High temperature neutron diffraction study of oxide-ion conductors

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Oxide-ion conductors attract significant interest because of their varied uses in oxygen separation membranes and cathodes for solid-oxide fuel cells (SOFCs). Investigation of mechanism of oxide-ion conduction will lead further development of SOFCs. In order to understand the mechanism of oxide-ion conduction, it is necessary to precisely determine the crystal structure (particularly position, occupancy factor, and anisotropic displacement parameters of oxygens) at high-temperature because oxide-ion conductors are generally used at high-temperature. Furthermore, combinations of high-temperature neutron diffraction data and maximum entropy method (MEM) can lead direct observation of ion diffusion pathway. In this context, we plan to carry out high-temperature and high-resolution neutron powder diffraction experiments for the oxide-ion conductors. There are several oxide-ion conductors for which the mechanism of the oxide-ion conduction is not clearly understood. In this study, we have investigated the crystal structure of oxide-ion conductor $A_2B_2O_7$ (A : rare earths, B : group 4 transition metal) at high temperature using high resolution neutron powder diffractometer Echidna installed at the research reactor OPAL, ACNS, ANSTO. The materials were prepared by the solid-state reactions. The sintered pellets of the reaction products were introduced into a vanadium can and used for the neutron diffraction experiment. The measurements were carried out from room temperature to high temperature (maximum 1400 °C) at 200 °C intervals. Each measurement time was few hours. The structural analyses for these data are carried out by Rietveld method using the program RIETAN-FP. The result of the Rietveld refinement at the room temperature 23 °C is shown in Figure (R_{wp} = 5.46 %, R_B = 1.72 %). For the diffraction data at 1400 °C, the final Rietveld plot is shown in Figure. The reliability factors are R_{wp} = 5.22 %, R_B = 5.80 %. There was no structure transition by heating up to 1400 °C. Now we carry out further structure analysis and MEM calculations for the data in order to the mechanism of the oxide-ion conduction in this material.

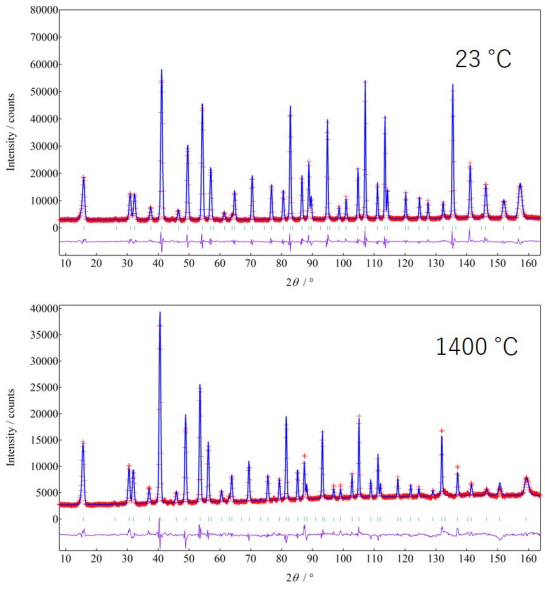

Fig. 1. Rietveld plots of A2B2O7 material