実験報告書様式（一般利用課題・成果公開利用）

（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。）

# MLF Experimental Report	提出日 Date of Report 2012/12/15
課題番号 Project No. 2012A0017 実験課題名 Title of experiment Investigation of possible disorders in multiferroic Pb(Fe0.5Nb0.5)O3) 実験責任者名 Name of principal investigator Je-Geun Park 所属 Affiliation Seoul National University, Korea	装置責任者 Name of responsible person Je-Geun Park 装置名 Name of Instrument/（BL No.） NOVA/BL21 実施日 Date of Experiment 2012/05/16 – 2012/05/19

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.

$PbFe_{0.5}Nb_{0.5}O_3$, powder

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.

Lead Iron Niobate $Pb(Fe_{0.5}Nb_{0.5})O_3$ (PFN) is a multiferroic disordered system. It is known to have a G-type antiferromagnetic transition at T_N=143 K [1] and a ferroelectric transition at T_C=385 K [2]. Near T_N, it shows a dielectric constant anomaly, which shows frequency dependence [1]. Because of its high dielectric constant it can be used in multilayer ceramic capacitors and other electronic devices [3]. Despite the interesting properties, there is still controversy over the room temperature structure: two possible space groups of R3m and Cm structure were proposed [4,5]. More importantly, it is not clear at all whether this material has Pb-disorder above the ferroelectric transition temperature. It is also interesting that negative thermal expansion behavior was reported below the antiferromagnetic transition [6].

In order to understand the properties and resolve some of controversy, we measured the crystal structure using a high resolution powder diffractometer, S-HRPD, to find that there is no negative thermal expansion behavior in our data unlike the reported results. However, our S-HRPD data could not be used to examine a possible Pb disorder effect. Thus the main purpose of this experiment carried out at NOVA was to determine both long- and short-range order simultaneously at room temperature. We also intended to examine a possible coupling mechanism between magnetism and electric polarization near T_N.

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

We used a total of 6.5g polycrystalline $Pb(Fe_{0.5}Nb_{0.5})O_3$ and carried out the total scattering measurements at 62, 127, 172, 298, and 453 K with the Q coverage of from 1 to 82 Angstrom−1. For the analysis of the long-range average structure, we used Fullprof while we employed Pdfgui to fit the radial distribution function. From our analysis, we conclude that it forms in the usual P m −3 m structure above the ferroelectric transition. But both R3m and Cm structures seem to fit our S-HRPD and NOVA data equally well below T_C. With further cooling new magnetic super lattice peaks emerge below T_N, which our analysis finds to be consistent with a G-Type antiferromagnetic ordering (Fig. 1).

On the other hand, we found several interesting features in the temperature dependence of the radial distribution data. First we can see a shoulder-type structure at r = 4 Å, which can be regarded as arising from Pb disorder above T_C (Fig 2). Second, we also observe that a peak at r = 2Å becomes asymmetric with cooling, which we think is related to possible oxygen octahedral motions (Fig. 2). However, we have tried to fit the radial distribution function with one of the long range structures (Fig. 2 right) and found that there exists certain discrepancy between the experimental data and our fitting results. We can see that several peaks cannot be explained well by the long range structure changes (Fig.2 blue arrow). This clearly indicates that the current model is not correct and we need to incorporate a local structure model in our analysis.

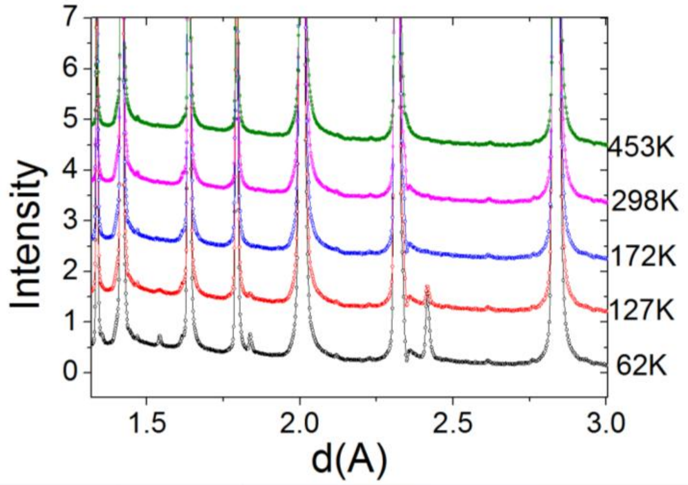

Fig. 1. With lowering temperature, new magnetic peaks emerge in consistent with a G-type structure (right, blue arrow) and these peaks show temperature dependency(left).

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

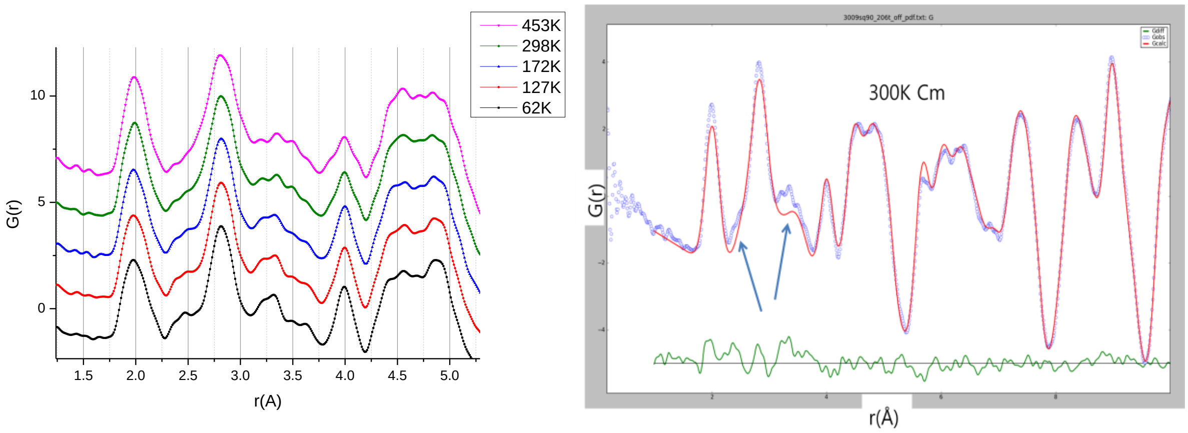

Fig. 2. Temperature dependence of radial distribution functions that cannot be explained by one of the long range structures.

Currently, we are trying to combine the long range structure with a local structure modeling in our analysis to explain both S-HRPD and NOVA data simultaneously. Once we are successful, we then will be able to understand the multiferroic phenomena in this material.

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