Structural changes of the high temperature proton conductor SrZr$_{1-x}$Yb$_x$O$_{3-\delta}$

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**Introduction**

Perovskite-type strontium zirconate SrZrO$_3$ exhibits appreciable proton conduction in hydrogen-containing atmosphere at high temperature when a few mol\% of trivalent cations such as Yb$^{3+}$, Y$^{3+}$, Ga$^{3+}$ and In$^{3+}$ are substituted for Zr$^{4+}$ ions. The chemical stability of SrZrO$_3$-based oxide is much better, and Yb-doped SrZrO$_3$ oxide shows the highest proton conductivity. The proton conductivity depends on the amount of dopant Yb ions and shows the maximum value when substituted for Yb ions by 10 mol\% [1, 2].

In order to understand the electrical properties of these materials, it is necessary to study the precise crystal structure of SrZrO$_3$ and doped SrZrO$_3$. In our previous study, it was found that SrZrO$_3$ undergoes a sequence of phase transitions as follows, $Pnma \rightarrow Imma \rightarrow I4/mcm \rightarrow Pm-3m$, at 790, 875 and 1120°C, respectively. Here we have used synchrotron X-ray diffraction technique, having higher angular resolution, to investigate the structural change and the phase transition temperature of SrZr$_{1-x}$Yb$_x$O$_{3-\delta}$ ($x = 0.05$ and 0.1).

**Experiments**

The powder samples of 5 and 10 mol\% Yb-doped SrZrO$_3$ were synthesized by solid-state reaction. To obtain higher angular resolution as possible with good counting statistics, we performed synchrotron X-ray powder diffraction experiments from 25°C to 1084°C for Yb-doped SrZrO$_3$ at the beam line BL-3A at the Photon Factory, High Energy Accelerator Research Organization (KEK), Japan. A monochromatized 0.99930Å X-ray was used for high-temperature diffraction measurements. To improve the angular resolution a Si (111) analyzer crystal was installed between the sample and the scintillation counter. The temperature was kept constant within ± 0.5°C during each data collection.

**Results and discussion**

Figure 1 shows the synchrotron X-ray diffraction patterns of 10 mol\% Yb-doped SrZrO$_3$ in the 2θ range of 27.8° to 28.0°. Figure 2 shows the transition temperatures against $x$ in SrZr$_{1-x}$Yb$_x$O$_{3-\delta}$. The transition temperatures of the Yb-doped SrZrO$_3$ decrease with increasing amount of dopant Yb ions in spite of substitution of Zr$^{4+}$ ions by Yb$^{3+}$ ions with a large ionic radius. This suggests that there exist much oxide ion vacancies introduced by substitution of tetravalent zirconium ions by trivalent ytterbium ions.

**References**


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