 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014B0114 実験課題名 Crystal Structure Analysis of Novel $A_3B_{11}O_{20}$ -Based Oxide-Ion Conductors 実験責任者名 Name of principal investigator Masatomo Yashima 所属 Affiliation [Present] Department of Chemistry, School of Science, Tokyo Institute of Technology [Previous] Department of Chemistry and Materials Science, Graduate School of Science and Engineering, Tokyo Institute of Technology	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 November 26- November 28, 2016

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 $AA'BO_4$, and ABO_4 -type metal-oxides, which are oxide-ion conductors or its related materials. Here A and A' are relatively large cations such as rare earth ions and alkaline earths ions and B is relatively small cations.
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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 oxide-ion conducting metal-oxides 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 samples were put into 6 mm ϕ vanadium sample holders and were used for the diffraction measurements. The diffraction measurements were carried out with double frame mode. Experimental results In 2014, we discovered a new type of oxide-ion conducting material $NdBaInO_4$. Recently, we have synthesized several new materials which have $NdBaInO_4$ -type structure. 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 $AA'BO_4$ were characterized by indexing and Le Bail analysis. Then the crystal structures of $AA'BO_4$ were refined using the structural model of related materials.

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 $AA'BO_4$ 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. 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.

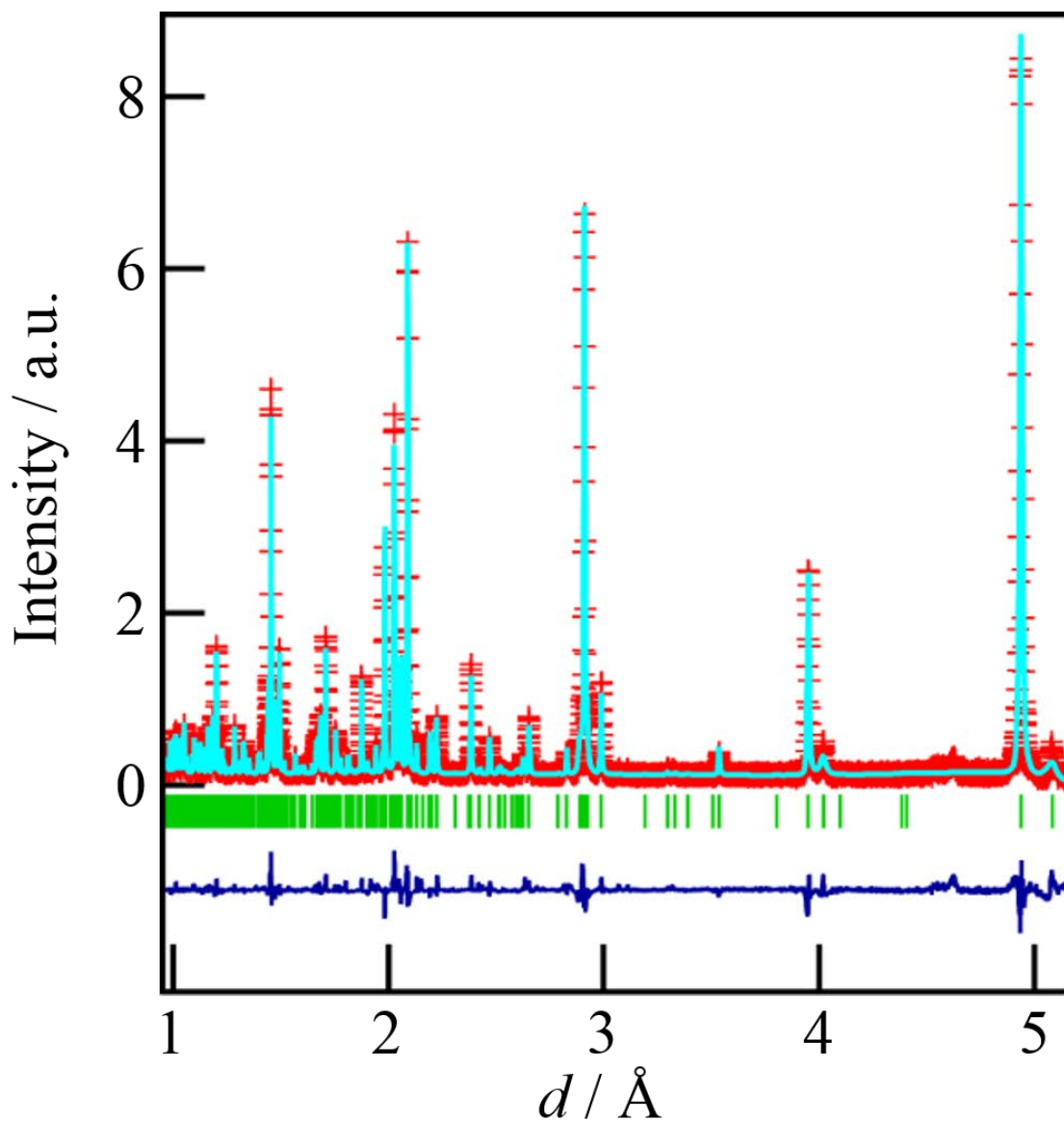


Figure 1 : Rietveld profile pattern of $AA'BO_4$.