(※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 June 24, 2011
課題番号 Project No. 2010A0074	装置責任者 Name of responsible person
実験課題名 Title of experiment C o spin-state ordering in $Sr_{1-x}R_xCo_4O_{10.5}$ (*R*=Rare E arth)	装置名 Name of Instrument/(BL No.) BL08
実験責任者名 Name of principal investigator Hironori Nakao	実施日 Date of Experiment 2010/6/22 12:00 〜 2010/6/24 12:00
所属 Affiliation High Energy Accelerator Research Organization	

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.

$Sr_3YCo_4O_{10.5}$

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.

$Sr_{1-x}R_xCo_4O_{10.5}$ (R = Y and lanthanide, 0.2 < x < 0.25) has been found recently as a room temperature ferromagnet with T_C ~ 360 K, which is the highest T_C among perovskite Co oxides. The crystal structure is formed with the CoO_6 octahedral layers and the $CoO_{4.25}$ layers, which stack along *c* axis alternatively. Recently resonant x-ray scattering provides direct evidence of not only e_g orbital ordering but also the existence of the intermediate spin (IS) state of Co^{3+} ($3d^6$). It was suggested that the ferrimagnetism is induced by the e_g orbital ordering of the IS state. Moreover, the peculiar e_g orbital, spin-state, and magnetic orderings were proposed.

To clarify the ferromagnetism and the spin-state ordering, neutron magnetic scattering experiment is quite important. Therefore neutron powder diffraction experiments have been performed at BL08. Two successive structural transitions were already known at 509K and 360 K. The highest temperature phase is a tetragonal structure (HTT, space group: I4/mmm) of $2a_0 \times 2a_0 \times 4a_0$, where a_0 is the cell length of the primitive perovskite unit cell. The first transition at 509K is driven by ordering of the oxygen vacancies in the $CoO_{4.25}$ layer, and the structure becomes the monoclinic one (HTM , space group: A2/m) of $2\sqrt{2}\, a_0 \times 2\sqrt{2}\, a_0 \times 4a_0$.

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

The second transition at 360K is of first order, at which the ferromagnetic state appears, and the unit cell becomes $4\sqrt{2}a_0 \times 2\sqrt{2}a_0 \times 4a_0$ with monoclinic structure (LTM). However, the crystal structures in each phase are not clear so far. In order to clarify the crystal structures and magnetic structure, we measured the diffraction patterns in the three phases, at 303 K, 453 K, and 573 K., utilizing a furnace.

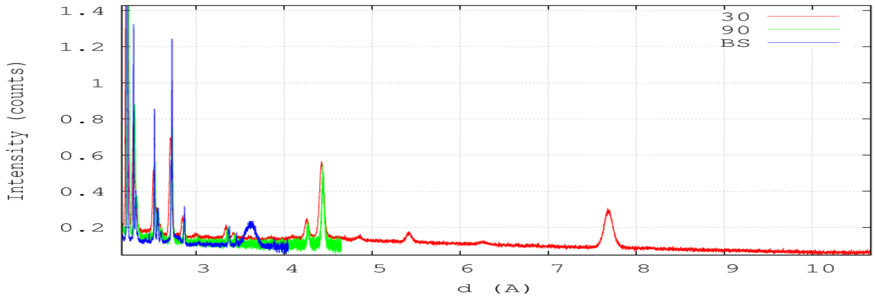

Figure.1

The diffraction patterns were observed at 303 K using 30 degree, 90 degree, and back scattering (BS) banks as shown in Fig. 1. The observable d-space range depends on the observed bank. The d resolution of the BS bank is the highest in the world. Using the BS bank, however, large d value cannot be measured fundamentally. In order to measure magnetic scattering, large d-space region is quite important. The temperature dependence of the diffraction patterns obtained by the 30 degree bank is shown in Fig.2

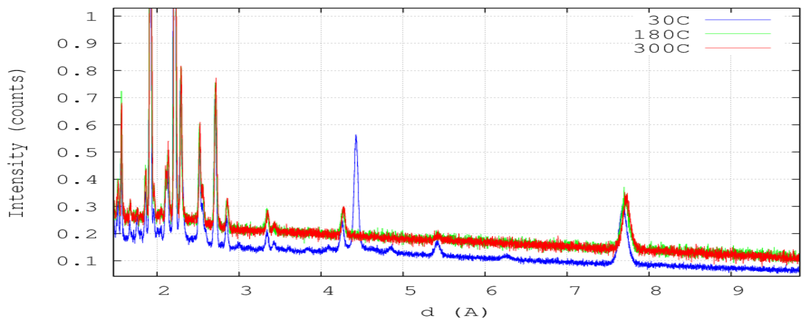

Figure. 2

Many new peaks, which are expected to be magnetic scattering, emerge in data at 303K. We also calculated the diffraction pattern based on the proposed peculiar spin-state ordering model as shown in Fig. 3.

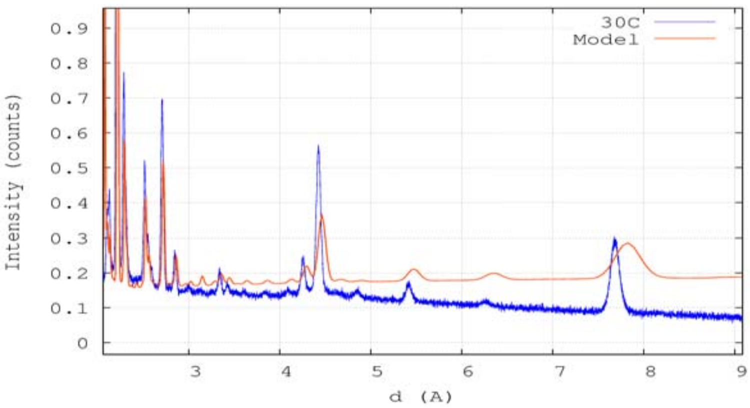

Figure.3

The simulation can explain well the experimental data. The detailed structural analysis using the Fullprof is in progress now.