

High temperature neutron diffraction study of $(\text{La}_{0.9}\text{Sr}_{0.1})\text{MnO}_{3+d}$ perovskite

K. Nomura (A), H. Kageyama (A), K. Kakinuma (B), T. Maekawa (C), S. Nakamura (C), H. Miyazaki (C), H. Imabayashi (C), and T. Ito (C)

(A) National Institute of Advanced Industrial Science and Technology (AIST), (B) Kanagawa University, (C) New Cosmos Electric Co., Ltd.

Strontium-doped lanthanum manganese perovskites, $(\text{La}_{1-x}\text{Sr}_x)\text{MnO}_{3+d}$ have been investigated as the electrode materials of solid oxide fuel cells, because of the high electronic and relatively high oxide-ion conductivity [1]. However, the detailed crystal structures at elevated temperatures have not been reported yet. In this study, we measured high temperature neutron diffraction data of 10 mol% Sr-doped LaMnO_3 , $(\text{La}_{0.9}\text{Sr}_{0.1})\text{MnO}_{3+d}$ (LSM), to investigate the crystal structure and the conduction path of oxide-ions.

Neutron diffraction measurements were performed in air with a 150-detector system, HERMES [2], installed at the JRR-3M reactor in JAEA (Tokai). The neutron wavelength was $1.8265(1)\text{\AA}$ and the diffraction data were collected in the 2θ range from 20 to 153 deg in step interval of 0.1 deg, in the temperature range from 297 to 1473K and oxygen partial pressure, $P(\text{O}_2)$, range between 2×10^{-4} and 0.21atm. 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. A tubular-type LSM sinter (outer diameter: 10 mm, inner diameter: 7 mm, length: 50 mm) was prepared, in order to obtain equilibrium conditions between the sinter and atmospheres at short times. The diffraction data obtained were analyzed using the Rietveld program RIETAN-2000 [3]

The diffraction data of LSM could be indexed assuming an orthorhombic symmetry ($Pnma$, No.62) (at 297 and 373K) or a trigonal one ($R\bar{3}c$, No.167) (between 473 and 1473K) in $P(\text{O}_2) = 0.21$ atm. Figure 1 shows the Rietveld refinement result of LSM measured at 1473K in $P(\text{O}_2) = 0.21$ atm. The number of chemical formula per

unit cell, refined cell parameters, and refined unit cell volume were as follows: $z = 6$, $a = 5.6029(5)\text{\AA}$, $c = 13.679(2)\text{\AA}$, $V = 371.87(7)\text{\AA}^3$. The reliability factors were $R_{wp} = 5.51\%$, $RI = 2.35\%$, and $RF = 1.74\%$ $R_e = 2.96\%$. Goodness of fit ($S = R_{wp}/R_e$) was 1.86.

References

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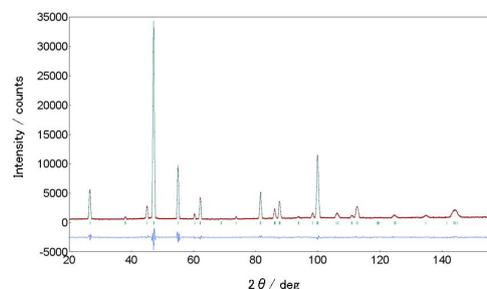


Fig. 1. Rietveld refinement result of $(\text{La}_{0.9}\text{Sr}_{0.1})\text{MnO}_{3+d}$ at 1473K in $P(\text{O}_2) = 0.21$ atm.