MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2008A0069 実験課題名 Title of experiment Ferroelectric transition on breaking quantum paraelectricity in $SrTiO_3$ 実験責任者名 Name of principal investigator Yukio Noda 所属 Affiliation IMRAM Tohoku University	装置責任者 Name of responsible person T. Kamiyama 装置名 Name of Instrument/(BL No.) BL08 SHRPD 実施日 Date of Experiment 2009.2.20-2009.2.23

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.

Powder sample of $SrTiO(18)_3$ was prepared by replacing oxygen atoms with isotope oxygen-18 in a sealed tube at high temperature for few months, by Professor Ito of TITEC. Prepared sample is kept in a vanadium can filled with He gas.

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.

Neutron powder diffraction of $SrTiO(18)_3$ was performed at BL08 (SHRPD) for 3 days. During the experiments, the condition of the accelerator was not so good and the beam was available for about 24 hours with the power 18kW. We have taken the data at 10K, 60K and 124K. The intensity statistics is not enough but we could take a preliminary data. Obtained data were analyzed by using the program Z-code. The analyzed data for 124K, high temperature Pm-3m phase is shown in Fig. 1. Fitting seems about satisfactory, but still we need improvement because profile functions are slightly insufficient to reproduce each peak. Obtained resolution $\Delta d/d$ is about 0.1%. To extend the procedure to the low temperature phase, I4/mcm tetragonal phase at 60K, we fixed all of the profile functions by the data obtained at the cubic phase, simply to reduce the number of the fitting parameters. Further, we tried structure analysis of the lowest ferroelectric phase, 10K, as the same manner.

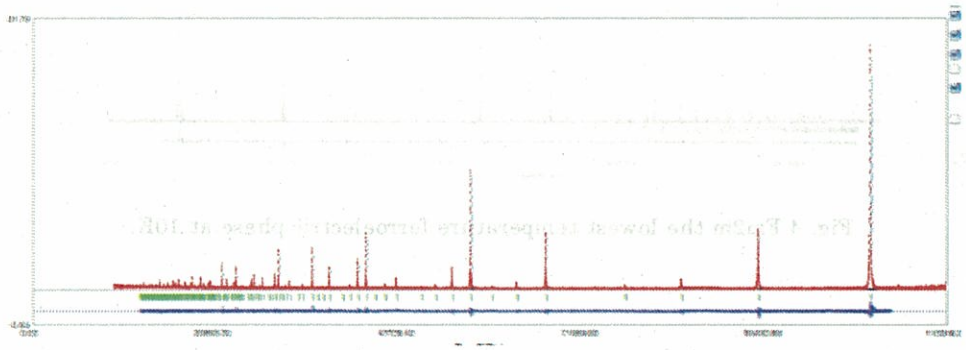

Fig. 1 Pm-3m high temperature phase

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

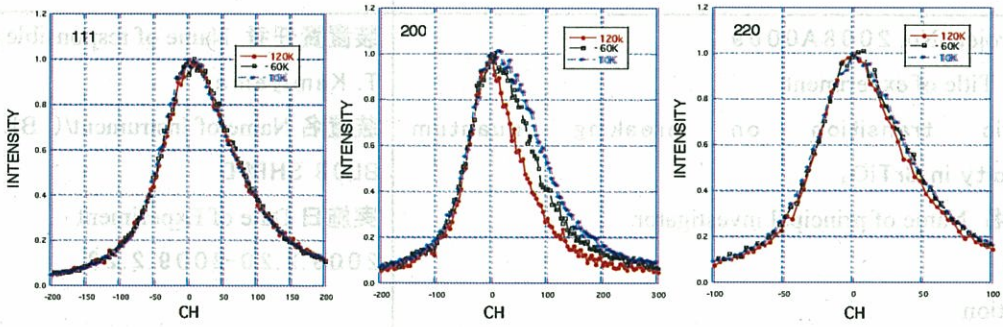

Fig. 2 (111), (200) and (220) peaks indexed with cubic cell for T=124K, 60K and 10K.

The ferroelectric phase is unknown phase and most interesting phase to consider the phase transition mechanism of the perovskite structure. We assumed orthorhombic unit cell, and the possible space group is Fm2m(2a x 2b x 2c cell) or I2cm($\sqrt{}$a x $\sqrt{}$b x 2c cell). In Fig.2, three typical indices (111), (200) and (220) peaks taken at 124K, 60K and 10K are shown. Since (111) seems to be a single peak for all of phases, the unit cell at 10K might be tetragonal or orthorhombic with 2a x 2b x 2c cell. The space group at 60K is well established and I4/mcm with a $\sqrt{}$a x $\sqrt{}$b x 2c cell. Thus, (200) peak has two components at 60K, (220) and (004) referred to the tetragonal unit cell. Z-code analysis was performed for the data taken at 60K. Fitting is almost the same level with that shown in Fig.1 of the cubic phase. Question is that the profile of (200) or (400) peak at 10K can be decomposed to two peaks or three peaks. Both models gave the solution for least square fitting procedures with Gaussian profiles, as shown in Fig.3. It seems that two peaks corresponding to Ic2m space group is favorable. In Fig.4, we will show the Z-code analysis result by assuming Fm2m space group (2a x 2b x 2c unit cell). Other possibility of I2cm space group was also tried but the fitting seem to be the same level. We definitely require better resolution and better statistics to distinguish them.

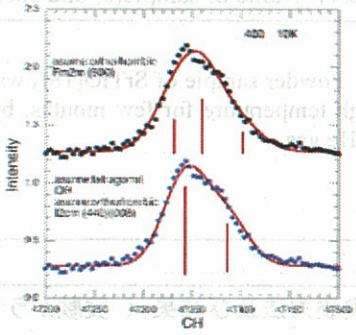

Fig.3 (400) peaks at 10K.

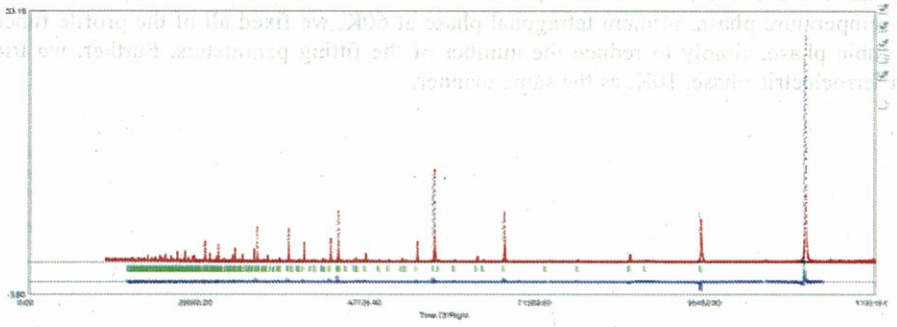

Fig. 4 Fm2m the lowest temperature ferroelectric phase at 10K.