表題：高温中性子回折による亜鉛を含む酸化物イオン伝導体の結晶構造解析

Crystal structure analysis of high temperature neutron diffraction data of Zn containing oxide-ion conductors

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Oxide-ion conductors, which include pure ionic conductors and mixed oxide-ion and electronic 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, several structures, such as fluorites, perovskites, K_2NiF_4, mellilites, and apatites, are known to show high oxide-ion conductivities. For further developments, it is necessary to find new structure families of oxide-ion conductors. According to such background, we are exploring new structure family of oxide-ion conductors. For example, we previously discovered new structural families of oxide-ion conductors $BaNdInO_4$, $Ca_{0.8}Y_{2.4}Sn_{0.8}O_6$, $Ca_3Ga_4O_9$, and $BaHo_2ZnO_5$. Recently, we found a new structure family of oxide-ion conductor, which containing zinc (Zn) as an essential element. 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. In the present study, we investigated the crystal structure of this new Zn-containing oxide-ion conductor at high temperature using high resolution neutron powder diffractometer Echidna installed at the research reactor OPAL, ACNS, ANSTO. The material was prepared by the solid-state reaction. 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 (1100 °C). Each measurement took about 3 hours. The reflection positions were shifted toward low angle by heating, which suggests the lattice parameters were expand by heating (see figure). Structural analyses are now undergoing by Rietveld method using the program Z-code. Our structure analysis reveal the present material contains positional disorder for the oxygen atoms, which has not been reported in the previous studies. This result indicate the neutron diffraction study is very important to lead the precise and correct atomic position and displacement parameters of oxygen atoms.

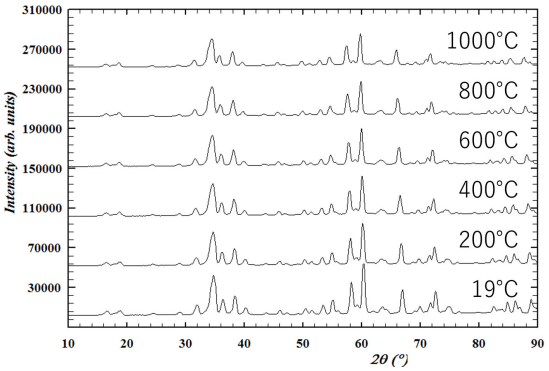

Fig. 1.

使用施設：JRR-3M，装置：T1-3:HERMES
分野：Structures and Excitations