実験報告書様式(一般利用課題・成果公開利用)

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

MLF Experimental Report	提出日 Date of Report
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課題番号 Project No.	装置責任者 Name of responsible person
2014A0186	Shuki Torii
実験課題名 Title of experiment	装置名 Name of Instrument/(BL No.)
Magnetic structure of ferrimagnetic spinel compound CoV_2O_4	BL08
実験責任者名 Name of principal investigator	実施日 Date of Experiment
Hiroki Ishibashi	2014/5/16 21:00 - 2014/5/20 21:00
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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.

cobalt vanadate (CoV₂O₄) 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. Spinel vanadium oxide CoV_2O_4 shows ferrimagnetic transition at $T_C = 145$ K and another transition is observed at $T_1 = 60$ K, however, the origin of the transition at T_1 as well as the magnetic structure of CoV_2O_4 is still unclear.

Neutron powder diffraction experiments were performed using a time-of-flight (TOF) diffractometer at BL08 beamline. The temperature dependence of the powder patterns of CoV_2O_4 was measured in the temperature range of 10 - 300 K using a closed-cycle refrigerator. We measured the diffraction patterns with long scan time (10 h) at 160 K, 70 K and 10 K (set temperature) corresponding to the paramagnetic and two ferrimagnetic phases, respectively, to refine the magnetic structure and those with short scan (2 h) to investigate the temperature dependences of lattice constant and intensities of the magnetic reflections.

Figure 1 shows a part of the powder diffraction patterns at 12, 81 and 171 K (sample temperature) obtained by the back scattering bank. All peaks can be indexed with the space group Fd-3m, and neither forbidden reflection nor superlattice one was detected in the diffraction pattern. This result indicates that the clear structural phase transition does not occur in CoV_2O_4 unlike the similar compound such as MnV_2O_4 .

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

Figure 2 shows the temperature dependence of the lattice constant estimated by the peak positions of the Bragg reflections. An anomalous behavior is clearly observed at around T_1 , which may correspond to the phase transition at T_1 .

On the other hand, intensities of some peaks such as 220 and 311 reflections change with decreasing temperature as shown in Fig. 1. Figure 3 shows the temperature dependences of the intensities of 220 and 311 reflections. Abrupt increases in the intensities are observed at the ferrimagnetic transition temperature $T_c = 145$ K, caused by the magnetic ordering. However, it is unclear whether there is an anomaly at T_1 . We constructed the magnetic structure model of the ferrimagnetic phases based on the space group Fd-3m with the propagation vector $\mathbf{k} = (0, 0, 0)$ in order to refine them by the Rietveld method. The simplest model is the collinear configuration one, i.e., the magnetic moment of Co^{2+} is antiparallel to that of V³⁺. We carried out the Rietveld analysis by assuming the collinear model using the FullProf program. Figure 4 shows the result of the Rietveld fitting of the data at 81 K, and the fitting is almost good. The refined magnitudes of the magnetic moments of Co^{2+} and V³⁺ are 2.60(2) and 0.45(3) μ_{B} , respectively, which indicates that V³⁺ has much smaller magnetic moment than that expected from the spin moment (2 μ_{B}). The analysis based on of the non-collinear model is now in progress.



Fig. 1. Neutron powder diffraction patterns of CoV_2O_4 at 12, 81, and 171 K.



Fig. 3. Temperature dependence of the intensities for 220 and 311 Bragg peaks.



Fig. 2. Temperature dependence of lattice constant of CoV_2O_4 .



Fig. 4. Observed and calculated diffraction patterns at 81 K from the Rietveld refinement.