Crystallography

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Crystal structural change in $Ce_{0.5}Zr_{0.5}O_2$ solid solution through synchrotron powder diffraction data

Takahiro Wakita[1], Masatomo Yashima[1,*], Hiroki Ishibashi[2], Takafumi Komatsu[1] and Yong Phat [1]
[1] Department of Materials Science and Engineering, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology, Nagatsuta-cho 4259, Midori-ku, Yokohama, 226-8502; [2] Department of Physical Science, Graduate School of Science, Osaka Prefecture University, Gakuen-cho 1-1, Naka-ku, Sakai, 599-8531

Introduction

Three-way catalyst has been known to oxidize CO and HC, and to reduce NOx at the same time. CeO_2-ZrO_2 solid solutions are used as the subcatalysts for purification of automotive exhaust gases. The development of CeO_2-ZrO_2 catalysts requires a better understanding of the crystal structure and structural change.The crystal structure of the CeO_2-ZrO_2 solid solutions has been investigated by Yashima et al. [1-6]. They reported the existence of three metastable tetragonal forms of t, t' and t''. The three tetragonal forms belong to the $P4_2/nmc$ space group. However, the crystal change in $Ce_{0.5}Zr_{0.5}O_2$ at high temperatures has not been investigated *in situ* yet. The purpose of this study is to investigate the structural change in the $Ce_{0.5}Zr_{0.5}O_2$ solid solution between 1639 K and 1680 K using the synchrotron powder diffraction data.

Experiment

Synchrotron powder diffraction experiment was conducted using a three-axis four circle diffractometer installed at the beam line BL-6C of the Photon Factory, KEK, Japan. Monochromatized 1.55330(7) Å x-ray was used for the diffraction experiment. A furnace with $MoSi_2$ heaters [7] was attached to a goniometer of the triple-axis/four-circle diffractometer, and used for synchrotron x-ray diffraction measurements at high temperatures. Individual profile fits were performed for the powder data using a profile-fitting program *PRO-FIT* [8].

Results and discussion

Fig. 1 shows the synchrotron x-ray diffraction profiles of the $Ce_{0.5}Zr_{0.5}O_2$ solid solution measured between 1639 K and 1680 K. All reflections are indexed by a tetragonal cell ($P4_2/nmc$) between 1639 K and 1658 K. The peak splitting between the 004_t and 220_t reflections was clearly observed between 1639 K and 1658 K (Fig. 1). All reflections in the synchrotron x-ray diffraction profile measured between 1664 K and 1680 K are indexed by a cubic fluorite-type cell ($Fm\bar{3}m$; Fig. 1). The 400_c reflection exhibits a single feature without splitting between the 004_t and 220_t reflections. The $Ce_{0.5}Zr_{0.5}O_2$ solid solution was found to transform from the tetragonal t' to cubic phase between 1658 K and 1664 K.

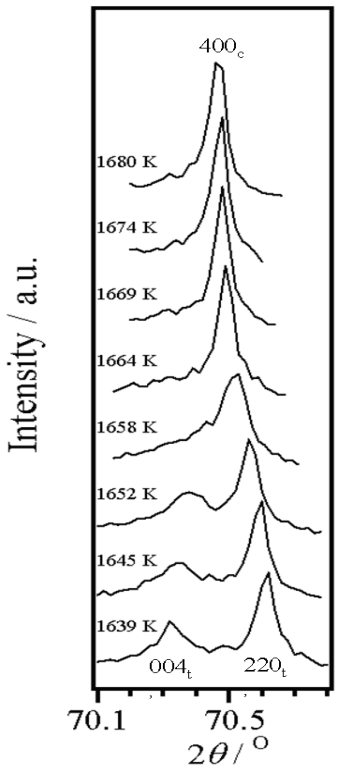

Fig.1 Synchrotron x-ray diffraction profiles from 400 reflection of the $Ce_{0.5}Zr_{0.5}O_2$ measured from 1639 K to 1680 K.

References

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* yashima+@+materia.titech.ac.jp