MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014B0316 実験課題名 Title of experiment Crystal structure analysis of $Fe_{1-x}Sr_2YCu_{2+x}O_{6+\delta}$ superconductor with intrinsic magnetic Josephson junction 実験責任者名 Name of principal investigator Takashi Mochiku 所属 Affiliation National Institute for Materials Science	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/(BL No.) BL-20 実施日 Date of Experiment March 8-9, 2015

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.

We measured the $Fe_{1-x}Sr_2YCu_{2+x}O_{6+\delta}$ power samples (x = 0, 0.05, 0.1, 0.2, 0.3, 0.32, 0.33, 0.34, 0.36, 0.38, 0.4, 0.5, 0.6 and 0.7), which were prepared using solid-state reaction of mixture of Fe_2O_3, $SrCO_3$, Y_2O_3 and CuO powers and annealing technique. A drop of a superconducting transition temperature, T_c, of 30 K is observed within the range of between 0.2 and 0.4. We study the cause of the drop of T_c from a viewpoint of the crystal structure.

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 TOF neutron powder diffraction data of all samples were collected at room temperature using the automatic sample changer, and the data were analyzed by the Rietveld refinement program Z-Rietveld. The structural model is based on the tetragonal $Ba_2YCu3O_{6+\delta}$-type structure (space group *P4/mmm*), which can be derived by stacking FeO_δ, SrO, CuO_2, Y, CuO_2 and SrO layers alternately along the *c*-axis. We assigned four sites for Cu and Fe: Cu(1) and Fe(1) on the FeO_δ layer, and Cu(2) and Fe(2) on the CuO_2 layer, and refined the occupation factors of those. The structural model is supported by the good fit between the observed and calculated patterns coupled with the low *R* factors (for example, R_{wp} = 7.41%, χ^2 = 7.38 for x = 0.2). Fig. 1 shows dependence of the lattice parameters, *a* and *c*, and the occupation factors of Cu(1), Cu(2) and O(1), $g_{Cu(1)}$, $g_{Cu(2)}$ and $g_{O(1)}$ on the Cu content, x. Although $g_{O(1)}$ decreases and $g_{Cu(1)}$ increases monotonously with increasing x, $g_{Cu(2)}$ is fixed around 0.95. Fig. 2 shows dependence of the selected interatomic distances on x.

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

While the Cu(1),Fe(1)–O(1) and Cu(2),Fe(2)–O(3) distances change monotonously, the Cu(1),Fe(1)–O(2) and Cu(2),Fe(2)–O(2) distances indicate anomaly within the range of x between 0.2 and 0.4, which corresponds to the range of the drop of T_c of 30 K. The anomaly of the interatomic distances is causes by the change of the charge distribution between the FeO_2 and CuO_2 layers, which induces the change of T_c.

