MLF Experimental Report

課題番号 Project No. 2012A0045 実験課題名 Title of experiment Magnetism and Superconductivity in $Rb_xFe_{2-y}Se_2$ 実験責任者名 Name of principal investigator Kazuki Ohishi 所属 Affiliation CROSS	提出日 Date of Report 装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/（BL No.） iMATERIA 実施日 Date of Experiment 2012/05/07 – 05/09

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.

Iron-based superconductor, $Rb_xFe_{2-y}Se_2$

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 recent discovery of superconductivity in iron selenide compounds $A_xFe_{2-y}Se_2$ (A = K, Rb, Cs), with transition temperatures up to $T_c \sim 32$ K, has led to a renewed interest for iron based chalcogenide systems. AFe_2Se_2 has $ThCr_2Si_2$ type crystal structure, isostructural to the 122-type iron pnictides. However, from the neutron powder diffraction (NPD) study, it was found that the chemically stable phase of $A_xFe_{2-y}Se_2$ is mainly contributed by $A_{0.8}Fe_{1.6}Se_2$ with a fivefold expansion of the parent $ThCr_2Si_2$ unit cell in the *ab* plane and a $\sqrt{5} \times \sqrt{5}$ Fe vacancy order. The ordered Fe-vacancy structure is accompanied by a strong magnetic order, with a transition around $T_N \sim 550$ K. The spin structure consists of antiferromagnetically (AF) coupled four-site ferromagnetic blocks, with large on-site moments of 3.3 μ_B. The key issue in $A_xFe_{2-y}Se_2$ is whether AF order and superconductivity cohabit due to phase separation or share a microscopic coexistence.

We have performed μSR measurements in single crystalline samples of superconducting (SC) $Rb_{0.8}Fe_{1.6}Se_2$ (T_c = 29 K) and non-SC $Rb_{0.8}Fe_{1.6}Se_2$, in order to elucidate whether there is difference of magnetic state between the SC and the non-SC samples and to answer above question (coexistence or phase separation). As a result, we found that (1) SC volume fraction in the SC sample is only ~6% and the rest is AFM phase, suggesting SC and AFM ordering is separated. It is consistent with a result of Rb-NMR, which is done by our collaborators.

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

(2) While no change in the μSR time spectra was observed in the SC sample, muon spin depolarization increases with decreasing temperature in the non-SC sample. It suggests the appearance of new magnetic state below 40 K, which is also consistent with Rb-NMR results, where the Rb signal disappears below ~40 K.

Our μSR and NMR results reveal two issues. (1) AF order and superconductivity cohabit due to phase separation. (2) New magnetic state appears below 40 K only in non-SC sample. In order to elucidate whether or not new magnetic state is a long-range ordered state, we have performed NPD measurements in the SC and the non-SC samples at BL20/iMATERIA in J-PARC/MLF. Figure 1 and 2 show the NPD results in the SC and the non-SC samples, respectively.

While the detailed analysis is still underway, we have found that multiple phases exist in the SC sample as shown in Fig. 1(a). It may correspond to the results observed by μSR and NMR which suggest the phase separation of SC and AFM. In the non-SC sample, more phases than those observed in the SC sample were observed. Comparing Fig. 1(a) with Fig. 2(a), the difference of phases is apparent. In the both samples, slight shifts of peaks corresponding to the temperature dependence of the lattice parameters were observed shown in Figs. 1(b) and 2(b). No new peak or broadening of peak was recognized at base temperature (7 K) in the SC sample, consistent with the μSR result which shows no change in the μSR time spectra. In the non-SC sample, however, a broadening of peak at Time of Flight ~ 34 ms, as shown in Fig. 2(b), was observed below 50 K. It suggests the magnetic ordering and is consistent with the results of μSR and NMR.

We are now proposing the next experiment in 2012B; we would like to measure the nuclear neutron diffraction pattern for the same SC and non-SC samples which we used this measurements in order to clarify the magnetic structure observed below 50 K in the non-SC sample. It is difficult to determine the magnetic structure observed in the non-SC sample at this stage, because multiple phases were observed in both samples shown in Figs. 1(a) and 2(a). In order to determine the new magnetic structure, we propose to measure NPD pattern at high temperature ($T > T_N$ = 550 K).

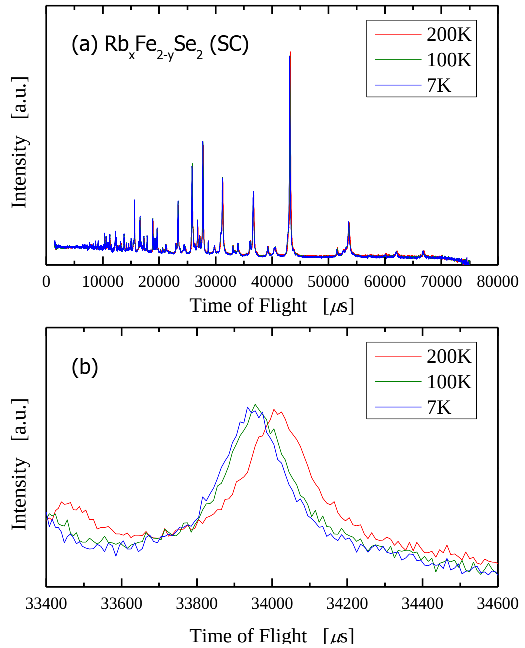

Fig. 1: Neutron powder diffraction patterns of the **SC** $Rb_{0.8}Fe_{1.6}Se_2$ obtained at several temperatures.

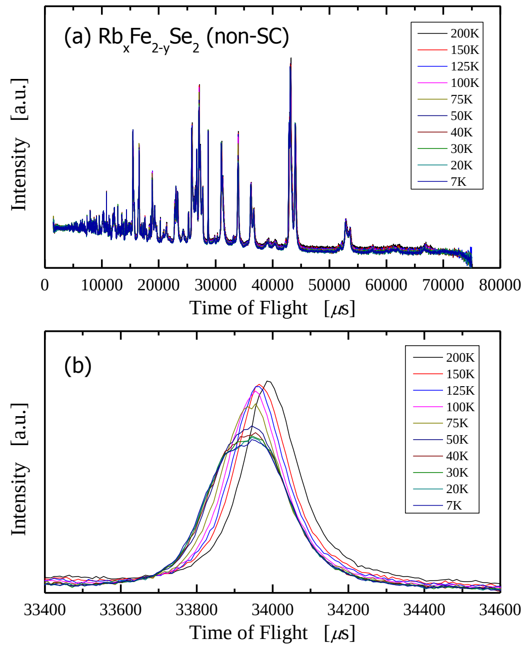

Fig. 2: Neutron powder diffraction patterns of the **non-SC** $Rb_{0.8}Fe_{1.6}Se_2$ obtained at several temperatures.