High temperature and high resolution neutron diffraction study of oxide-ion conductors

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1. Introduction

Oxide-ion conductors attract significant interest because of their varied uses in oxygen separation membranes and cathodes for solid-oxide fuel cells (SOFCs). The oxide-ion conductivity is strongly dependent on the crystal structure. At present, most researches about oxide-ion conductors only focus on the specific structure-type such as fluorites, perovskites, K_2NiF_4, mellilites, and apatites. However, investigation of the new oxide-ion conductors with new structure family is necessary for further development in this field. According to such background, our group investigates oxide-ion conductors with new structure type. For example, we have reported new materials $BaNdInO_4$ (*Chem. Mater.* **2014**, *J. Mater. Chem. A* **2015**, *J. Electrochem. Soc.* **2017**) and $SrYbInO_4$ (*J. Phys. Chem. C* **2017**) as new oxide-ion conductors. The crystal structures of these materials have been analyzed from the neutron powder diffraction data taken at J-PARC. Investigations of the crystal structure at high-temperature are also important for oxide-ion conductors because these materials usually used at high-temperature (above 600 °C). Thus, we also investigates the crystal structures at high temperature for the oxide-ion conductors and related materials. The target materials of this proposal are $BaNdScO_4$ and its doped materials and $AB_2C_3O_{10}$-type new oxide-ion conductors. We have previously measured the diffraction data of $BaNdScO_4$, but we took the data again because we found some problems in the previous data.

2. Experiment

TOF-neutron data of $BaNdScO_4$, its doped materials, and $AB_2C_3O_{10}$-type new oxide-ion conductors were measured at SuperHRPD diffractometer installed at BL08 of MLF, J-PARC. After the room temperature measurements, a vacuum furnace was set and high-temperature data collections were conducted. The data reductions were carried out using HistMaker and the data analyses were carried out using the Z-code.

3. Results

Fig. 1 shows the TOF-neutron diffraction patterns of $BaNdScO_4$ at various temperature. The peak shift due to the thermal expansions were observed for the all samples. In all cases, we could not observe significant pattern change, which indicated no phase transition up to 800 °C. The data analyses are in progress. Our one of the purposes is the investigatoin of the structural change by doping. To determine the small but important structure difference between non-doped and doped samples, careful data analyses are required. Now we are analyzing the data with several dfferent structure models, and different refinement conditions to lead clear and correct conclusions.

4. Conclusion

The data analysis is now in progress and the result may obtain later. The data quality seems fine, so that we wil be able to lead new insights about the target materials which we have discovered.

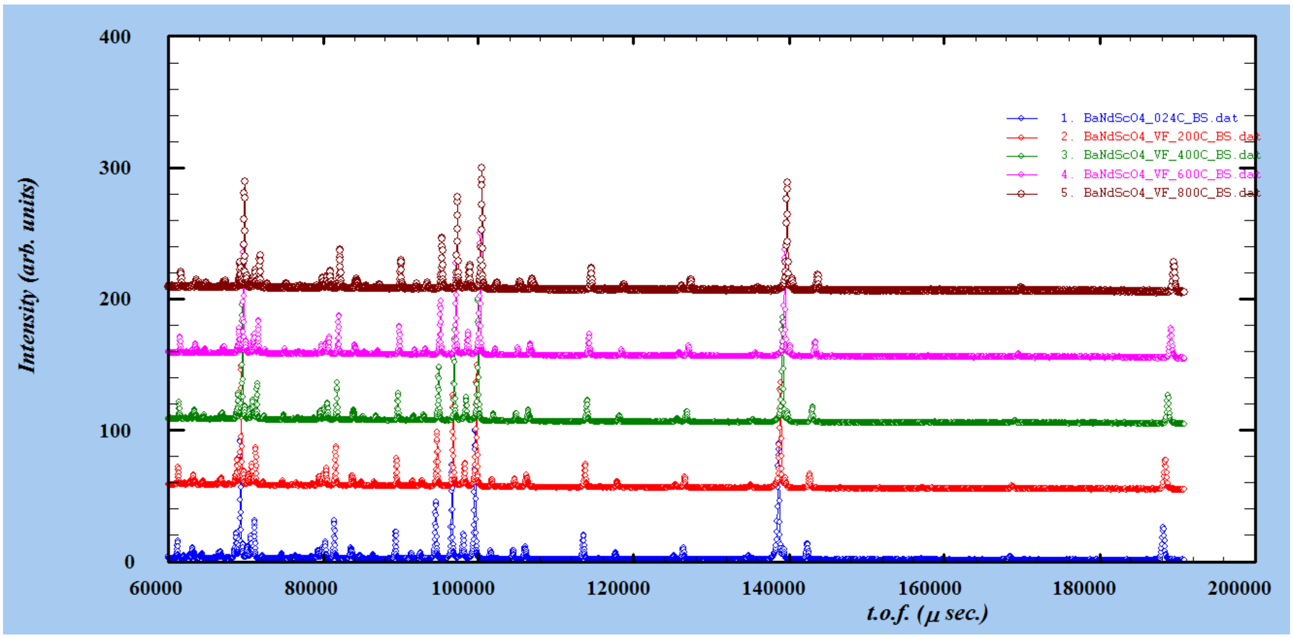

Fig.1 The diffraction data taken at SuperHRPD diffractometer. Room temperature, 200, 400, 600, and 800 °C (from bottom to top).