

## High Temperature Neutron Diffraction Study of (La<sub>0.5</sub>Sr<sub>0.5</sub>)CoO<sub>3-d</sub> Perovskite

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Recently, strontium-doped lanthanum cobaltate perovskites, (La<sub>1-x</sub>Sr<sub>x</sub>)CoO<sub>3-d</sub> have been investigated as the cathode materials of solid oxide fuel cells, because of the high electronic and high oxide-ion conductivity [1]. However, the detailed crystal structures under cell operation conditions, i.e., at elevated temperatures under oxygen partial pressures,  $P(\text{O}_2) \leq 0.21 \text{ atm}$ , have not been reported yet. In this study, we have measured high temperature neutron diffraction data of 50 mol% Sr-doped LaCoO<sub>3</sub>, (La<sub>0.5</sub>Sr<sub>0.5</sub>)CoO<sub>3-d</sub> (LSC), at elevated temperatures,  $298 \leq T \leq 1273 \text{ K}$ , under  $0.0002 \leq P(\text{O}_2) \leq 0.21 \text{ atm}$ , to investigate the detailed crystal structures.

Neutron diffraction measurements were performed with a 150-detector system, HERMES [2], installed at the JRR-3M reactor in JAEA (Tokai). The neutron wave length was  $1.8265(1) \text{ \AA}$  and the diffraction data were collected in the  $2\theta$  range from 20 to 153 deg. in step interval of  $2\theta = 0.1$  deg. A furnace with Pt-Rh heaters installed in a vacuum chamber was placed on the sample stage, and used for neutron-diffraction measurements at high temperatures under different  $P(\text{O}_2)$  conditions. The diffraction data obtained were analyzed using the Rietveld program RIETAN-2000 [3]. The diffraction data of LSC could be indexed assuming a trigonal symmetry (R-3c, No.167) between 298 and 608K, or a cubic one (Pm-3m, No.221) between 723 and 1273K under  $P(\text{O}_2) = 0.21 \text{ atm}$ . Almost all the diffraction peaks could be indexed as a tetragonal system (P4/mmm, No.123) at 1073K in  $P(\text{O}_2) = 0.0002 \text{ atm}$ . Figure 1 shows the Rietveld refinement result of LSC measured at 1273K in  $P(\text{O}_2) = 0.0004 \text{ atm}$ . Under this condition, almost all the diffraction peaks could be indexed as

a cubic perovskite phase (Pm-3m, No.221) (In addition, trace amount of CoO phase was detected). The refined cell parameters of perovskite phase were as follows:  $Z = 1$ ,  $a = 3.9395(3) \text{ \AA}$ ,  $\beta = 90$  deg.,  $V = 61.138(8) \text{ \AA}^3$ . The reliability factors were  $R_{\text{wp}} = 5.81\%$ ,  $R_{\text{I}} = 3.93\%$ ,  $R_{\text{F}} = 2.14\%$ , and  $R_{\text{e}} = 2.12\%$ . Goodness of fit ( $S = R_{\text{wp}}/R_{\text{e}}$ ) was 2.73.

### References

- [1] N. Minh, J. Am. Ceram. Soc., 76, 563 (1993).
- [2] K. Ohoyama, T. Kanouchi, K. Nemoto, M. Ohashi, T. Kajitani, and Y. Yamaguchi, Jpn. J. Appl. Phys., 37, 3319 (1998).
- [3] F. Izumi and T. Ikeda, Mater. Sci. Forum, 321-324, 198 (2000).

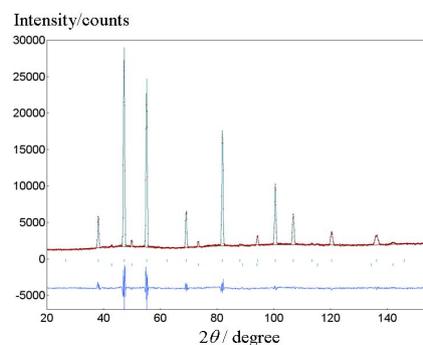


Fig. 1. Rietveld refinement result of (La<sub>0.5</sub>Sr<sub>0.5</sub>)CoO<sub>3-d</sub> at 1273K in  $P(\text{O}_2) = 0.0004 \text{ atm}$ .