MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2017A0074 実験課題名 Title of experiment Relationship between the local lattice distortion with Aem2 symmetry in parent compound and higher Tc in iron-based superconductor 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 2017/6/18-21

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 compounds of iron-based superconductors, LaFeAsO and NdFeAsO 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.

We have observed the local lattice distortion in the parent compound of iron-based superconductor PrFeAsO in the previous measurement (2015A0061). The broad Pr-As atomic correlation peak observed in the atomic pair distribution function (PDF) at 20 K cannot be reproduced by the averaged structure with space group Cmma, and can be reproduced by the structure model with space group Aem2, indicating the existence of the local lattice distortion with symmetry Aem2. This space group is the same as the space group of the overdoped antiferromagnetic phase, AF2, in $LaFeAsO_{1-x}H_x$ ($x>0.4$) [1]. In $LaFeAsO_{1-x}H_x$ system, two superconducting phases SC1 and SC2 appear at x～0.1 and x～0.33[2]. The AF2 phase is regarded as the parent phase of the SC2 phase. The maximum value of Tc of the SC2 phase (～36 K) is larger than the value of the SC1 phase (～26 K). The maximum Tc of the superconducting phase of Pr1111 systems whose parent compound PrFeAsO has the local lattice distortion with Aem2 symmetry, is about 50 K which is one of the highest values among iron-based superconductors. These results suggest that the long and short-range lattice distortions with Aem2 symmetry in the parent phase advantageous to higher Tc in the superconducting phase. To reveal the relationship between the Aem2 lattice distortion in the parent phase and Tc-value in the superconducting phase,

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

parent compounds LaFeAsO and NdFeAsO whose maximum Tc-values in the superconducting phases are about 26 K and 50 K, respectively, are studied by PDF analysis.

The powder diffraction measurements have been performed at NOVA. The data were collected at 5, 20 and 160 K, for both samples. To obtain the PDF, 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 $Å^{-1}$. In Fig. 1, PDF of LaFeAsO at 20 K is shown by open circle. The blue line is the PDF calculated by using the average structure with space group Cmma. The line almost reproduces the observed PDF. The red line is the PDFs calculated by using the structure models with space group Aem2. The red line almost overlap with the blue line. The estimated values of the atomic shifts of Fe and As along a-direction giving the breaking the inversion symmetry are much smaller than the atomic shifts in PrFeAsO. These indicate that the local lattice distortion with Aem2 symmetry is negligibly small in LaFeAsO, supporting the above suggestion on the relationship between the local lattice distortion and maximum Tc-value. The local structural analysis on NdFeAsO is being performed to further reveal the validity of the above suggestion.

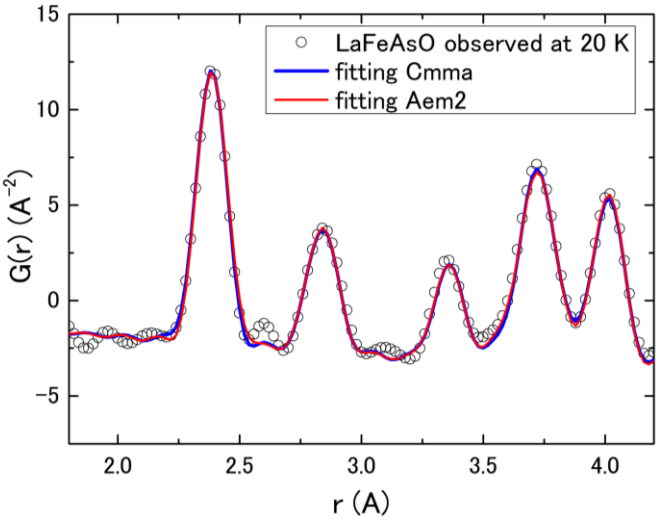

Fig. 1 PDF of LaFeAsO obtained at 20 K (open circle). Blue and red lines are the PDFs calculated by using the structure models with space groups Cmma and Aem2, respectively

references

[1] M. Hiraishi et al. Nature Physics 10, 300 (2014).

[2] S. Iimura et al., Nature Commun. 3, 943 (2012).