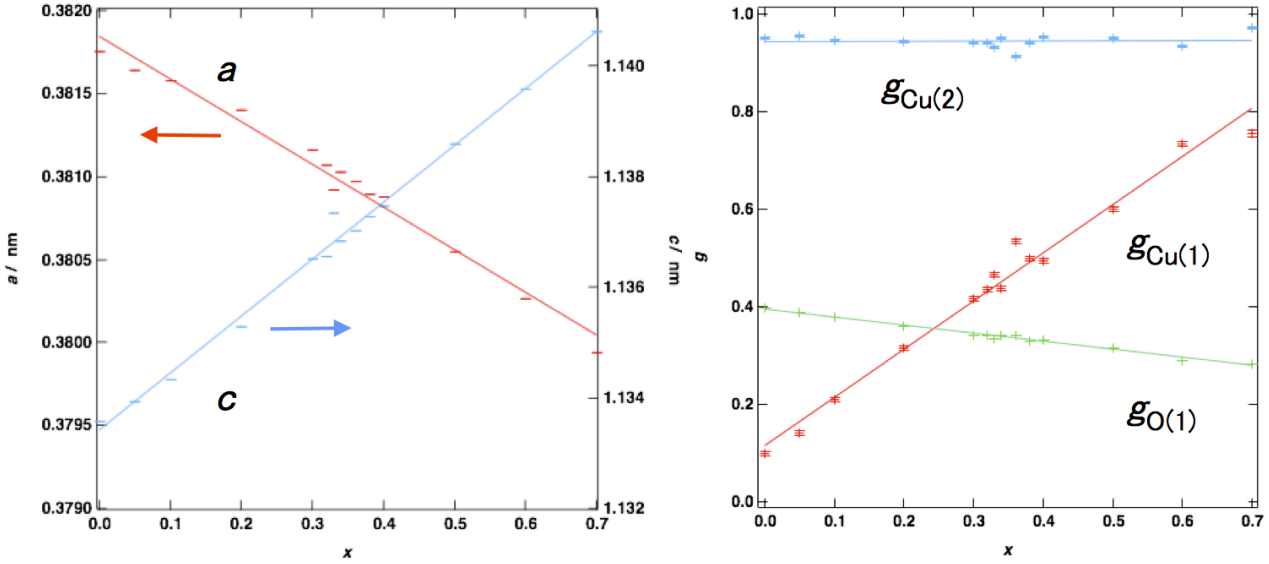

Fig. 1. Dependence of the lattice parameters, *a* and *c* and the occupation factors of Cu(1), Cu(2) and O(1), gCu(1), gCu(2) and gO(1).

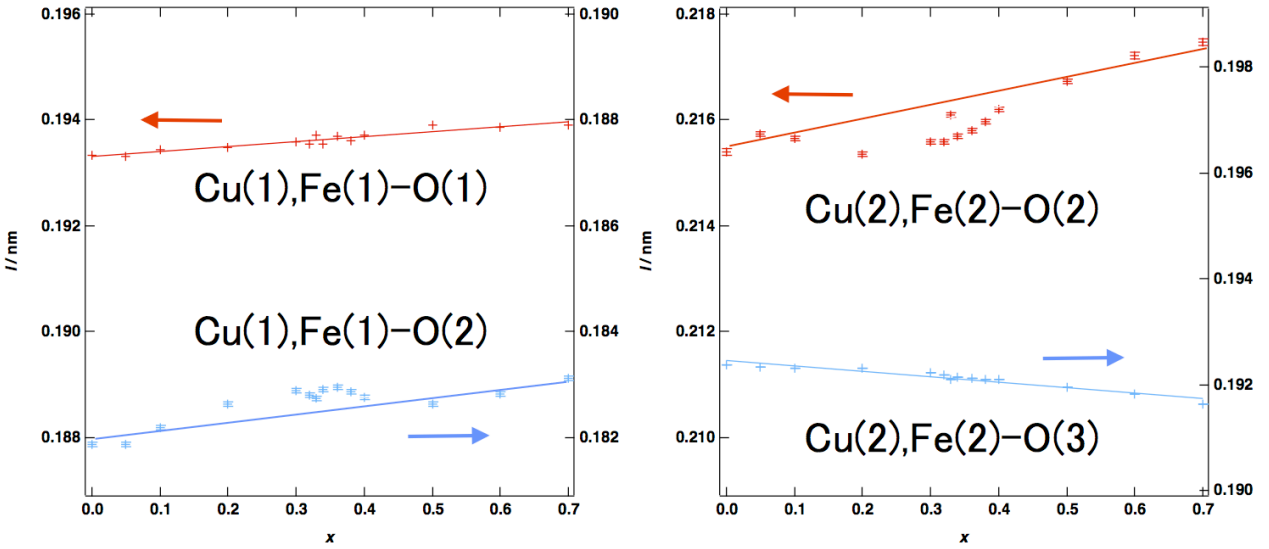

Fig. 2. Dependence of the selected interatomic distances between Cu(1),Fe(1) and O(1), Cu(1),Fe(1) and O(2), Cu(2),Fe(2) and O(2), and Cu(2),Fe(2) and O(3).