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Temperature dependence of the unit-cell parameters of double perovskite-type $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$

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Introduction

Double perovskite-type compounds Ba_2LnBO_6 (*Ln* = lanthanoid and Y, *B* = Sn, Sb, Nb, Ta) are candidates for electrolytes of solid oxide fuel cells (SOFCs) [1]. The purpose of this study is to investigate existing phases and their unit-cell parameters of $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$ between 790 K and 1673 K.

Experimental procedure

Synchrotron powder diffraction measurements of $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$ were carried out from 790 to 1672.6 K by a high-angular-resoluion multi-detector system [2] and a furnace [3,4] installed at the BL-4B$_2$ beam line of Photon Factory. Wavelength of synchrotron X-ray was 1.1960 Å.

The experimental data were analyzed assuming the cubic (space group $Fm\bar{3}m$) double-perovskite-type structure using Rietveld method with a computer program RIETAN-FP [5].

Results and discussion

Figure 1 shows a part of synchrotron powder diffraction pattern of $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$ at 790 K. There exist two 440 reflections, which indicates the coexistence of two cubic phases. The weight fraction of one phase with the unit-cell parameter of 8.5932(2) Å was estimated to be 83.4% at 790 K. The weight fraction of the other with lower cell parameter of 8.56821(12) Å was estimated to be 16.6%. The unit-cell parameters of two $Fm\bar{3}m$ phases increase with an increase of temperature (Fig. 2).

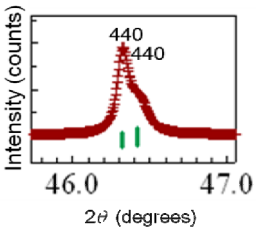

Figure 1. A part of synchrotron powder diffraction pattern of $Fm\bar{3}m$ $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$ at 790K. Wavelength of synchrotron X-ray was 1.1960 Å. The crosses represent the observed pattern. The vertical lines are the Bragg reflection markers.

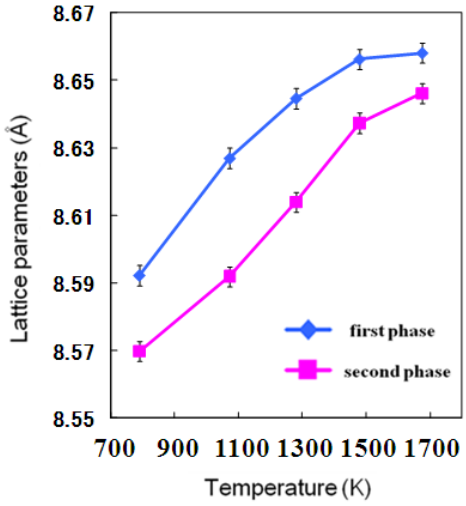

Figure 2. Temperature dependence of the unit-cell parameters for $Ba_2NdSn_{0.6}Sb_{0.4}O_{6-\delta}$ obtained from Rietveld analysis of synchrotron X-ray powder diffraction data at high temperatures.

References

[1] P. J. Saines, M. M. Elcombe, B. J. Kennedy, Physica B, 385-386, 187 (2006)

[2] H. Toraya, H. Hibino, K. Ohsumi, J. Synchrotron Rad. 3, 75 (1996).

[3] M. Yashima, K. Oh-uchi, T. Ida, J. Appl. Crystallogr. 38, 854 (2005).

[4] M. Yashima, K. Oh-uchi, M. Tanaka and T. Ida, J. Am. Ceram. Soc. 89, 1395 (2006).

[5] F. Izumi and K. Momma, Solid State Phenom. 130, 15 (2007).

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