

Structure analysis of novel ionic conductors and mixed-anion materials from neutron powder diffraction data

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Our research group explore novel ceramic ionic conductors and mixed-anion materials. These materials attract many interests because of their possible applications. In the present work, we aim to analyze crystal structures of novel ionic conductors and mixed-anion materials based on the neutron diffraction data in order to understand relationship between structure and properties. Neutron diffraction techniques enable us to reveal the precise structural information of anion species of ceramic materials.

Constant-wavelength neutron powder diffraction data of the prepared samples were measured at the HERMES diffractometer installed at the JRR-3 reactor of the Japan Atomic Energy Agency with the measurement conditions of wavelength: 1.34170(5) Å, step interval: 0.05° in 2θ / step. For some novel ionic conductors, we performed the high-temperature measurements using our furnace.

Fig. 1 shows the measured diffraction patterns of a novel ionic conductor taken at room temperature (17 °C), 500 °C and 1000 °C. With increasing temperature, lattice volume expansions were observed as the peak position shifts toward lower angle. We are now analyzing the neutron diffraction data by Rietveld method.

Fig. 2 shows the Rietveld patterns for neutron diffraction patterns of a novel mixed-anion material Ba_{0.5}Sr_{0.5}Sn_{0.7}Y_{0.30}O_{2.65}H_{0.14}. We have

successfully observed hydride ion exits in this material by Rietveld structure refinement. This is a direct evidence for an existence of hydride ion at an oxygen site in this material. We have reported this outcome in *Inorg. Chem.* [1].

[1] M. Nakamura *et al.*, *Inorg. Chem.* **61**, 6584 (2022).

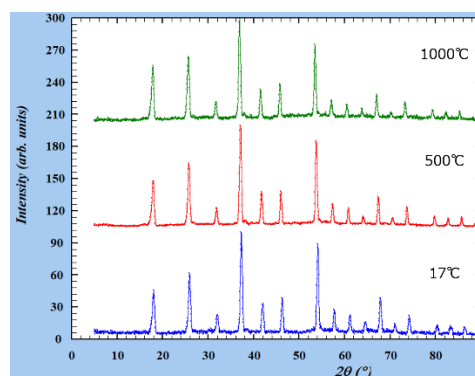


Fig. 1. Neutron diffraction patterns of novel ionic conductor taken at 17 °C (blue), 500 °C (red), and 1000 °C (green).

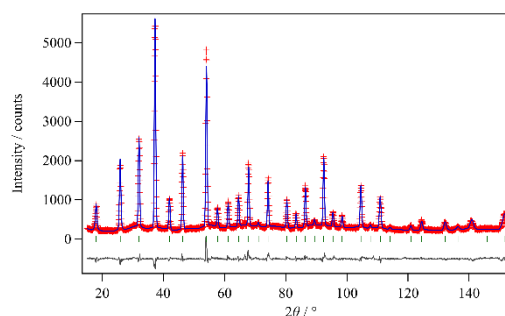


Fig. 2. Rietveld pattern of neutron diffraction data for Ba_{0.5}Sr_{0.5}Sn_{0.7}Y_{0.30}O_{2.65}H_{0.14}. (red: observed, blue: calculated, and grey: difference patterns; green tick marks: Bragg reflection positions).