MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2015A0061 実験課題名 Title of experiment Local structural analysis on parent compound of iron-based superconductor, PrFeAsO 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 Toshiya Otomo 装置名 Name of Instrument/（BL No.） NOVA (BL21) 実施日 Date of Experiment 2016/6/7-8

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.

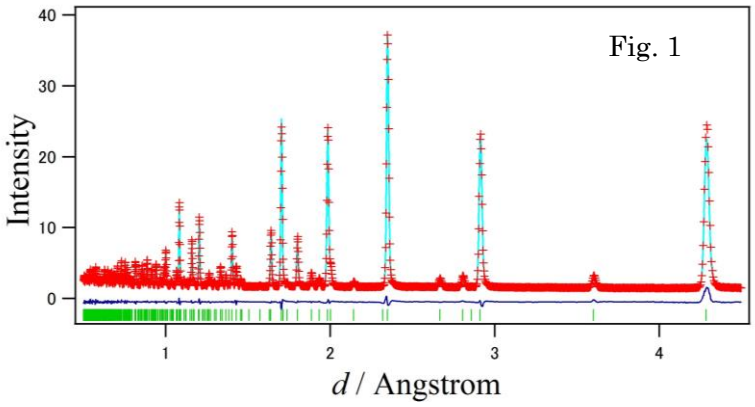
Parent compound of iron-based superconductor, PrFeAsO powder

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.

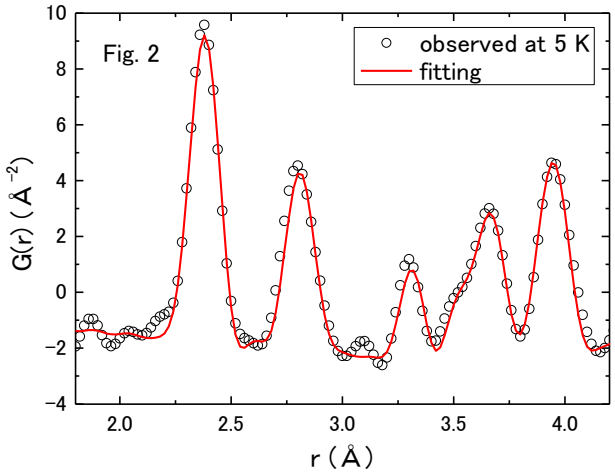
The parent compound of iron-based superconductor PrFeAsO exhibits the structural phase transition from the tetragonal to orthorhombic structure at about 140 K. The Fe and Pr moments have antiferromagnetic ordering below about 130 K and 12 K, respectively. In the Mossbauer spectroscopy, the amplitude of the electric field gradient at Fe nuclear rapidly decreases accompanied with the magnetic ordering of Pr moment.[1] This rapid decrease of the electric field gradient have been explained by the reorientation of the Fe moment; the Fe moment has large component along *c*-direction below 12 K, although the moment is parallel to a-axis above 12 K.[1], [2] However, if the change of the electronic state of Fe 3d electron causes the change of the electric field gradient, it can be related to the nematicity which is one of the most interesting issues in the iron-based superconductors. Then, we have planned to investigate the change of the electronic state of Fe 3d electron through the structural information. Because the orthorhombic lattice distortion is remarkable in the local structure obtained by the atomic pair distribution function (PDF),[3] we have performed PDF analysis on powder neutron diffraction data of PrFeAsO obtained by using NOVA.

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

The diffraction data were collected at 5, 20 and 160 K. Figure 1 shows the diffraction pattern at 160 K and the fitting result by Rietveld analysis. In the analysis, the intensity obtained at 90 degree bank is used. The line calculated using reported tetragonal structure with a space group P4/nmm almost reproduces the observed diffraction pattern. The diffraction patterns at 20 K and 5 K are fitted by the reported average structure with a space group Cmma.



In Fig. 2, the atomic pair distribution function G(r) obtained at 5 K is shown by open circles. The Bragg reflection at the smallest Q position (～0.7 $Å^{-1}$) cannot be detected by 90 degree bank. To obtain G(r), the structure function S(Q) obtained at 90 degree bank with 1.1 < Q < 40 $Å^{-1}$ is connected with S(Q) obtained at 45 degree bank with 0.6 < Q < 1.1 $Å^{-1}$. The red line shows the fitting result using the structure with Cmma corresponding with the averaged structure. The line almost reproduces the observed G(r). The lattice parameters obtained by the fitting are roughly consistent with the parameters obtained by the Rietveld analysis. To investigate the change of the local structure accompanied with the magnetic ordering of the Pr moment and the discrepancy between the local and average structures, the detailed local structural analysis should be performed on the data obtained at several temperature.



References

[1] McGuire et al. New J. Phys. 11, 025011 (2009).

[2] Maeter et al., Phys. Rev. B 80, 094524 (2009).

[3] Niedziela, McGuire, and Egami, Phys. Rev. B 86, 174113 (2012).