MLF Experimental Report	提出日 Date of Report July 14, 2011
課題番号 Project No. 2010A0030 実験課題名 Title of experiment Structural Origin of Large Oxygen Permeability in the Pr_2NiO_4-Based Mixed Conductors 実験責任者名 Name of principal investigator Masatomo Yashima 所属 Affiliation Department of Chemistry and Materials Science, Graduate School of Science and Engineering,, Tokyo Institute of Technology	装置責任者 Name of responsible person Takashi Kamiyama 装置名 Name of Instrument/（BL No.） BL-08 実施日 Date of Experiment November 25, 2010

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.

Powders of Pr_2NiO_4-based materials

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.

Neutron powder diffraction data of a Pr_2NiO_4-based material $Pr_{1.9}(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05}O_{4+\delta}$ were measured at room temperature by a high-resolution neutron powder diffractometer installed at the beam line BL08 of J-Parc facility, Japan. The diffraction data were analyzed by the Rietveld method with a computer program Z-Rietveld. Neutron diffraction profiles include useful information on oxygen, because the scattering ability of the oxygen nucleus (amplitude of coherent scattering length) is relatively large and independent of diffraction angle. The crystal structure of $Pr_{1.9}(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05}O_{4+\delta}$ was refined by the *I*4/*mmm* K_2NiF_4-type structure. Figure 1 shows the refined crystal structure of tetragonal *I*4/*mmm* K_2NiF_4-type $Pr_{1.9}(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05}O_{4+\delta}$. This structure consists of $Pr_{1.9}(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05}O_3$ perovskite and $Pr_{1.9}O$ rock salt units. It should be noted that (1) the apex O2 oxygen exhibits a large anisotropic thermal motions and that (2) there exists an interstitial O3 oxygen. The oxide ions would diffuse through the anisotropic O2 and interstitial O3 sites as shown by the arrows in Fig. 1. Thus, the interstitial oxygen has an essential role in the oxygen diffusion. These results are consistent with our previous works obtained for $(Pr_{0.9}La_{0.1})_2(Ni_{0.74}Cu_{0.21}Ga_{0.05})O_{4+\delta}$ (References).

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

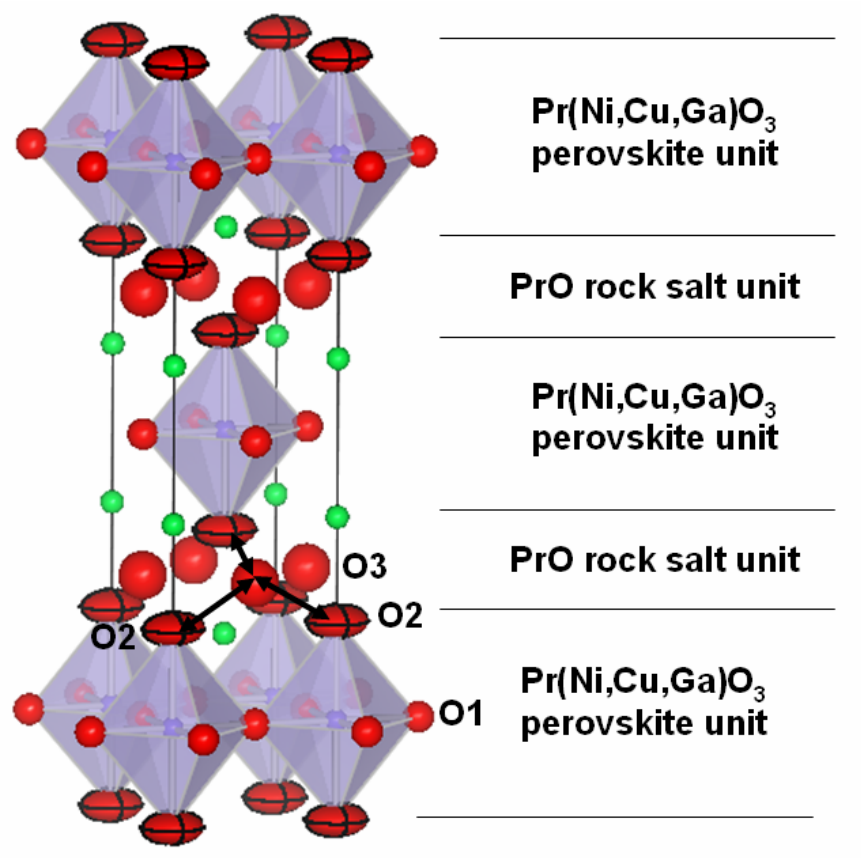

Figure 1. Refined crystal structure of $Pr_{1.9}(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05}O_{4+\delta}$.

References:

1. M. Yashima, M. Enoki, T. Wakita, R. Ali, Y. Matsushita, F. Izumi and T. Ishihara, "Structural Disorder and Diffusional Pathway of Oxide Ions in a Doped Pr_2NiO_4-Based Mixed Conductor", *J. Am. Chem. Soc. (Communications)*, **130**, [9] 2762-2763 (2008).
2. M. Yashima, N. Sirikanda and T. Ishihara, "Crystal Structure, Diffusion Path and Oxygen Permeability of a Pr_2NiO_4-Based Mixed Conductor $(Pr_{0.9}La_{0.1})_2(Ni_{0.74}Cu_{0.21}Ga_{0.05})O_{4+\delta}$", *J. Am. Chem. Soc.*, **132**, [7] 2385-2392 (2010).