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Crystal Structure of Perovskite-type $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ at a 1010°C

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Introduction

Solid oxides that exhibit high ionic conductivity have attracted widespread interest in recent years owing to their technological importance in a number of applications, such as oxygen sensors, separation membranes and solid oxide fuel cells. From this point of view recently significant interest has been aroused in lanthanum cobaltite-based materials having perovskite-type structure as they exhibit high oxide-ion and electronic conductivities. Crystal structure and electrical properties of perovskite-type lanthanum cobaltite compounds have been studied by a number of researchers. To improve their properties, it is important to understand the crystal structure at high temperatures, but very less studies have been reported on crystal structure of perovskite-type $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$. Here, we have determined the crystal structure and electron density distribution of $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ by combining a Rietveld method, a maximum-entropy method (MEM) and whole pattern fitting using synchrotron X-ray diffraction intensity measured at 1000°C.

Experimental

Synchrotron X-ray powder diffraction data were collected using the multi-detector diffractometer and a furnace[1] installed at BL-4B$_2$ of Photon Factory, KEK, Tsukuba. The wavelength was λ=1.2 Å. Diffraction data were collected at 1010 °C in the 2θ range from 7.00470° to 154.384° in the step interval of 0.005° in 2θ. The diffraction data were analyzed by the Rietveld method, RIETAN-FP[2] followed by an application of MEM-based pattern fitting (MPF).[3]

Results and discussion

Rietveld analysis of the perovskite-type $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ were analyzed with a cubic $Pm\bar{3}m$ space group. La and Sr atoms were placed at the 1b 1/2, 1/2, 1/2 site. Co and Fe atoms were placed at the 1a 0, 0, 0 site. O atom was placed at the 3d 1/2, 0, 0 site. The calculated profiles fit well with that of observed one (Fig. 1). The occupancy at the O site was refined to be 0.950(4), which was consistent with thermogravimetric measurements. The MEM analyses were performed using the structure factors obtained from the Rietveld analysis. The number of structure factors was 33. The MEM calculations were done with the unit cell divided into 64 × 64 × 64 pixels and whole-pattern fitting using RIETAN-FP.[2] Then, the MEM-based pattern fitting was applied which improved the reliability factors. Electron-density image is shown in Fig.2 to visualize the density derived from the MEM calculations. The electron density distribution map (Fig.2) indicates covalent bonding between the (Co,Fe) and O atoms, which might be formed by the overlap of (Co,Fe) 3d and O 2p electrons.

References

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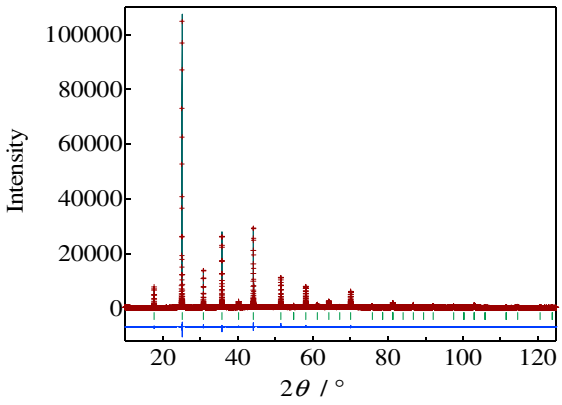

Fig.1 Rietveld fitting pattern of $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ measured at 1010°C. Crosses (+) and line denote observed and calculated profile intensities, respectively. Short vertical bars represent Bragg reflection position.

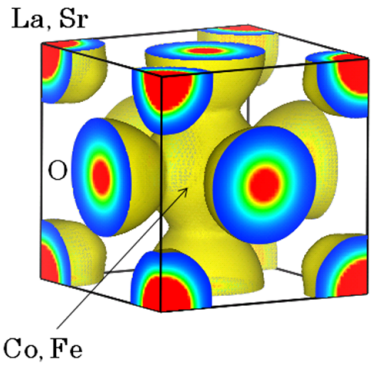

Fig.2 Equi-electron density surfaces at 0.5 Å^{-3} of perovskite-type $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$.

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