Materials Science

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X-ray magnetic circular dichroism of (La,Ba)CoO_3

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Introduction

$LaCoO_3$ perovskite is of particular interest because it shows two spin-state transitions. Namely, nonmagnetic insulator continuously changes to a paramagnetic insulating state above about 100 K and transforms to a metallic state around 500 K. The two transitions are considered to relate to low-spin (LS, $t_{2g}^6e_g^0$, S = 0), intermediate-spin (IS, $^3T_1$; $t_{2g}^5e_g^1$, S = 1) and high-spin (HS, $t_{2g}^4e_g^2$, S = 2) states of Co atoms. When La^{3+} in $LaCoO_3$ is replaced by divalent alkaline-earth metals, the magnetic atate increase with increasing x, where the constituent Co^{3+} ion changes to Co^{4+} or Co^{3+} with a hole. For doped $LaCoO_3$ crystals, most studies have been done on $La_{1-x}Sr_xCoO_3$ (*e.g.* [1]), while there are only a few studies on $La_{1-x}Ba_xCoO_3$ [2-4].

In this paper we present a site- and valence-selective XMCD study at the Co *K* absorption edge to elucidate the relationship between magnetic property and crystal structure in terms of the hybridization between the 3*d* and 4*p* states of Co atom through the ligand 2*p* state

Experimental

XANES and XMCD experiments were carried out on the BL-6C(3A). The horizontally polarized white X-rays were monochromatized by the Si(111) double-crystal monochromator. The beam size limited by a slit was $3^{(H)}$ x $2^{(V)}$ mm^2 at the sample position. The intensity after transmitting through the sample was measured with 300 mm ionization chamber which was filled with 75% N_2 + 25% Ar gas. The difference in the absorption coefficients for right- and left-circularly polarized X-rays was measured with spins parallel and antiparallel to the direction of light travel. The incident beam was guided into a synthetic single crystal of (001) diamond with a thickness of 0.492 mm in order to produce circularly polarized X-rays. A standard transmission setup was used with the Faraday arrangement, where X-rays irradiates the sample through a pair of pinholes in rare-earth magnets in a magnetic field of 0.4 T.

Results and discussion

A negative XMCD peak was clearly observed at E = 7.719 keV within the threshold region of the main edge for the solid solution of $La_{1-x}Ba_xCoO_3$ ($0.2 \le x \le 0.4$), which can be assigned a similar peak of pure $LaCoO_3$ [1]. A positive XMCD peak appeared at E = 7.723 keV by Ba substitution of La in $LaCoO_3$ in the region of $x \ge 0.2$. A negative XMCD peak was also observed at the pre-edge for the samples of $x \ge 0.2$, which can be explained as the hybridization with the neighboring Co^{4+} in the dipole transition. The dispersion-type XMCD signals at the main edge may be rationalized with the hypothetical double-exchange interaction between Co^{3+} and Co^{4+}. The first-principles calculations reproduced well the experimental spectra of X-ray magnetic circular dichroism (XMCD) at the Co *K*-absorption edge, where a hybridization of Co 3*d* and O 2*p* can stabilize a magnetic state of $La_{1-x}Ba_xCoO_3$.

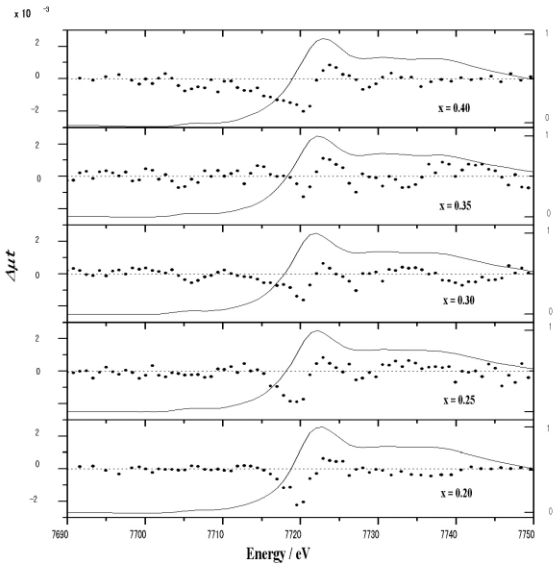

Fig. 1: XMCD spectra of $La_{1-x}Ba_xCoO_3$ ($0.2 \le x \le 0.4$) at the Co *K* edge.

References

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