MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2010A0037 実験課題名 Title of experiment Structural Positional Disorder and Crystal Structure of Ceria-Zirconia Catalysts; Structural Origin for High Bulk Oxygen Diffusivity and High Catalytic Activity? 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 26, 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.

$Ce_xZr_{1-x}O_2$ materials (Powders)

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.

Experimental Procedure: Neutron powder diffraction data of $Ce_xZr_{1-x}O_2$ materials (x=0, 0.5, 1) 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.

Results and discussion: Figure 1 shows the Rietveld pattern of nano-sized $Ce_{0.5}Zr_{0.5}O_2$, which were prepared by the Pechini method. Atomic displacement parameter of oxygen atom in $Ce_{0.5}Zr_{0.5}O_2$ was found to be larger than those in CeO_2 and ZrO_2. Thus, the positional disorder of oxygen atoms in $Ce_{0.5}Zr_{0.5}O_2$ is also larger, which might lead to higher oxygen diffusivity in $Ce_{0.5}Zr_{0.5}O_2$. The high atomic displacement parameter of oxygen atom in $Ce_{0.5}Zr_{0.5}O_2$ would be an important factor of high catalytic activity of this material.

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

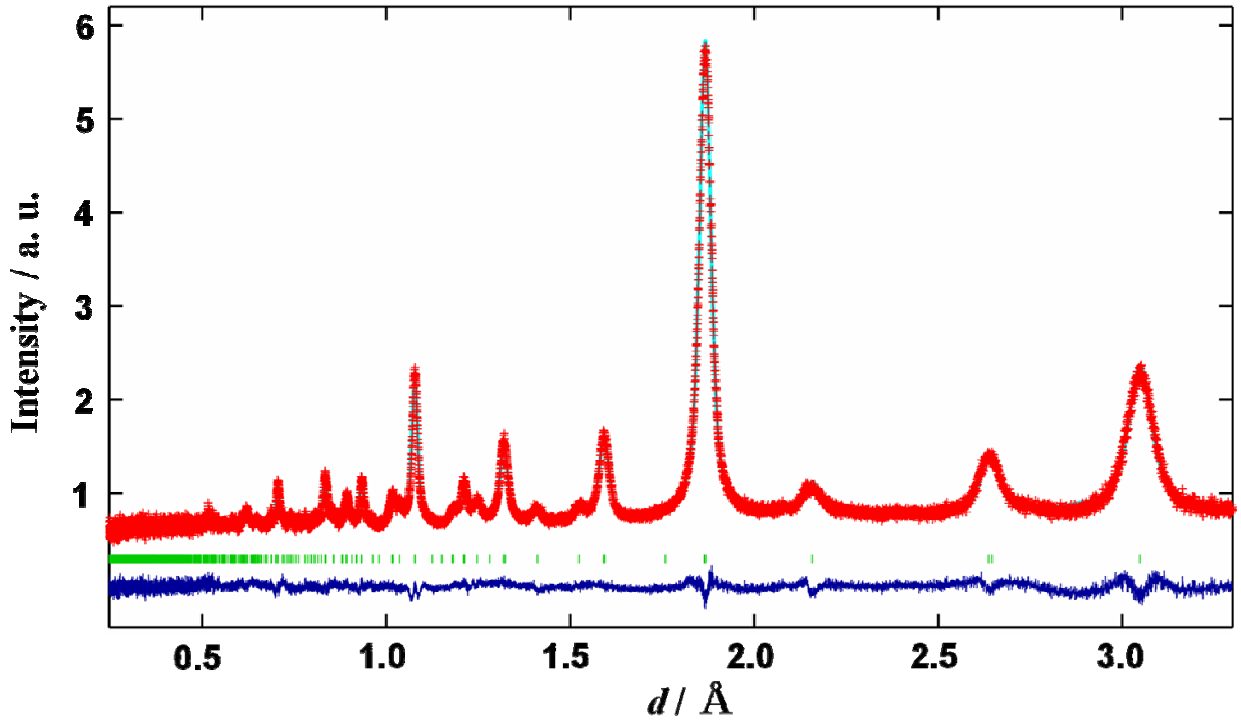

Fig. 1. Rietveld fitting pattern for neutron diffraction data of $Ce_{0.5}Zr_{0.5}O_2$ nano particles prepared by the Pechini method.