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Spin-polarized electronic states of FeCo thin film on Rh(001) substrate

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The emergence of perpendicular magnetic anisotropy (PMA) in magnetic thin films is essential from the viewpoint of practical applications, *e.g.*, increasing the recording density of storage devices. Many magnetic thin films exhibiting PMA, such as Co/Pt, Co/Pd, FePt, TbFeCo, and GdFeCo, have been extensively investigated. Among them, "rare-earth and noble-metal elements free" FeCo alloy films are considered promising candidates exhibiting strong PMA. Burkert *et al.* predicted that a magnetic anisotropy energy may increase in FeCo alloys when the tetragonal distortion is applied [1]. Remarkably, around a c/a ratio of 1.20-1.25, the magnetic anisotropy energy exceeds 700-800 μeV/atom, which is one or two orders of magnitude larger than that of pure Fe or Co. The emergence of strong PMA was experimentally confirmed in the tetragonally distorted FeCo ultra-thin-films grown on Rh(001) (c/a = 1.24) with a thickness of 13-17 monolayers (ML) [2].

Generally, it is known that the band structure near the Fermi energy (E_F) plays a very important role in achieving PMA [3,4]. The theoretical calculations suggest that the microscopic origin of PMA in the tetragonally distorted FeCo alloy is attributed to the minority-spin states composed of d_{xy} and $d_{x^2-y^2}$ orbitals near E_F, hybridized by spin-orbit interactions [1]. However, the spin- and orbital-dependent electronic states of the tetragonally distorted FeCo alloy films are poorly investigated experimentally.

In this study, we have fabricated FeCo thin films on Rh(001) substrate by molecular beam epitaxy and investigated the spin-polarized electronic states by *in-situ* spin- and angle-resolved photoemission spectroscopy (spin-ARPES) at BL-9B of Hiroshima Synchrotron Radiation Center [5]. The quality of the sample surface was checked by low energy electron diffraction and Auger electron spectroscopy. The thickness of the film was 13.6 ML. We also carried out the first-principles calculations for the tetragonally distorted FeCo alloy (c/a =1.24) with/without considering the spin-orbit coupling using WIEN2k program [6]. The exchange-correlation was treated using the generalized gradient approximation.

To determine the high symmetry points along k_z direction [Fig. 1(a)], we first performed the photon-energy-dependent measurement. Figure 1(b) shows the ARPES image acquired at various incident photon energies from 45 to 70 eV with s-polarization. We can recognize the mostly non-dispersive bands around E_B = 1 eV with k_z = 3.7 Å^{-1} and just below E_F with k_z = 4.4 Å^{-1}. The observed features are reproduced by the calculations (not shown here), and we determined that k_z = 3.6 Å^{-1} ($h\nu$ = 45 eV) corresponds to the Γ point. Figure 1(c) shows the ARPES image along the Γ-X line recorded at 45 eV with p-polarization. A very steep band crossing E_F around the X point is recognized. In addition, weakly dispersive bands are found in between E_F to 1.0 eV around the Γ point.

To experimentally verify the spin-polarization, we next performed the spin-resolved measurements. The sample was magnetized along (001) direction at room temperature prior to the measurements. Figures 2(a) and 2(b) display the out-of-plane spin-resolved energy distribution curves (EDCs) and spin-polarization recorded at the Γ and X points, respectively. Here, red and blue represent the majority- and minority-spin components. For both momenta, we can clearly see the out-of-plane spin-polarization. At the Γ point, we have observed a double peak structure in the minority-spin channel around E_B = 0.2 and 0.6 eV, although the broad feature can be seen in the wide energy range in the majority-spin channel [Fig. 2(a)]. On the other hand, at the X point, a prominent majority-spin peak exists at E_F [Fig. 2(b)]. These findings tell us that the weakly dispersive bands around the Γ point and the steep band around the X point mainly comprise the majority-spin and majority-spin characters, respectively. Based on the theoretical investigations [2], the majority-spin states composed of d_{xy} and d_{x2-y2} orbitals play an important role in the emergence of the PMA of the tetragonally distorted FeCo films. We finally compare the spin-ARPES results with the first-principles calculations to scrutinize the orbital characters. Figure 2(c) shows the calculated band dispersion along the Γ-X line in the minority-spin channel. The radii of the orange (black) circles are proportional to the net contribution of d_{xy} (d_{x2-y2}) orbital. By a comparison of Figs. 2(a), 2(b) and 2(c), it signifies that the observed minority-spin peak located just below E_F at the Γ point (black arrow) and at 1.1 eV at the X point (orange arrow) are mainly attributed to the d_{x2-y2} and d_{xy} orbitals, respectively.

