MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2013A0068 実験課題名 Title of experiment Observation of self-organization process of “charge glass state” in $^{7}LiMn_2O_4$ by using PDF 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 2013/4/30-5/1

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 ^{7}Li-enriched $^{7}LiMn_2O_4$

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.

$LiMn_2O_4$ exhibits a structural phase transition from cubic structure with space group Fd3-m to orthorhombic structure with Fddd at around 260K with decreasing temperature. In the orthorhombic phase, the system is in the charge ordering state because inequivalent Mn sites with the valences of +3 and +4 arrange periodically [1]. However, even in the cubic phase, the electrical resistivity is not metallic although all Mn atoms are equivalent and their valence is +3.5 [2]. These results suggest that the valence electron of Mn site is localized like a glass and the arrangement of Mn^{3+} and Mn^{4+} has only short range periodicity in the cubic phase. Actually, atomic pair distribution function (PDF) of $^{7}LiMn_2O_4$ in cubic phase (at 300K) obtained at NOVA, can be reproduced by orthorhombic structure with Mn^{3+} and Mn^{4+}, supporting above suggestion [3].

In this beam time, we have performed powder neutron diffraction measurements on $^{7}LiMn_2O_4$ at above 300K in order to investigate the temperature (T) development of the orthorhombic local lattice distortion caused by the localization of valence electron with the short range periodicity. Fig. 1 shows the temperature dependence of PDF in the temperature region of $200 < T < 450$K. The data at 200K is obtained at iMATERIA. The shape of the PDF is almost independent of T. Mn-O distances averaged in five kinds of inequivalent MnO_6 octahedra

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

which are estimated by the local structural analysis on the PDF is also independent of *T* as shown in Fig. 2, indicating that the local lattice distortion and the distribution of the electrons localized at Mn sites are almost independent of *T*, in the whole *T*-region including the orthorhombic phase at low temperature.

[1] Rodriguez-Caravajal et al. Rhys. Rev. Lett. 81 (1998) 4660.

[2] for example, Sugiyama et al. J. Phys. : Condens. Matter 9 (1997) 1729.

[3] Kodama et al. J. Phys. Soc. Jpn. 82 (2013) 094601.