) to achieve sufficient thermal stability in microsized magnetic random access memories (MRAMs). Although various ferromagnets such as $D0_{22}$ $Mn_3Ga(Ge)$, $L1_0$ MnGa, and $L1_0$ FePt exhibit large PMA, MTJs with these ferromagnets did not show high tunnel magnetoresistance (TMR) ratios, which is another important requirement for MRAMs. Therefore, the mainstream of current research for PMA in MTJs is in interface-induced PMA at interfaces between ferromagnetic electrodes and tunnel barrier layers. A typical system with such interface-induced PMA is Fe(Co)/MgO, where relatively large values of interfacial anisotropy constant K_i have been observed [1,2]. Several theoretical studies have supported these results and found that the interfacial hybridization between Fe $d_{3z^2-r^2}$ and O p_z states is the key for the PMA [3,4]. Recently, similar interface-induced PMA has been demonstrated in another heterostructure $Fe/MgAl_2O_4$ [5,6]; however, no theoretical studies have addressed this issue so far.

In this work, we investigated interfacial magnetic anisotropy at $Fe/MgAl_2O_4$ interface by means of the first-principles calculations [7]. We found PMA with K_i~1.2 mJ/m^2, which is a little bit smaller than that of the Fe/MgO with a similar barrier thickness (K_i~1.5-1.7 mJ/m^2). By carrying out the second-order perturbation analysis on the PMA (Fig. 1), we clarified that the difference in K_i between $Fe/MgAl_2O_4$ and Fe/MgO comes from the different contributions from spin-flip scattering terms. In order to find a way to enhance K_i in $Fe/MgAl_2O_4$, we further considered tungsten (W) insertion into the interface of $Fe/MgAl_2O_4$. A giant value of K_i (K_i>3.0 mJ/m^2) was obtained by inserting 5 layers of W into the interface.

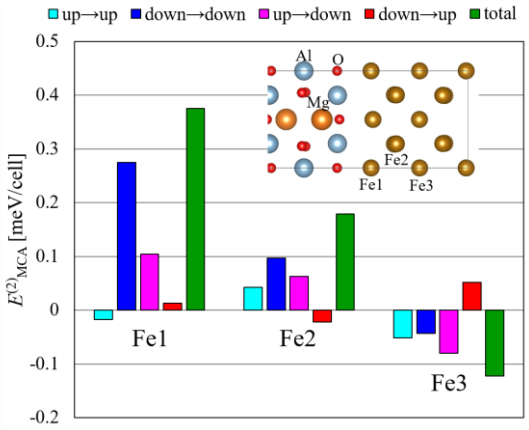

Fig.1. Results of the second-order perturbation analysis on the interfacial PMA in $Fe/MgAl_2O_4$.

This work was partly supported by the Grant-in-Aid for Scientific Research (S) (Grant No. 16H06332) and (B) (Grant No. 16H03852), NIMS MI^{2}I and by the ImPACT Program.

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

[2] J. W. Koo *et al.*, Appl. Phys. Lett. **103**, 192401 (2013).

[3] K. Nakamura *et al.*, Phys. Rev. B **81**, 220409(R) (2010).

[4] A. Hallal *et al.*, Phys. Rev. B **88**, 184423 (2013).

[5] J. Koo, H. Sukegawa, and S. Mitani, Phys. Status Solidi RRL **8**, 841 (2014).

[6] Q. Xiang *et al.*, Appl. Phys. Express **11**, 063008 (2018).

[7] K. Masuda and Y. Miura, arXiv: 1803.10428.