MLF Experimental Report

課題番号 Project No. 2014B0265	提出日 Date of Report
実験課題名 Title of experiment Magnetic Structure of $Cs_2Cu_2Mo_3O_{12}$ with CuO_2 ribbon chains	装置責任者 Name of responsible person Ishigaki, Toru
実験責任者名 Name of principal investigator Yasui, Yukio	装置名 Name of Instrument/（BL No.） iMATERIA
所属 Affiliation Meiji Universuty	実施日 Date of Experiment 2015/4/10 ～ 2015/4/13

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.

$Cs_2Cu_2Mo_3O_{12}$

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.

Magnetically frustrated quantum spin 1/2 chain system $Cs_2Cu_2Mo_3O_{12}$ with CuO_2 ribbon exhibits the ferroelectric transition at ~7.5K induced by applying the magnetic field. The nagnetic ground state of $Cs_2Cu_2Mo_3O_{12}$ have been found to be antiferromagnetic long range ordered state below antiferromagnetic transition temperature T_N=1.85K. This behavior is contrast to the nonmagnetic ground state for isostructural system $Rb_2Cu_2Mo_3O_{12}$. In order to understand the mechanism of multiferroic phenomenon and the reason why varies in ground state between $Cs_2Cu_2Mo_3O_{12}$ and $Rb_2Cu_2Mo_3O_{12}$, it is important to clarify the detailed magnetic structure of $Cs_2Cu_2Mo_3O_{12}$. We have carried out the powder neutron diffraction measurements by using neutron diffractometer (iMateria BL20).

First, we analyzed the obtained nuclear Bragg peaks at room temperature by Rietveld refinement, considering the crystal structure of $Rb_2Cu_2Mo_3O_{12}$. As a results of having analyzed it, we confirm that the crystal structure system of $Cs_2Cu_2Mo_3O_{12}$ is consistent with the reported crystal structure system by S. F. Solodovnikov *et al.*(J. Structual Chem. **38** (1997) 765-771.)

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

Next, we have measured the neutron diffraction patterns at T=12 K (> T_N) and T=0.58K (<T_N), which is shown in Fig. 1. All the observed peaks at 12 K correspond to the nuclear Bragg reflections of $Cs_2Cu_2Mo_3O_{12}$. At 0.58 K, the magnetic reflections derived from the antiferromagnetic ordering are observed at several nuclear Bragg *d*-positions, as shown in Fig. 1. The magnetic diffraction intensitis I_{mag} evaluated by difference intensity $I(T$=0.58K)-$I(T$=12K) are shown in Fig. 2.. We can assign all the observed magnetic reflections of $Cs_2Cu_2Mo_3O_{12}$ by displayed indices in Fig.2. As a results of preliminaly analysis of the magnetic Bragg peaks at 0.58K (< T_N), we have obtained the periodic spin cofiguration of 16 spins in a unit cell of $Cs_2Cu_2Mo_3O_{12}$. Figure 3 show the obtained periodic spin cofiguration of $Cs_2Cu_2Mo_3O_{12}$. The magnetic structure is call ed as “Neel state”, which is not a helical or a sinusoidal type. Now, we are quantitatively analyszing the detailed magnetic structure including the each spin direction.

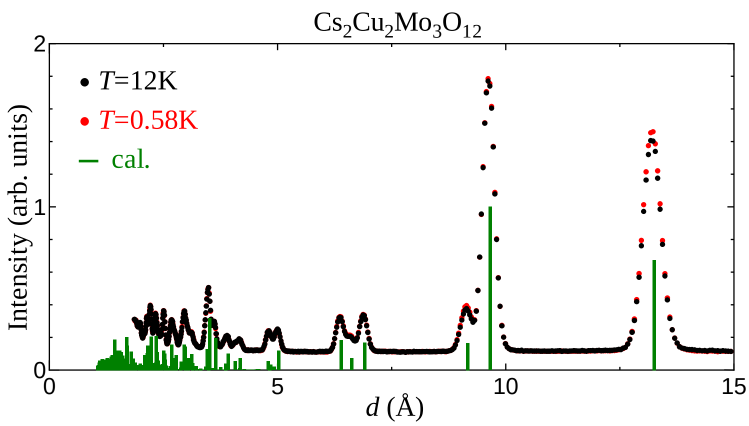

Fig. 1: Neutron powder diffraction patterns of $Cs_2Cu_2Mo_3O_{12}$ taken at T =12 K and 0.58 K. The bars indicate the calculated nuclear diffraction intensities and *d*-positions.

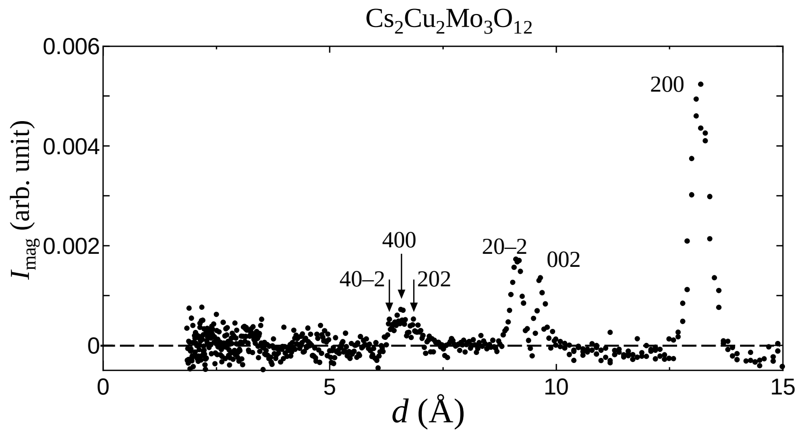

Fig. 2: Magnetic diffraction patterns of $Cs_2Cu_2Mo_3O_{12}$ evaluated by difference intensity $I(T$=0.58K)-$I(T$=12K) The observed magnetic reflection can be assigned by the displayed indices.

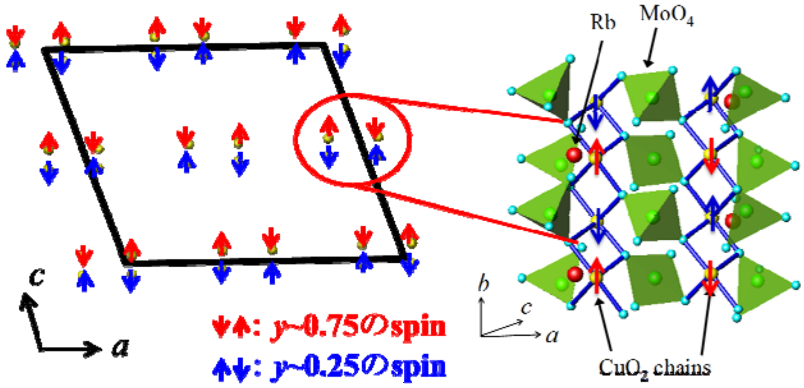

Fig. 3: Schematic figure of the periodic spin cofiguration of $Cs_2Cu_2Mo_3O_{12}$, which can reproduce the *d*-positions of the observed magnetic reflections. The determination of detailed magnetic structure including the each spin direction is in progress.