MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2009AP0010 実験課題名 Title of experiment Observation of "charge amorphous" in charge frustrated system LaPd2O4 by means of PDF analysis 実験責任者名 Name of principal investigator Katsuaki Kodama 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/(BL No.) iMATERIA/(BL20) 実施日 Date of Experiment 2010/5/28-29

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.

BaBiO3

Ba0.8K0.2BiO3

V

All samples are powders.

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.

The measurements of powder diffraction were performed for all samples. All samples were mounted in a closed-cycle refrigerator. Data of $BaBiO_3$ and V were collected at room temperature and data of $Ba_{0.8}K_{0.2}BiO_3$ were collected at 10 K, 150 K and room temperature. All diffraction data were corrected for about 4 hours because we need precise intensity data over wide Q-range, which can be transformed to the atomic pair distribution function (PDF). V-data were collected in order to estimate the absolute values of diffraction intensities of $BaBiO_3$ and $Ba_{0.8}K_{0.2}BiO_3$, which are necessary to get PDF.

The diffraction patterns of $BaBiO_3$ and $Ba_{0.8}K_{0.2}BiO_3$ observed at room temperature are shown by red crosses in Figs. 1(a) and 1(b), respectively. The reported crystal structures of $BaBiO_3$ and $Ba_{0.8}K_{0.2}BiO_3$ are monoclinic and orthorhombic structures, respectively. The preliminary results of the analyses using Z-Rietveld based on the reported structure models are shown by the black solid lines in the figures. The calculated lines almost reproduce the observed data for both samples. The structural parameters, lattice constants and atomic positions obtained by using Z-Rietveld, are almost consistent with the parameters determined by the analysis on the diffraction data which are collected by using HRPD at JRR-3.

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

In $Ba_{0.8}K_{0.2}BiO_3$, unexpected peak splits are observed in several diffraction peaks at low temperatures, suggesting the some structural phase transition. However, the structural phase transition has not been observed in $Ba_{0.8}K_{0.2}BiO_3$ below room temperature in the current studies on this compound. The crystal structure at the low temperature is considered to be monoclinic because the diffraction patterns at low temperatures are similar to the diffraction patterns of $BaBiO_3$. However, the successful fitting are not obtained by using the structural model same as $BaBiO_3$. Further analysis using possible structural models is necessary for the determination of the structure of $Ba_{0.8}K_{0.2}BiO_3$ at low temperatures.

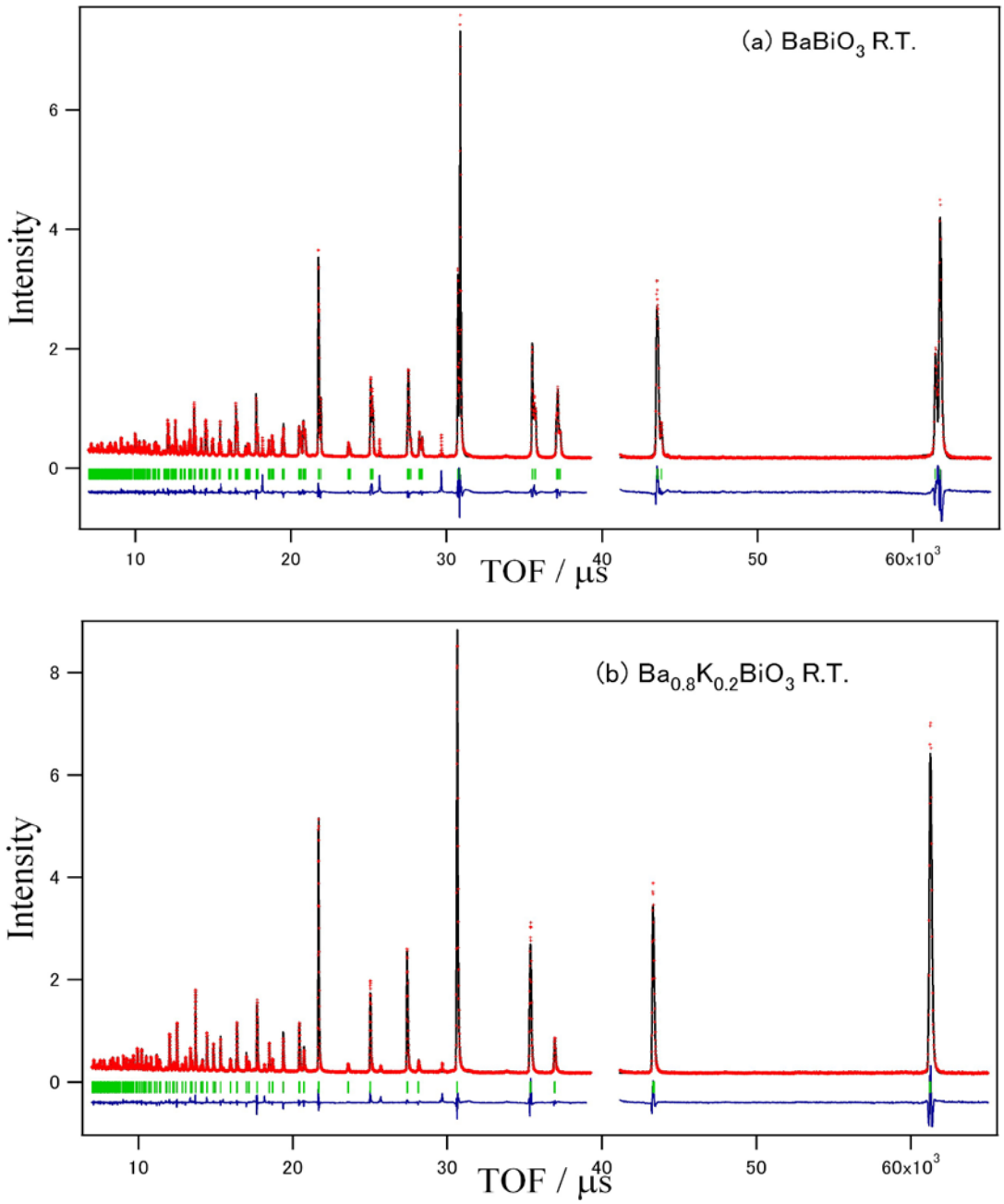

Fig. 1 Observed (red crosses) and calculated (black solid lines) diffraction patterns of BaBiO3 (a) and $Ba_{0.8}K_{0.2}BiO_3$ (b) at room temperature. Vertical bars show the calculated positions of Bragg reflections. The blue solid lines at the bottom of the figures are the difference between observed and calculated intensities.