MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014AM0011 実験課題名 Title of experiment 中性子回折による固体酸化物形燃料電池材料の結晶構造解析 実験責任者名 Name of principal investigator 中島 靖 所属 Affiliation 第一稀元素化学工業(株)	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/(BL No.) iMATERIA / BL-20 実施日 Date of Experiment June 24, 2014

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Neutron powder diffraction measurements were carried out for sintered pellets of AB_4O_7, AB_2O_4, RSrInO$_4$ and powdered samples of ABO$_2$N, ABO$_2$N-($A'B'$O$_2$N)$_{0.005}$, ABO$_2$N-($A'B'$O$_2$N)$_{0.01}$. Here A and A' are relatively large cations such as rare earth ions, R is rare earth ions, and alkaline earths ions and B is relatively small cations.

2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。)
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Experimental methods

Time-of-flight (TOF) neutron powder diffraction data of materials for solid oxide fuel cells (SOFCs) were measured at room temperature by a high-resolution neutron powder diffractometer iMATERIA installed at the beam line BL20 of J-PARC facility, Japan. The sintered or the powder samples (0.49 – 3.8 g) were put into 6 mm ϕ vanadium sample holders and were used for the diffraction measurements. The diffraction measurements were carried out ca. 1 hour for each sample with double frame mode (MLF beam power 280kW).

Experimental results

Recently we have successfully synthesized new materials RSrInO$_4$ (R is a rare earth element) which are possible candidates of materials for solid oxide fuel cells (SOFCs). In this work, we aimed to determine their crystal structures from TOF neutron diffraction data. Based on the measured TOF neutron diffraction data and preliminary measured X-ray diffraction data, the crystal structures of RSrInO$_4$ were characterized by indexing and Le Bail analysis. Then the crystal structures of RSrInO$_4$ were refined using the structural model of related

2. 実験方法及び結果（つづき） Experimental method and results (continued)

One of the results of Rietveld structure refinements of RSrInO$_4$ is shown in Figure 1. The Rietveld analysis of TOF neutron diffraction data was carried out using the program Z-Code. The refinement gave good quality of fitting (R_{wp} 0.0348, R_p 0.0285, R_B 0.0391, R_F 0.0305). We are now carrying out further detailed structure analyses, which include determination of anisotropic displacement parameters and site occupancy factors. After the refinement, we will discuss the relationship between crystal structures and electrical conductivities combined with the result of X-ray diffraction analysis and theoretical calculations using density functional theory for these materials.

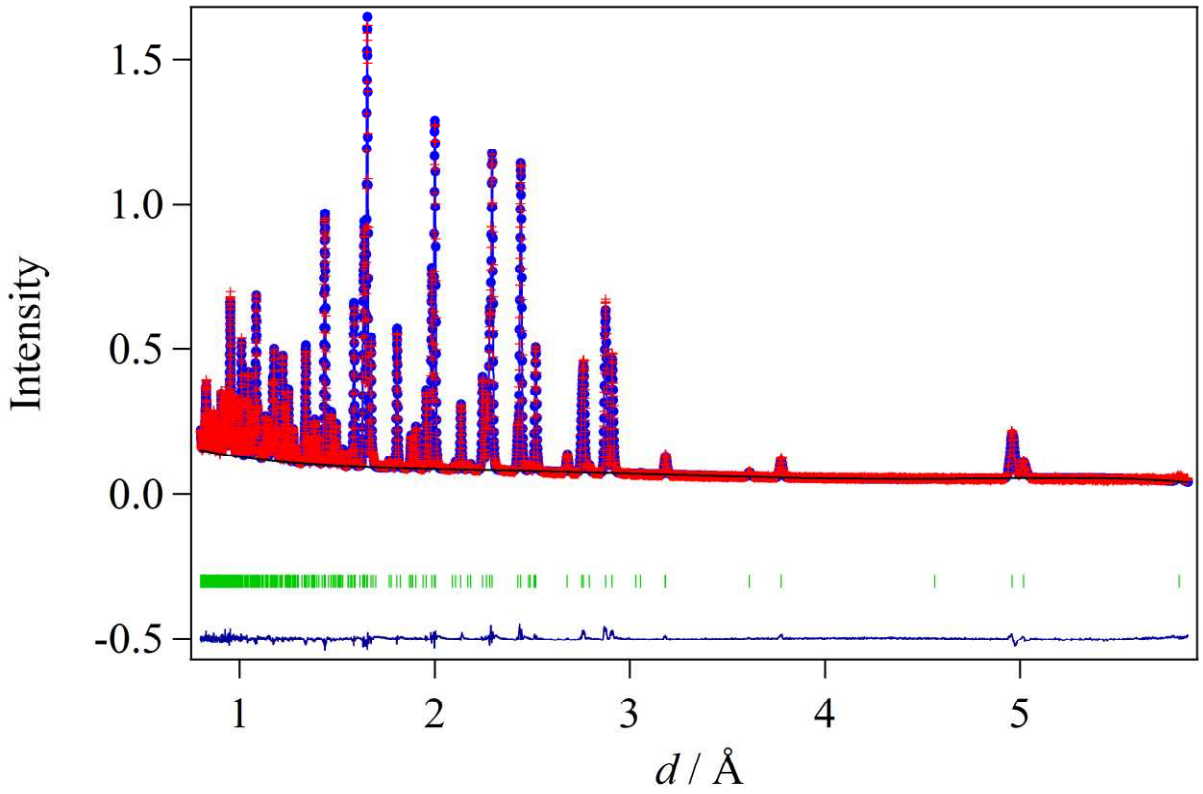

Figure 1 : Rietveld profile pattern of RSrInO$_4$ (R is a rare earth element). Measurement time : 40 min, sample weight 3.85 g.