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Crystallographic Mn site in the icosahedral cluster of $LaCo_{13-x}Mn_x$ compounds

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Introduction

$LaCo_{13-x}Mn_x$ compounds are the cubic $NaZn_{13}$-type structure and consists of La atoms and icosahedral clusters composed of thirteen Co and Mn atoms. With increasing Mn content, the magnetic moment exhibits a maximum at around x = 1.0.

The transition metals in the icosahedral cluster in this structure have two different crystallographic sites; one is the center of the icosahedron, the other is its corner. The magnetic moment and the exchange interaction of the Mn atom are sensitive to its local environment such as the interatomic distance and the coordination number. However, it is uncertain that Mn atom occupies either of two sites. In this report, the study on the crystallographic site of Mn in $LaCo_{13-x}Mn_x$ compounds was carried out by using XAFS of the Mn K-edge.

Experiments

The specimens of $LaCo_{13-x}Mn_x$ (x = 0.0 ~ 3.0) were prepared by arc melting under a pure argon atmosphere and were annealed in an argon atmosphere at 1273 K. The lattice constants were obtained by X-ray powder diffraction with Cu Kα radiation. XAFS spectra of the Mn K-edge were measured by a transmission method at 20 K using a double Si(111) monochromator. UWXAFS programs are used for data analyses (AUTOBK) and calculations (FEFF).

Results and Discussion

Fig. 1 presents the obtained $\chi(k)$ curves for the $LaCo_{13-x}Mn_x$ compounds in terms of $k^3\chi(k)$ versus k. The XAFS results show nearly the same spectra for all the compounds. This fact indicates that the Mn site in the these compounds does not change with the Mn concentration.

The Fourier transform of the fitting results for the Mn K-edge XAFS spectrum for $LaCo_{13-x}Mn_x$ compound with x = 1.0 are shown in fig. 2. The calculated curve for the Co(II) site well reproduces the observed curve, but that for the Co(I) site can not reproduce the peaks in the range r > 2.5. Therefore, The Mn atoms preferentially occupy the corner site Co(II) in the icosahedral cluster of the $LaCo_{13-x}Mn_x$ compounds.

From the model calculations and the curve fittings using the program FEFF and FEFFIT, the average of Mn-Co interatomic distance obtained by the present XAFS analyses is 2.52(4) Å which is larger than 2.50(8) Å obtained by X-ray powder diffraction. On the other hand,

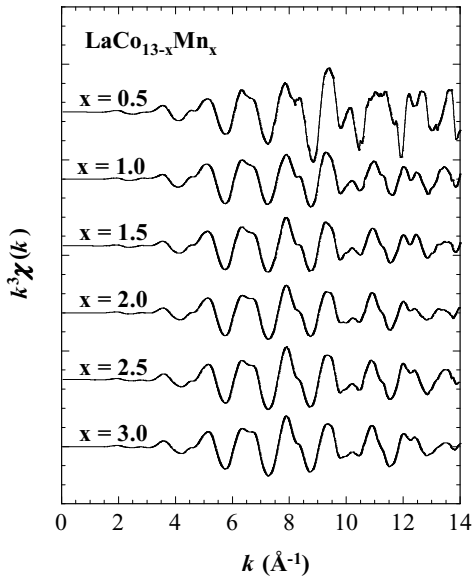

Fig. 1 XAFS spectra of the Mn K-edge represented as $k^3\chi(k)$ vs. k for the $LaCo_{13-x}Mn_x$ compounds with x = 0.5 ~ 3.0.

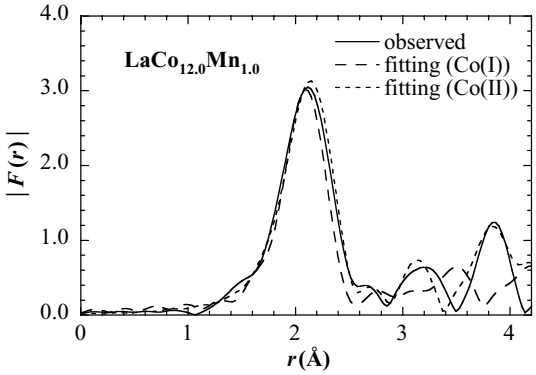

Fig. 2 Fourier transformations of $k^3\chi(k)$ of the Mn K-edge for the $LaCo_{12.0}Mn_{1.0}$ compound. The solid lines stand for the observed results.

the Mn-La interatomic distance obtained by the XAFS analyses is smaller than the value obtained by X-ray diffraction. It appears that the size of an icosahedral cluster including Mn atoms expands, and hence the crystallographic Mn position slightly shifts toward the La atom[1].

References

[1] K.Asada et al., *J. Alloys Comp*. 350 (2003) 47.

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