

Development of Ba-Sc Oxide Electrolyte Material  
with Defective Perovskite Type Structure

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Introduction

Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub> with defect perovskite-related structure has a characteristic order-disorder transition at about 930°C, and shows high oxide ion conductivity at the higher temperature. In order to utilize as the electrolyte for solid oxide fuel cells (SOFCs), various attempts to stabilize the high temperature phase had been made until now, and it was clarified that the high conductivity was maintained even at low temperature by doping Ga, Gd or La to Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub>[1-3]. However, there was a problem for the utilization as a solid electrolyte because In ion is reduced at the oxygen partial pressure as low as that of the fuel electrode. In this study, we have developed Ba-Sc oxide where Sc is used instead of In in Ba-In oxide, because Sc ion is stable even at low oxygen partial pressure.

Experimental

Barium carbonate (Wako, 99.0%), lanthanum oxide (Wako, 99.9%), scandium oxide (Mitsuwa, 99.9%), and zirconium oxide (Mitsuwa, 99.9%) were weighed at various ratios and mixed for 5h in an electric mortar. The mixtures were pressed into disks, heated at 1600°C for 7h in air, and then left to cool in the furnace. The products were powdered and analyzed by the X-ray diffraction (XRD) using CuKα radiation at room temperature. The above heating procedures were repeated twice.

The crystal structures of the products were determined by the Rietveld analysis. For the Rietveld analysis, a powder XRD pattern was collected with MoKα radiation using a powder X-ray diffractometer (Model RINT-TTR, Rigaku, Tokyo, Japan) equipped with a curved-crystal graphite monochromator. The computer program named RIEVEC [1,45] was used for the Rietveld calculation.

Powder of the product was pressed into disk, pressed by cold isostatic press in 392MPa and sintered at 1600°C for 7h. The sintered product was cut into a prism 4×10×2 mm<sup>3</sup> in size. The total electrical conductivity of the sample prism was measured by the DC 4 probes method in the range of 500-1000°C.

Results and discussion

XRD patterns of Ba<sub>1-x</sub>La<sub>x</sub>Sc<sub>1-y</sub>Zr<sub>y</sub>O<sub>3-α</sub> was indexed by the cubic perovskite structure (space group : *Pm3m*) for 0≤x≤0.2 and 0.3≤y≤0.8 region. In Fig.1, the lattice constant of Ba<sub>1-x</sub>La<sub>x</sub>Sc<sub>1-y</sub>Zr<sub>y</sub>O<sub>3-α</sub> versus the Zr content determined by the Rietveld analysis is shown. The lattice constant decreased with increasing Zr content and La content. This may result from the ionic radii of Zr<sup>4+</sup> and La<sup>3+</sup>, each of which is smaller than that of Sc<sup>3+</sup> and Ba<sup>2+</sup>, respectively[6].

Fig.2 shows the Arrhenius plots of the total electrical conductivities of Ba<sub>1-x</sub>La<sub>x</sub>Sc<sub>1-y</sub>Zr<sub>y</sub>O<sub>3-α</sub>. These were very close to that of Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub> at high temperature, and they kept high values at lower temperature without the transformation. The slopes of Arrhenius plots became gentle with decreasing

temperature. It was suggested that these samples have the proton conduction.

Novel Ba-Sc oxide electrolyte material with defective perovskite type structure was developed.

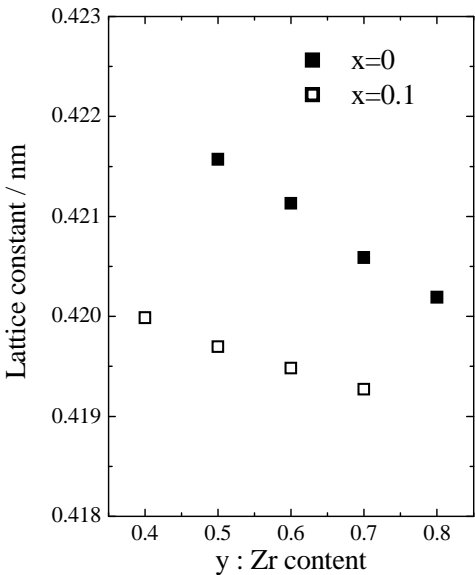


Fig.1 Lattice constant of Ba<sub>1-x</sub>La<sub>x</sub>Sc<sub>1-y</sub>Zr<sub>y</sub>O<sub>3-α</sub> as a function of Zr content

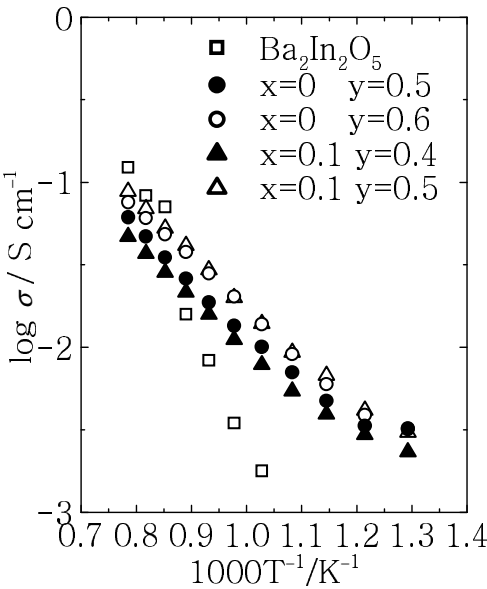


Fig.2 Electric conductivities of Ba<sub>1-x</sub>La<sub>x</sub>Sc<sub>1-y</sub>Zr<sub>y</sub>O<sub>3-α</sub>

Reference

[1]T. Yao, Y.Uchimoto, M. Kinuhata et al., *Solid State Ionics*, **132**, 189-198 (2000).  
[2]Y. Uchimoto, T. Yao, H. Takagi et al., *Electrochemistry*, **68**, 531-533 (2000).  
[3]K. Kakinuma et al., *Solid State Ionics*, **140**, 301-306(2001).  
[4]T. Yao, T. Ito and T. Kokubo, *Journal of Materials Research* **10**, 1079-1082 (1995)  
[5]T. Yao, Y. Oka and N. Yamamoto, *Materials Research Bulletin*, **27**[6], 669-675(1992)  
[6] R. D. Shannon, C. T. Prewitt, *Acta Cryst.*, **B25**, 925, (1969)