MLF Experimental Report	提出日 Date of Report June 30, 2011.
課題番号 Project No. 2010B0094 実験課題名 Title of experiment High-resolution neutron diffraction study of $La_2O_2Fe_2OSe_2$ 実験責任者名 Name of principal investigator Sungdae Ji 所属 Affiliation Tohoku University	装置責任者 Name of responsible person Takashi Kamiyama 装置名 Name of Instrument/（BL No.） BL-08 実施日 Date of Experiment 2011/01/31 11:00 - 2011/02/02 11:00

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.

Fe-oxychalcogenide ($La_2O_2Fe_2OSe_2$) 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.

Recently, a Mott-insulating Fe-oxychalcogenide ($La_2O_2Fe_2OSe_2$) has drawn a lot of attention with respect to an abnormal magnetic ground state behavior. It crystalizes in tetragonal, I4/mmm structure and has magnetic transition at T_N = 90 K. The magnetic structure below transition temperature forms double diagonal stripe magnetic order which is geometrically frustrated up to the 2nd nearest neighbor interaction and has been exceptionally realized in metallic but iso-structural $Fe_{1+y}Se_xTe_{1-x}$ among Fe-based superconductors. While the magnetic frustration effect in Fe- is still controversial due to de-localized electrons and lattice distortion accompanied by the magnetic order, that in $La_2O_2Fe_2OSe_2$ has been believed to be very strong since electron are localized and lattice distortion has not been observed. There have been experimental reports showing some precursors of magnetic frustration effect. Curie-Weiss temperature obtained from the inverse magnetic susceptibility is 650 K seven times higher than T_N and we observed a strong spin fluctuation still exists even at 300 K above T_N, which implies that magnetic frustration suppresses to form a long-range order below Curie-Weiss temperature being consistent with the magnetic susceptibility measurement. A heat capacity measurement showed that the magnetic entropy is not fully released by magnetic transition which indicates

still remains below magnetic transition, but it has not been examined by a microscopic measurement. Moreover, if we remind that most geometrically frustrated magnets undergo a structural transition when they form a full or partial magnetic order, it is demanded to re-confirm existence of structural distortion using higher-resolution diffractometer.

Our main goals are 1) to find a magnetic frustration effects below magnetic transition such as magnetic peak broadening and 2) to confirm global or local distortion of crystal structure in Fe-oxycha using BL-8 beamline in J-PARC, a time-of-flight powder diffractometer with high flux and resolution. Since magnetic Bragg peaks appear mostly in the lower-Q region but lattice distortion effect is more distinctive in the higher-Q region, three detector banks were utilized simultaneously for the purpose. Temperature dependence of whole powder patterns cover to from 5 K to 300 K using a closed-cycle refrigerator.

Fig. 1 shows a selected region of the powder pattern at T = 5 K with the lower bank. While the peak profile of nuclear Bragg peaks is a shape of Gaussian and resolution limited, that of magnetic Bragg peaks is a shape of Lorentzian and broader than nuclear Bragg peaks. This indicates that magnetic order $La_2O_2Fe_2OSe_2$ is suppressed by geometrical magnetic frustration in magnetically ordered phase. More quantitative analysis is now on process. However, as shown in Fig. 2, it is confirmed that any clear change of lattice distortion below and above T_N was not observed even using the back scattering bank which is the option of highest instrumental resolution in BL-8. The result gives us clear evidences that $La_2O_2Fe_2OSe_2$ is the first system realizing a frustrated double diagonal stripe magnetic order without a lattice distortion and moreover, it will shed light on understanding of geometrical frustration effect on newly emerged Fe-based superconductors.

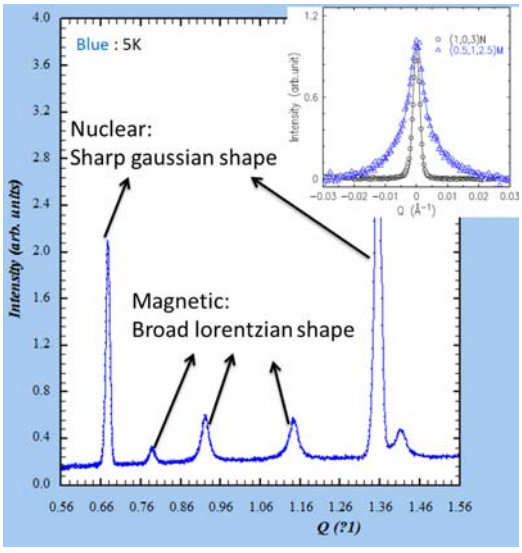

Fig. 1: Selected region of powder pattern at 5 K

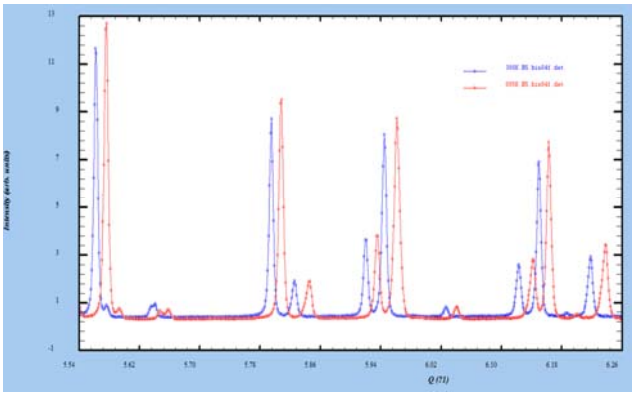

Fig. 2: powder patterns of 5 K and 300 K in high-Q region