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Large anisotropic Fe orbital moments in perpendicularly magnetized Co<sub>2</sub>FeAl Heusler alloy thin films revealed by angular-dependent x-ray magnetic circular dichroism

Jun Okabayashi,<sup>1\*</sup> Hiroaki Sukegawa,<sup>2</sup> Zhenchao Wen,<sup>2</sup> Koichiro Inomata,<sup>2</sup> and Seiji Mitani<sup>2</sup>
<sup>1</sup>Research Center for Spectrochemistry, The University of Tokyo 113-0033, Japan
<sup>2</sup>National Institute for Materials Science (NIMS), Tsukuba 305-0047, Japan

## 1 Introduction

MgO-based magnetic tunnel junctions have been developed by exploiting the strong perpendicular magnetic anisotropy (PMA) at the interfaces between MgO and CoFeB transition metal alloys, measuring 2.1  $\times 10^5$  J/m<sup>3</sup> [1], which is comparable to PMA in Co/Pt multilayers. Co-based Heusler alloys Co<sub>2</sub>YZ (Y: transition metal; Z: main group element) have attracted much attention owing to their excellent properties that give rise to high spin polarization. In particular, Co<sub>2</sub>FeAl is a promising alloy owing to its low magnetic damping constant at room temperature (RT) and its better lattice matching with MgO as well as a high spin polarization. Recently, Heusler alloys were used to discover PMA in Co<sub>2</sub>FeAl thin layers sharing an interface with MgO, with a lattice mismatch of 3.4% [2]. However, the physical origin of PMA at the interface of Co<sub>2</sub>FeAl/MgO remains elusive. Clarifying the mechanism of PMA in Co2FeAl may help design materials with high spin polarization and PMA to be used in future high performance spintronics applications. Here, we report the origin of PMA in Co<sub>2</sub>FeAl/MgO interface structures, revealed by the X-ray magnetic circular dichroism (XMCD) technique with element specific orbital magnetic moments.

## 2 Experiment

Samples were fabricated using the magnetron sputtering method. The films were deposited on MgO (001) substrates. Thin Co<sub>2</sub>FeAl samples of 0.8, 2, and 10 nm layer thicknesses with a 2 nm thick MgO layer were deposited at RT. Using the vibrating sample magnetometer (VSM), we confirmed that 0.8 nm thick Co<sub>2</sub>FeAl has perpendicular magnetization at RT, while 2 and 10 nm thick Co<sub>2</sub>FeAl samples are characterized by in-plane magnetization, as previously reported [2].

The XMCD was performed at BL-7A (Research Centre for Spectroschemistry, The University of Tokyo). A magnetic field of 1 T was applied along the incident polarized soft x-ray. The total electron yield mode was adopted. All measurements were carried out at RT. Samples were rotated from the surface normal to 60°, defined as normal incidence (NI) and grazing incidence (GI), respectively.

## 3 Results and Discussion

Figure 1 shows the x-ray absorption spectra of Fe and Co  $L_{2,3}$  edges in Co<sub>2</sub>FeAl/MgO layers of different thicknesses. Clear metallic peaks are observed, which confirm that there is no mixing of oxygen atoms in the thin Co<sub>2</sub>FeAl layer. For a 0.8nm thick Co<sub>2</sub>FeAl sample,

the asymmetry between the  $L_2$  and  $L_3$  edges is slightly enhanced in Fe L edges, resulting in large residuals for the integrated XMCD intensities of  $L_{2,3}$  edges. On the other hand, the Co  $L_{2,3}$  edge XMCD yields almost the same results in both NI and GI geometries. Orbital and spin magnetic moments are deduced separately for Fe and Co 3d electrons using the magneto-optical sum rules. We found that PMA is determined mainly by the contribution of Fe atoms with the large orbital magnetic moments, which are enhanced at the interface between  $\text{Co}_2\text{FeAl}$  and MgO [3].

According to the first principles calculations for the Fe/MgO and Co/MgO interfaces, the Fe-O bonding induces PMA that is stronger as compared to the case of the Co/ MgO [4]. Therefore, we conclude that, for a Co2FeAl, a FeAl layer that shares an interface with MgO, with hybridization between Fe  $3d_{z2}$  and O 2p orbitals, is more energetically stabilized as compared to the Co layer sharing an interface with MgO.

## References

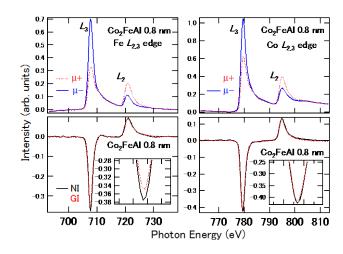


Fig. 1: X-ray absorption spectra and angular-dependent XMCD of the 0.8 nm thick  $Co_2FeAl$  / MgO for Fe and Co L edges. Inset shows the expanded view around the  $L_3$  edges.

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<sup>\*</sup> jun@chem.s.u-tokyo.ac.jp