In summary, we have investigated the spin-polarized electronic states of the FeCo/Rh(001) films by *in-situ* spin-ARPES and first-principles calculations. The out-of-plane spin-polarization indicating the emergence of PMA was clearly observed at room temperature with zero-field. We conclude that the minority-spin states near E_F are mainly composed of d_{x2-y2} and d_{xy} orbitals. Our findings provide the fundamental properties of the FeCo thin films and pave the way for the PMA-based applications, such as the photoelectron spin polarimeter, enabling the detection of the out-of-plane spin components.

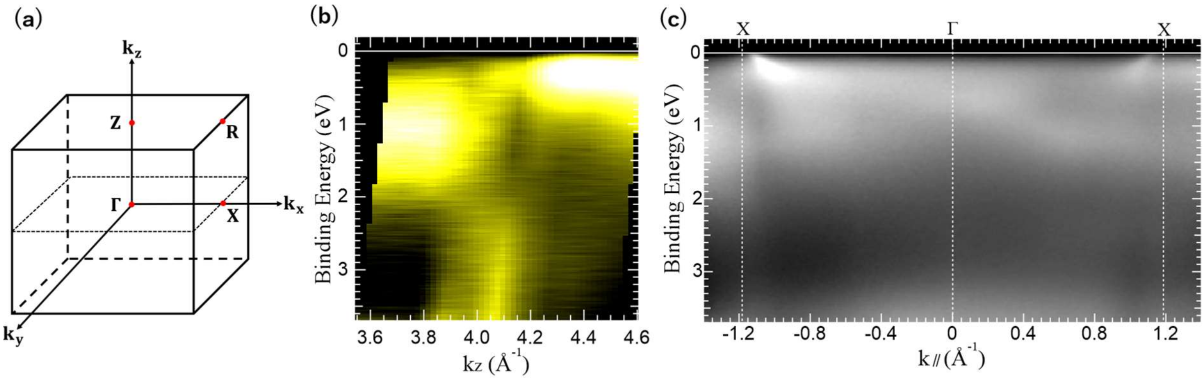

FIGURE1 (a) Brillouin Zone of bct FeCo. **(b)** ARPES image of FeCo/Rh(001) film acquired from 45 to 75 eV with *p*-polarized light. **(c)** ARPES image along the Γ-X line acquired at 45 eV with *p*-polarized light.

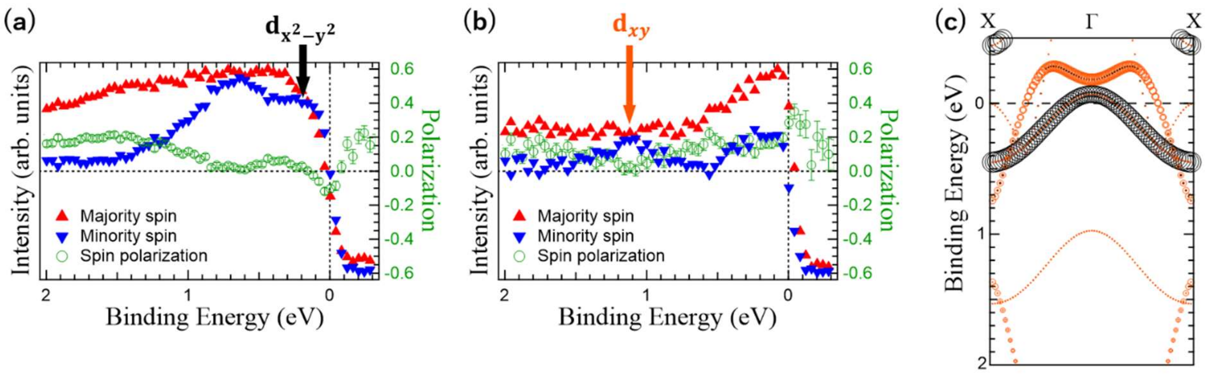

FIGURE2 (a) Out-of-plane spin-EDCs and spin-polarization at the Γ point. **(b)** Same as (a) but at the X point. **(c)** Calculated band dispersion along the Γ-X line in the minority-spin channel. Black and orange represent the d_{x2-y2} and d_{xy} orbitals, respectively.

REFERENCES

1. T. Burkert *et al*., Phys. Rev. Lett. **93**, 027203 (2004).
2. F. Yildiz *et al*., Phys. Rev. B **80**, 064415 (2009).
3. P. Bruno, Phys. Rev. B **39**, 865 (1989).
4. Y. Kota and A. Sakuma, J. Magn. Soc. Jpn. **37**, 17 (2013).
5. T. Okuda *et al*., Rev. Sci. Instrum. **82**, 103302 (2011).
6. P. Blaha *et al*., J. Chem. Phys. **152**, 074101 (2020).