MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2016A0284 実験課題名 Title of experiment Local structure analysis of the element-substituted $SrTiO_3$ 実験責任者名 Name of principal investigator Ryoichi Kajimoto 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Toshiya Otomo 装置名 Name of Instrument/（BL No.） NOVA/BL21 実施日 Date of Experiment June 28-29, 2016

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.

Powder samples of:

$SrTiO_3$

$SrTi_{0.98}Mn_{0.02}O_3$

$Sr_{0.95}La_{0.05}TiO_3$

$Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$

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.

$SrTiO_3$ is known as an incipient ferroelectric material which is characterized by a soft TO phonon at the Γ point. In addition, it shows a cubic to tetragonal structure transition at 105 K, which is caused by antiferrodistortive distortions of TiO_6 octahedra characterized by softening of a phonon mode at the *R* point. Recently it was found that a few percent co-doping of electrons (substitution of Sr^{2+} by La^{3+}) and Mn ions in $SrTiO_3$ reduces the thermal conductivity substantially at room temperature (RT) [1]. One of the possible effects of the co-doping is that Jahn-Teller (JT) active Mn^{3+} ions are created. The local JT distortions may couple with the inherent structural instability of $SrTiO_3$, and obstruct heat flow. Accordingly, we performed a powder neutron diffraction study of doped $SrTiO_3$ to study their crystal structures.

Powder samples of $SrTiO_3$, $SrTi_{0.98}Mn_{0.02}O_3$, $Sr_{0.95}La_{0.05}TiO_3$, and $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$ were prepared by crushing their single crystals grown by the floating-zone method. Each sample is about 5 g in weight. The measurements were performed at room temperature, and measurement time is about 5 hours for $SrTiO_3$ and 2.5 hours for each of the other three samples.

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

Figure 1 shows powder diffraction patterns of $SrTiO_3$ and $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$, and the results of their Rietveld refinements using Z-Rietveld. All the four samples measured in the present study were successfully refined with the cubic crystal structure (space group *Pm*-3*m*). However, the *R*-factor for $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$ (4.5%) is larger than those for the other three samples (3.5-3.7%), which suggests that the true crystal structure of $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$ has some deviation from the *Pm-3m* symmetry. Then, we checked whether superlattice peaks characterizing the low-temperature tetragonal structure of $SrTiO_3$ (space group *I*4/*mcm*) appear in $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$, but we did not observe any of this type of superlattice peaks within the statistics of the present data. Therefore, we found no observable difference in the average crystal structure between the four samples. On the other hand, if we look into the pair distribution function (PDF) profiles derived from the powder patterns, we found that only the profile for $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$ shows a shoulder at r ~ 2.1 Å in the peak corresponding to the Ti-O bond length at r = 1.9 Å (Fig. 2). We should note that this r value of the shoulder is quite similar to the value of the long Mn-O bond in the Jahn-Teller distorted $Mn^{3+}O_6$ octahedra in $LaMnO_3$ [2]. We are trying more detailed analysis of the PDF profiles.

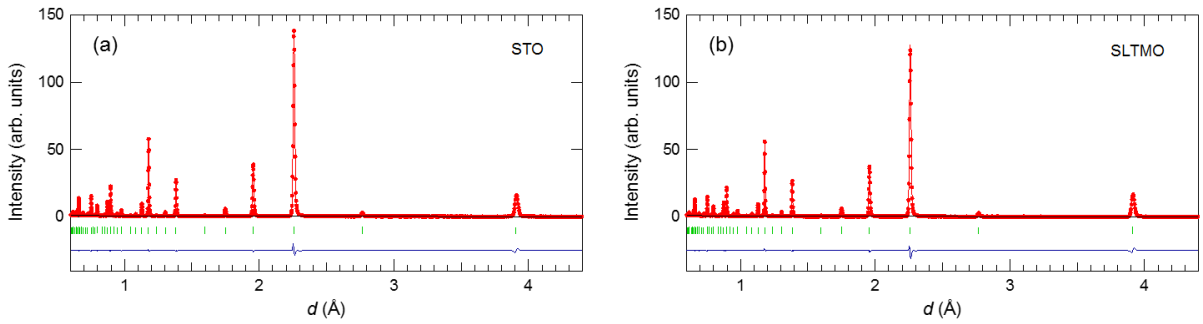

Fig. 1. Powder diffraction patterns and their Rietveld refinements for (a) $SrTiO_3$ and (b) $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$.

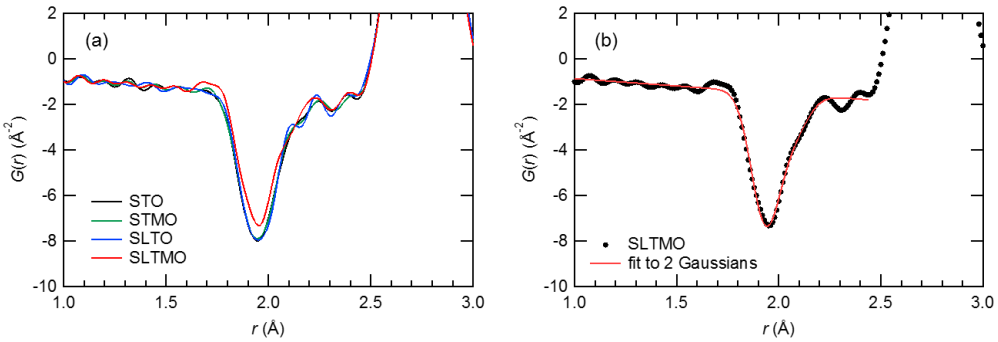

Fig. 2. (a) PDF profiles for $SrTiO_3$ (STO), $SrTi_{0.98}Mn_{0.02}O_3$ (STMO), $Sr_{0.95}La_{0.05}TiO_3$ (SLTO), and $Sr_{0.95}La_{0.05}Ti_{0.98}Mn_{0.02}O_3$ (SLTMO) around the Ti-O bond length. (b) PDF profile for $Sr_{0.95}La_{0.05}Ti_{0.98}M_{0.02}O_3$. Solid line shows a fit to two Gaussians.

[1] T. Okuda *et al.*, J. Phys. Soc. Jpn. **85**, 094717 (2016).

[2] X. Qiu *et al.*, Phys. Rev. Lett. **94**, 177203 (2005).