

## Crystal structure analysis of a zirconia-scandia solid solution through synchrotron powder diffraction data at 1497 °C

Toshikazu Ueda, Masatomo Yashima\*, Takahiro Wakita, Roushown Ali\*\*, Takayuki Tsuji, Qi Xu, Yoshiaki Ando, and Yoichi Kawaike

Department of Materials Science and Engineering, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama, 226-8502, Japan

\*\*Quantum Beam Center, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan

### Introduction

Zirconia-scandia solid solutions are some of the highest oxygen ion conductors in the zirconia-based materials. Here, we report the crystal structure of a zirconia-scandia solid solution using the high-temperature synchrotron X-ray powder diffraction data at 1497 °C.

### Experiment

Synchrotron powder diffraction experiment was conducted using a diffractometer installed at the beamline BL-3A(6C) of the Photon Factory, KEK, Japan. Monochromatized 0.899392 Å X-ray was used for the diffraction experiment. The sample was heated at 1497 °C using a furnace with molybdenum silicide heaters. An analyzer crystal was set between the sample and scintillation counter in order to improve the angular resolution and S/N ratio. The diffraction data were analyzed by the Rietveld method with a computer program RIETAN-2000.

### Results and discussion

All the reflections of the zirconia solid solution ( $Zr_{0.81}Sc_{0.19}O_{1.905}$ ) sample measured at 1497 °C were indexed with a cubic cell of  $a=b=c=5.17419(1)$  Å,  $\alpha = \beta = \gamma = 90$  deg. Rietveld analysis was performed with the fluorite-type structure ( $Fm\bar{3}m$ ). The cations were put at the special position of  $4a$  0,0,0 site of the fluorite-type structure. The oxygen ions were put at the  $8c$   $1/4, 1/4, 1/4$  site. Calculated profile agreed well with the observed data as shown in Fig.1. It was confirmed that the  $Zr_{0.81}Sc_{0.19}O_{1.905}$  has the fluorite-type structure (Fig. 2).

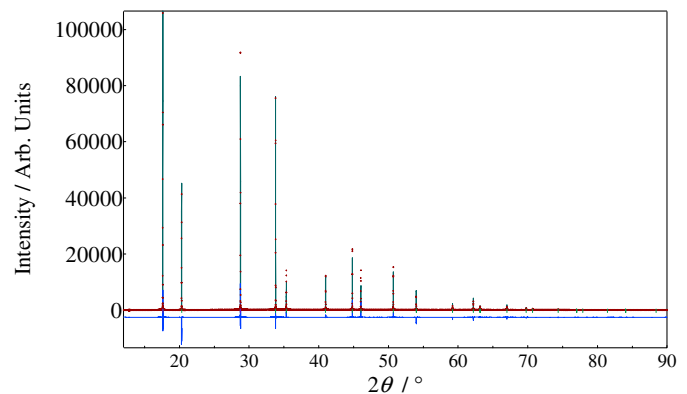


Fig. 1. Rietveld analysis pattern of  $Zr_{0.81}Sc_{0.19}O_{1.905}$  at 1497 °C.

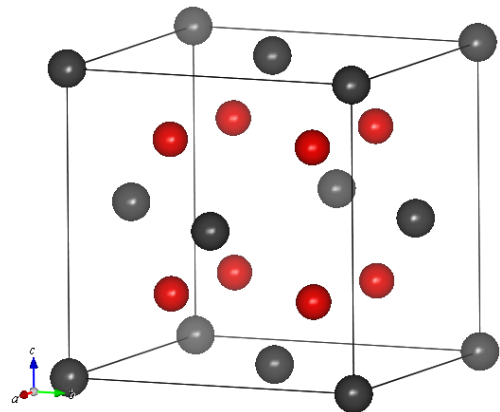


Fig. 2. Refined crystal structure of  $Zr_{0.81}Sc_{0.19}O_{1.905}$  at 1497 °C. Red and black spheres indicate the anion and cation, respectively.

\* yashima@materia.titech.ac.jp