BL-9A/2023G069

Operando EXAFS for detecting changes of lattice distances by reversible strain at Co_2FeSi/PMN-PT interface

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Multiferroic heterostructures using an artificial ferromagnetic/ferroelectric interface have been widely investigated from both fundamental and technological aspects. The electric field (***E***) control of magnetism through the interfacial strain in the ferroelectric material modulates the lattice distance, resulting in the changes of magnetic anisotropy in the magnetic layer. Controlling the magnetic anisotropy by the interfacial strain is one of the hot topics related to the orbital magnetic moments (m_{orb}), which has a potential for future devices using both spins and orbitals. To understand the relationship between strain and m_{orb}, the modulation of element-specific lattice distances has to be clarified explicitly [1]. We have developed the ***E***-induced extended x-ray absorption fine structure (EXAFS) technique by applying piezo-strain into the ferroelectric substrate $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT), which tunes the interfacial lattice constants of the Co_2FeSi (CFS) magnetic layer [2]. In this study, we discuss the microscopic origin of inverse magneto-striction effects concerning the lattice strain, especially the changes of element-specific lattice distances by using the *E*-induced EXAFS [3,4].

We prepared the samples of 10-nm-thick CFS (422) layer grown on single-crystal PMN-PT(011) substrates with the insertion of 0.3-nm-thick Fe layer by molecular beam epitaxy. To apply an ***E*** to the PMN-PT substrate along the [011] direction, a Au(100 nm)/Ti(3 nm) electrode was deposited on the backside of the PMN-PT substrate, where the CFS film was utilized as a top electrode [4]. The ***E***-induced modulation of the in-plane magnetic properties was characterized by X-ray magnetic circular dichroism (XMCD). The EXAFS measurements at the Fe and Co *K* edge under an applied *E* were performed at BL-9A at KEK-PF using the fluorescence yield mode with a 19-element solid-state detector at room temperature. A linearly polarized incident beam arrived at the sample from the 45° direction and enabled the detection of the signals along the $[01\bar{1}]$ direction. The system that applied the *E* was the same as that employed in *E*-induced XMCD.

As shown in Fig. 1**a**, the Fe and Co *K*-edge absorption spectra with EXAFS oscillatory behaviors are observed in the fluorescence yield mode. Clear XAFS oscillations are detected and plotted at wavenumber *k* in the inset of Fig. 1**b**. The XAFS oscillation function $k^3\chi(k)$ can be fitted by the FEFF8 program. The Fourier transformed EXAFS profile for the real-space view of the local structure is displayed in Fig. 1**b** and considers the information up to the second-nearest neighbor sites and using the range of $k = 3 - 13$ Å^{-1}. Owing to the effect of the phase shift, the peak position in the EXAFS was not directly related to the bond length. Using the fitting procedure, the nearest bond lengths in both Fe and Co sites are estimated to be 2.22 and 2.33 Å, respectively, for the +0.8 MV/m case; these values are almost identical to the bulk CFS. The linearly polarized incident beam is used to detect the absorption along the [011] direction in the CFS. Under a negative applied *E* on the PMN-PT substrate as a compressive strain, the nearest neighbor distances in the Fe and Co sites change −0.27% and 0.09%, respectively; these potentially originate from the orientation of the CFS layer in the high-index (422) plane. These element-specific distortions could not be detected by X-ray diffraction in the 10-nm-thick CFS films. These findings indicated that the tensile local distortion in Fe triggered a change in m_{orb} in the CFS layer.

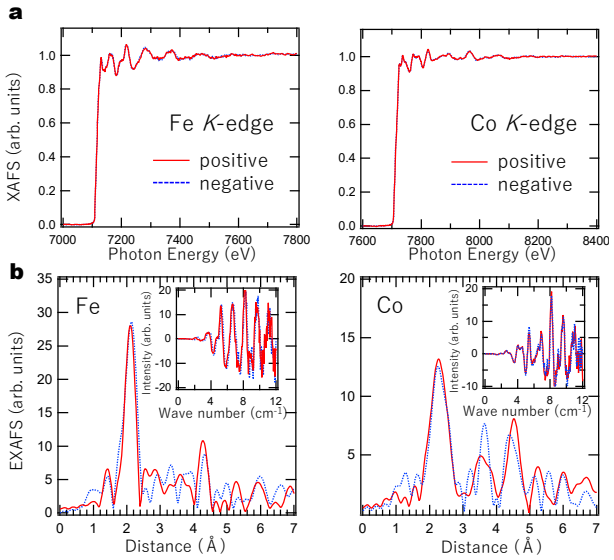

Fig. 1, XAFS and EXAFS analysis under an applied electric field in Co_2FeSi/PMN-PT. (**a**) XAFS spectra of Fe and Co *K*-edges under ±0.8 MV/m. (**b**) EXAFS analysis through the Fourier transform of the XAFS oscillation shown in the insets [4].

References

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