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# Crystal structural change in $Ce_{0.4}Zr_{0.6}O_2$ solid solution through synchrotron powder diffraction data

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## 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 $Ce_{0.4}Zr_{0.6}O_2$ at high temperatures has not been investigated in-situ yet. The purpose of this study is to investigate the structural change in the $Ce_{0.4}Zr_{0.6}O_2$ solid solution between 296 K and 1790 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 0.89679(10) Å X-ray was used for the diffraction experiment. A furnace with $MoSi_2$ heaters [7] was placed on the sample table, 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 $Ce_{0.4}Zr_{0.6}O_2$ solid solution measured at 1609, 1745 and 1790 K. All reflections are indexed by a tetragonal cell ($P4_2/nmc$) between 1609 K and 1745 K. The peak splitting between the $004_{t'}$ and $220_{t'}$ reflections was clearly observed between 1609 K and 1745 K (Fig. 1a and b). All reflections in the synchrotron x-ray diffraction profile measured at 1790 K are indexed by a cubic fluorite-type cell ($Fm\bar{3}m$; Fig. 1c). The $400_c$ reflection exhibits a single feature without splitting between the $004_{t'}$ and $220_{t'}$ reflections. The $Ce_{0.4}Zr_{0.6}O_2$ solid solution was found to transform from the tetragonal t' to cubic phase between 1745 K and 1790 K.

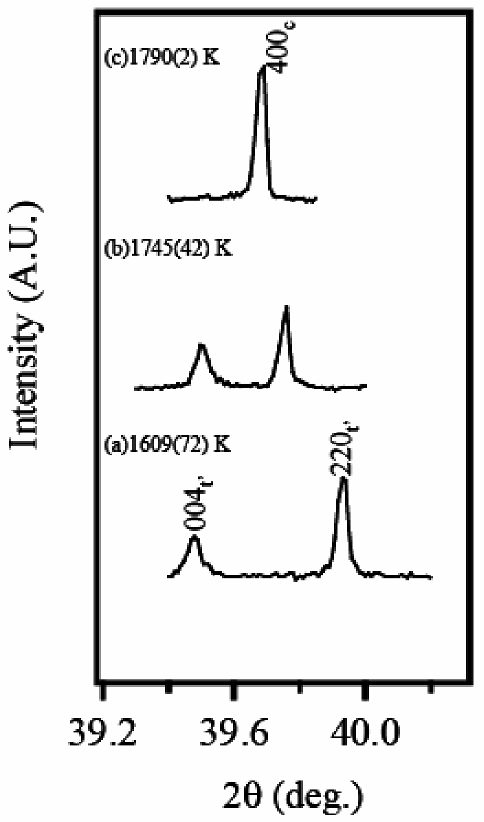

Fig.1 Synchrotron x-ray diffraction profiles for $004_{t'}$, $220_{t'}$ and $400_c$ peaks of the $Ce_{0.4}Zr_{0.6}O_2$.

## References

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