Crystallography

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Phase Transition of Doped Lanthanum Cobaltite through synchrotron powder diffraction

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Introduction

SOFC (Solid Oxide Fuel Cell) is an attractive energy-generation system due to high efficiency and cleaness. Some ABO_3 perovskite-related compounds such as doped lanthanum cobalt oxides can be utilized as electrode materials in the SOFCs due to excellent ionic and electronic conductivity. The development of better electrode materials requires a better understanding of the mechanism of ionic conduction, and crucial to this is a comprehension of the crystal structure and phase transition at high temperatures where the materials work efficiently. Here we report the phase transition of $La_{0.601}Sr_{0.394}Co_{0.802}Fe_{0.203}O_{3-\delta}$ (LSCF6482) at high temperatures.

Experiment

Synchrotron powder diffraction experiments of the LSCF6482 sample were conducted using the diffractometer installed at the beam line BL-3A of the Photon Factory, KEK, Japan. Monochromatized 0.908 Å X-ray and a furnace with the $MoSi_2$ heaters were used for the high-temperature diffraction experiments (Yashima & Tanaka, *J. Appl. Cryst.* **37** (2004) 786-790).We installed a Si(111) analyzer crystal between the sample and the scintillation counter to obtain high angular resolution of $\delta d/d$ ~0.03% .

Results and discussion

The diffraction profile of the LSCF 6428 at room temperature was identified to be the trigonal phase with a distorted perovskite-type structure (space group $R\bar{3}c$). Figures 1 and 2 show the temperature dependence of the synchrotron powder diffraction profiles. At room temperature the peak split into 4 0 4 and 0 0 12 reflections was clearly observed (Fig. 1). Similarly the peak split between the 2 2 0 and 2 0 8 reflections was also detected as shown in Fig. 2. The difference between the peak positions between 4 0 4 and 0 0 12 reflections became smaller with increasing temperature and merged between 773 K and 823 K (Fig. 1). The difference between the 2 2 0 and 2 0 8 peak positions also became smaller with increasing temperature and merged between 773 K and 823 K, indicating the trigonal ($R\bar{3}c$) to cubic ($Pm\bar{3}m$) phase transition. These peak splits continuously decreased and disappeared, suggesting that the phase transition is continuous.

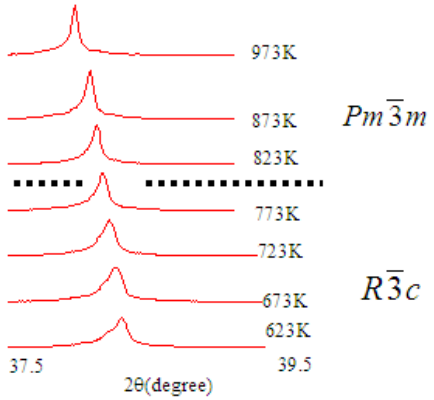

Fig. 1. Diffraction profiles of LSCF6482 around the 4 0 4 and 0 0 12 reflections measured at different temperatures.

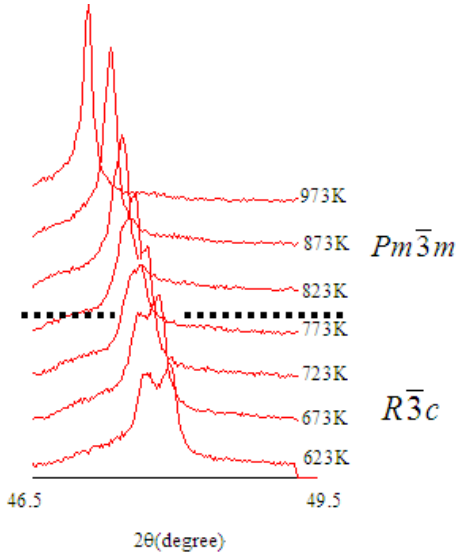

Fig. 2. Diffraction profile of LSCF6482 around the 2 0 2 and 2 0 8 reflections measured at different temperatures.

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