MLF Experimental Report	提出日 May 21, 2010
課題番号 Project No.2009A0020 実験課題名 Structural study on square-planar coordinated iron oxides 実験責任者名 Hiroshi Kageyama 所属 Graduate School of Engineering, Kyoto University	装置責任者 Toru Ishigaki 装置名 IMATERIA/(BL No.08) 実施日 Dec 9 –Dec 10, 2009

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.

$Sr_{0.075}Ca_{0.925}FeO_2$ (23.5 grams Powder sample)

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.

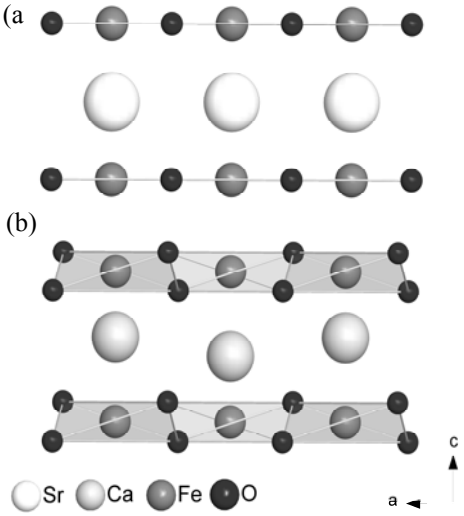
$SrFeO_2$ has an infinite layer (IL) structure with iron in corner sharing oxygen square planes. Layers are separated by strontium cations having an eight-fold coordination (Figure 1a). Following the synthesis of this material, we reported the successful substitution of strontium by calcium in the $Sr_{1-x}Ca_xFeO_2$ solid solution. At room temperature, the size of calcium being smaller than strontium, the lattice parameters a and c of $Sr_{1-x}Ca_xFeO_2$ are decreasing against x for $0 \leq x \leq 0.925$. Over this limit ($x = 0.925$) a transition is observed by the expansion of the c axis of the solution. $CaFeO_2$ has a distorted structure with FeO_4 square planes distorting to tetrahedra. Implying that Ca is in a 6-fold coordinated polyhedra. Following these experiments, we performed diffraction at low temperature which showed that the $0 \leq x \leq 0.925$ region exhibits phase transition between $SrFeO_2$-type and $CaFeO_2$-type structure. This is followed by the negative expansion of their unit cell. This implies that The low temperature phase for 0.25 to 0.925 exhibits negative thermal expansion. To understand the local structure of this material we performed time of flight diffraction which allow access to the atomic pair distribution function.

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

Neutron diffraction

The 25 g sample was inserted in a cell and cooled down to 10 K by using a …. Each neutron powder diffraction measurement was performed at. Scan to measure the contribution of the vanadium cell were performed to obtain the background. The samples, after being cooled down to 10 K were exposed to the beam. Following this, the temper Figure 1. Structure of $SrFeO_2$ (a) and ζ. The datas were collectedule and collected to the detector bank. $CaFeO_2$ (b).

In figure 2, we can observe the evolution of the whole patterns at 10K, 70 K, 130 K and 190 K. The 110 peaks and 001 peaks are presented in the figure 3. The 001 peak represents the evolution of the interlayer of FeO_4 square planes distance (*c* axis) and the 110 represents the *a* axis. The peaks are showing opposite evolution against temperature implying that the *c* axis decreases with increasing temperature.. The Rietveld refinement of these data is now in progress. Finally these data will be converted using the structure function and Fourier transformation to get pair distribution function which will provide clues on the local mechanism of the negative thermal expansion.



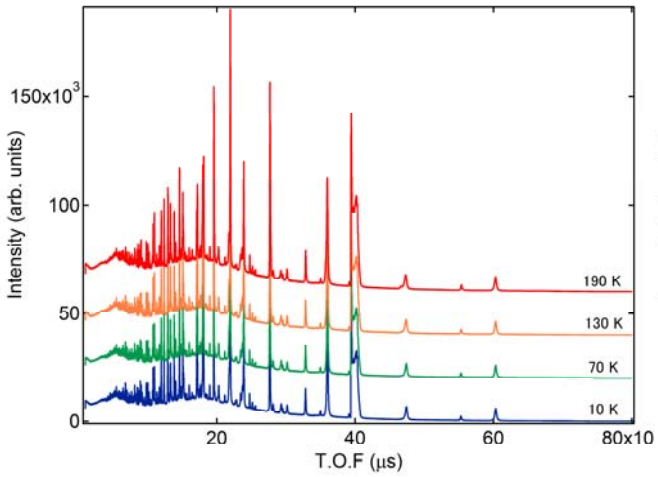


Figure 2. Time-of-flight measurement of $Sr_{0.075}Ca_{0.925}FeO_2$

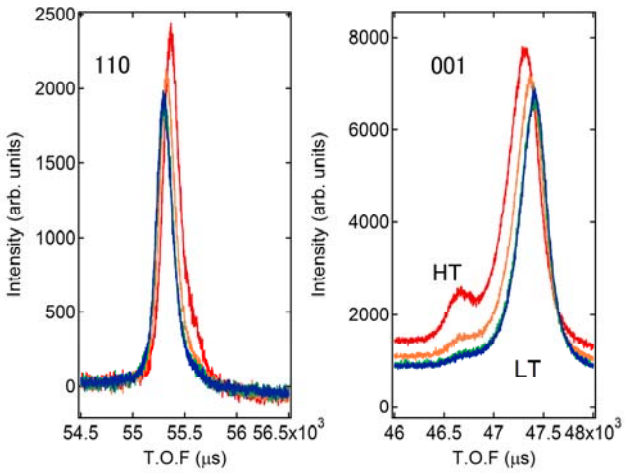


Figure 3. 110 and 001 peak evolution of $Sr_{0.075}Ca_{0.925}FeO_2$