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Structural phase transitions in strontium zirconate perovskite $SrZrO_3$

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Introduction

Perovskite-structured oxides have received recent attention as high-temperature proton conductors with potential applications as fuel cells and hydrogen sensors. Some doped zirconates possess appreciable levels of proton conductivity. In order to understand the electrical properties of these materials, it is necessary to study the precise crystal structure of $SrZrO_3$. Here we have used synchrotron X-ray diffraction technique, having higher angular resolution, to investigate the structural change and the phase transition temperature of $SrZrO_3$.

Experiments

To obtain higher angular resolution as possible with good counting statistics, we performed synchrotron X-ray powder diffraction experiments from 25°C to 1203°C for $SrZrO_3$ at the beamline BL-3A at the Photon Factory, High Energy Accelerator Research Organization (KEK), Japan. A monochromatized 0.99963(6)Å 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.

Results and discussion

Figure 1 shows the fitting result of a Rietveld analyses of *Pnma* $SrZrO_3$ at 25°C. The use of a sample spinner during the synchrotron radiation diffraction measurement was very effective to obtain accurate Bragg intensity data. The reliability factors were R_{wp} = 18.35%, R_I = 8.44% and R_F = 5.97%. Goodness of fit was 1.76. Refined unit-cell parameters were a = 5.82001(4) Å, b = 8.20718(6) Å and c = 5.79612(4) Å. Figure 2 shows parts of the diffraction patterns for $SrZrO_3$ at 849, 876 and 904°C. At 876°C the pattern exhibited both peaks of *Imma* and *I*4/*mcm* phases, indicating that the phase transition is discontinuous and of first order.

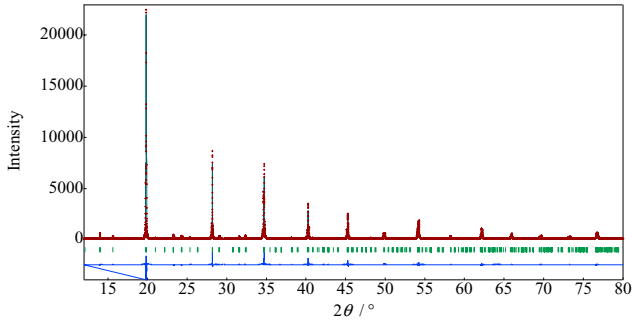

Fig.1. Rietveld pattern of $SrZrO_3$ measured at 25°C.

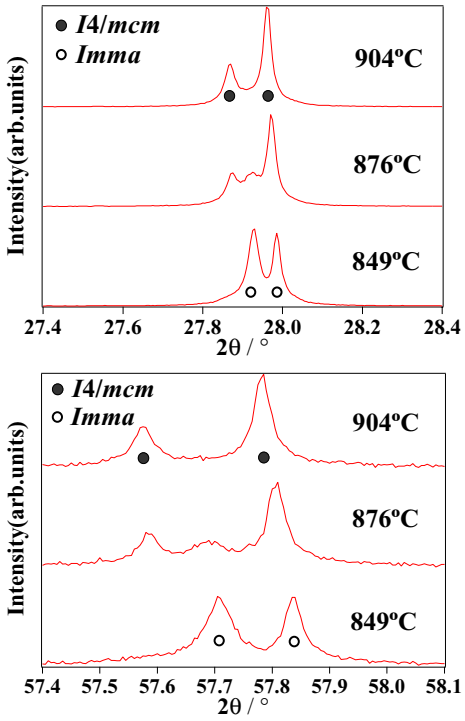

Fig.2. Segments from the observed diffraction patterns of $SrZrO_3$ recorded at 849, 876 and 904°C.

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