

 MLF Experimental Report	提出日 Date of Report 2013/4/15
課題番号 Project No. 2012B0045 実験課題名 Title of experiment Observation of charge glass state in $\text{Sr}_3\text{Fe}_2\text{O}_7$ by using PDF (atomic pair distribution function) 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 Toshiya Otomo 装置名 Name of Instrument/(BL No.) NOVA (BL21) 実施日 Date of Experiment H25/3/5-6

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 $\text{Sr}_3\text{Fe}_2\text{O}_{7-\delta}$ ($\delta \sim 0.08$) (2.2g)

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.
<p>$\text{Sr}_3\text{Fe}_2\text{O}_7$ exhibits metal-insulator transition at about 340K. In the insulating phase below 340K, Fe sites with valences of +3 and +5 are observed by Mossbauer spectroscopy whereas all Fe sites are equivalent above 340K. However, structural phase transition and/or superlattice reflections are not observed in the diffraction pattern at 340K, and all Fe sites are crystallographically equivalent in the averaged structure whole temperature region. These results suggest that the 3d electrons are localized at Fe sites like a glass and the arrangement of Fe^{3+} and Fe^{5+} has short range correlation.</p> <p>In order to detect the local lattice distortion caused by such glass-like electron localization we have performed PDF (atomic pair distribution function) analysis on powder neutron diffraction data of $\text{Sr}_3\text{Fe}_2\text{O}_{7-\delta}$ ($\delta \sim 0.08$) obtained by using NOVA. The diffraction data were collected at 160, 230, 300 and 390K. Figure. 1 shows the diffraction patterns at all temperatures and their fitting results by using z-Rietveld. In the analyses, the reported tetragonal structure with a space group $I4/mmm$ which has a single Fe site are used. The calculated lines reproduce the observed diffraction patterns, indicating that the averaged structure does not change below 340K</p>

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

as reported by preceding studies. In Fig. 2, the PDFs at all temperatures are shown by open circles. The solid lines are fitting results by using the averaged structures which are determined by the Rietveld analysis at each temperature. Even below 340K, the lines almost reproduce the observed PDFs, indicating that “apparent” local lattice distortion which is expected from the glass-like localization of 3d electrons is not observed in PDF.

However, as shown in Fig. 3, weighted R factor, R_{wp} , obtained by PDF analysis increases with decreasing temperature. It suggests that the local structure is not fitted perfectly by using averaged structure and slight local lattice distortion may exist at lower temperatures. If R_{wp} increases below 340K as shown in the figure by the guide line, the slight local lattice distortion is caused by the localized electrons like a glass with short range correlation.

