19B/2001G011

Co 2p x-ray absorption spectrum of $LaCoO_3$

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Introduction

$LaCoO_3$ exhibits a gradual nonmagnetic to paramagnetic transition around 100 K. The ground state of Co is the low-spin (LS) state with S=0. It is now considered that the intermediate-spin (IS) state with S=1 is the first excited state and populated thermally through the transition [1]. By assuming these spin states, the magnetic susceptibility is explained qualitatively but not quantitatively [2]. The nature of the transition has yet to be understood fully.

We have studied the Co 3d state of $LaCoO_3$ associated with the magnetic transition around 100 K by using Co 2p x-ray absorption spectroscopy (XAS) with the aid of a CoO_6-cluster model analyses.

Results and Discussion

The sample used was a $LaCoO_3$ single crystal, whose surface was cleaned *in situ* by scraping. Photon energies were calibrated by measuring Au 4f photoemission spectra.

Figure 1 shows the Co 2p XAS (total electron yield) spectra taken at 20 and 250 K. The overall features of the two spectra are like each other and in agreement with previous result [3]. Upon heating, the Co $2p_{3/2}$ and $2p_{1/2}$ peaks are shifted to higher energies, a shoulder around 779 eV decreases and that around 783 eV increases in intensity in comparison with the Co $2p_{3/2}$ peak. According to the magnetic susceptibility analyses [1], over half of Co is excited thermally at 250 K, whereas almost all Co remains in the LS state at 20 K.

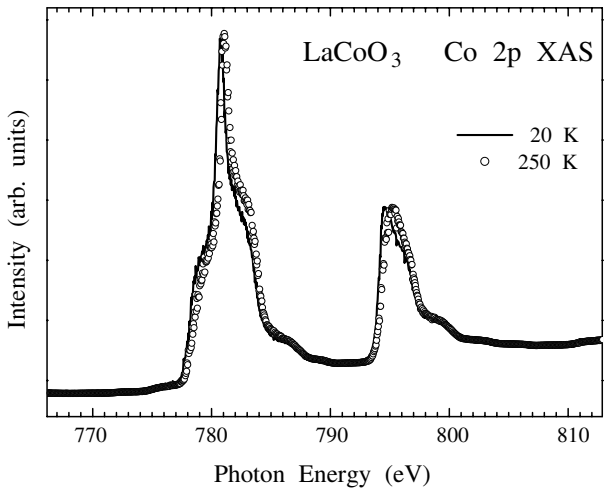

Fig. 1. Co 2p x-ray absorption spectra of $LaCoO_3$ taken at 20 K (solid line) and 250 K (open circles).

We have used a CoO_6-cluster model to analyze the obtained XAS spectra, and assumed that the population of each spin state of Co follows that predicted by the model described in Ref. 1. and that only the first excited state is excited thermally. The calculated results are shown in Figure 2. The parameters used are listed in Table 1.The calculation does not reproduce well the temperature dependence of the observed spectra. The refinement of the parameters used and more detailed simulation by taking into account higher excited states should be necessary.

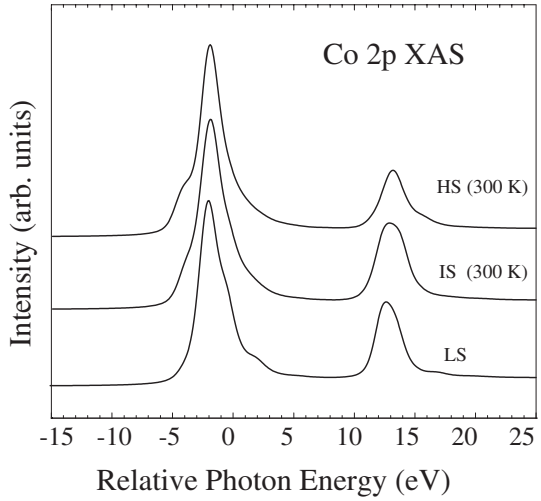

Fig. 2. Simulated results of temperature dependence of Co 2p XAS spectrum of $LaCoO_3$. Curve LS represents the 20 K-spectrum, and curves IS (300 K) and HS (300 K) the 300 K spectrum by assuming the IS and the high-spin state as the first excited state, respectively.

Table 1: Parameters used in calculation. Values are given in eV, except for Rc and Rv

Δ	U_{dd}	$V(t_{2g})$	U_{dc}	$10Dq$	Rc	Rv
2.0	5.0	3.0	6.0	0.75	0.8	0.9

References

[1] T. Saitoh *et al.*, Phys. Rev. B 55, 4257 (1997).
[2] S. Noguchi *et al.*, to be published in Phys. Rev. B.
[3] M. Abbate *et al.*, Phys. Rev. B 47, 16124 (1993).

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