MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2013B0198 実験課題名 Structural Understanding of the Electrical Properties in the Novel Structural Typed Mixed-Ionic and Electronic Conducting Materials 実験責任者名 Name of principal investigator Kotaro Fujii 所属 Affiliation 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 Takashi Kamiyama 装置名 Name of Instrument/（BL No.） SuperHRPD / BL-08 実施日 Date of Experiment March 27-April 1, 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.

$AA'BO_4$- and $A_3B_{11}O_{20}$-based materials (*A*: large cations such as rare earth La, Pr, Nd, Y, Ho, Yb and Ba, Sr, Ca; *B*: smaller cations as In, Ge, Ga, Ta, W).

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 $AA'BO_4$- and $A_3B_{11}O_{20}$-based materials were measured at room temperature and high temperature by a high-resolution neutron powder diffractometer SuperHRPD installed at the beam line BL08 of J-PARC facility, Japan. The sintered or the powder samples were put into 10 mm ϕ vanadium sample holders and were used for the diffraction measurements. The diffraction measurements were carried out with five frame mode.

Experimental results

TOF-neutron data of Sr_2TiO_4 measured at 23 °C were analyzed using the program Z-Code. As shown in Figure 1, it gave good quality of fitting and *R*-factors; R_{wp} = 10.16 % and R_B = 5.06 %). The anisotropic displacement parameters were successfully determined and the crystal structure of $SrTiO_4$ at room temperature has been determined precisely. High-temperature data were, then, analyzed in the same manner. However, the absorption of vanadium furnace would cause the energy dependent absorption and the structural analysis for high-temperature data have not been

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

completed. Now, we try to solve the absorption problem. At this stage, we could not obtain a good quality fitting and result from the high-temperature data. Especially, displacement parameters do not converge into the reasonable values.

Sr_2TiO_4 is most simple sample among measured sample. Thus, success of the structural analysis for Sr_2TiO_4 is necessary for the following structural analysis. As we'd like to reveal the structure and oxide-ion conducting behavior for new oxide-ion conducting materials, we first carefully exam the crystal structure analysis of Sr_2TiO_4 measured at several different temperature points.

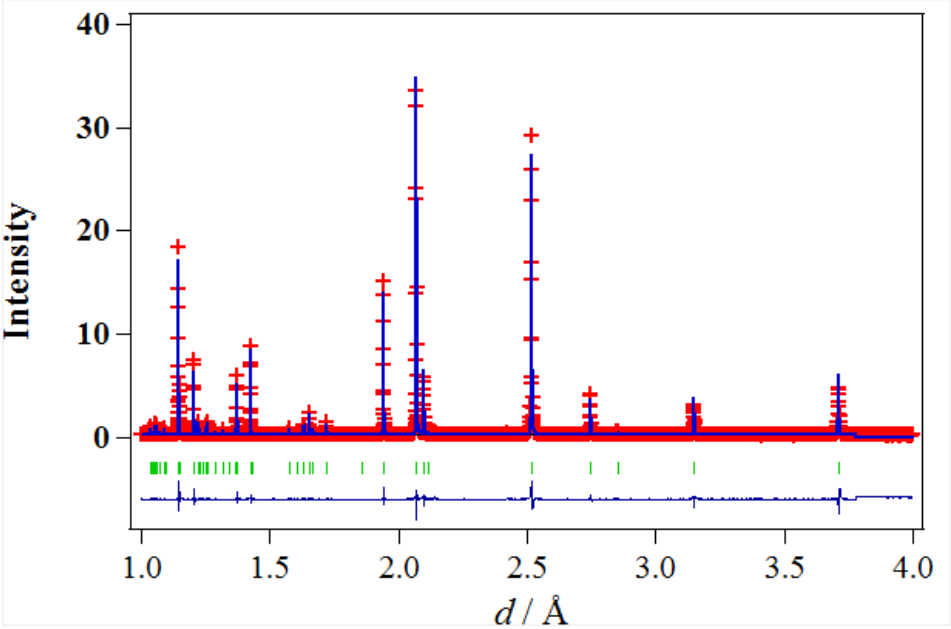

Figure 1：Rietveld plot of $SrTiO_4$ measured at 23 °C.