 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2011B0044 実験課題名 Title of experiment Crystal structure analysis of new cathode material $\text{Li}_{2-x/2}\text{Mn}_{1-x}\text{Co}_{3x/2}\text{O}_3$ with high cyclic performance 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 石垣 徹 装置名 Name of Instrument/(BL No.) BL20 iMATERIA 実施日 Date of Experiment from March 12, 2012 to March 13, 2012

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 following samples: #1 $\text{Li}_{1.95}\text{Mn}_{0.9}\text{Co}_{0.15}\text{O}_3$ cathode material (powder), #2 the cell for in-situ measurement of charge and discharge using the sample #1 as the cathode material.

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. <p>We used the sample changer for the measurement of the sample #1, and the flange specially made for the in-situ measurement of the sample #2 after uninstalling the robots for routine measurements, to complete the different kinds of measurements within the limited beam time. We collected the TOF diffraction data for the samples in the single frame operation.</p> <p>The data of the sample #1 was analyzed using the Rietveld refinement program Z-Rietveld (see Fig. 1). It indicates that the sample #1 has the Li_2MnO_3-type structure ($C2/m$), which is different from the reported structure ($\alpha\text{-NaFeO}_2$-type structure, $R-3m$). Not only the Li ions between the layers but also the Li ions in the layers contribute the charge and discharge, and consequently the cathode material with this structure has high cyclic performance.</p> <p>We also made the cell for in-situ measurement of the charge-discharge cycle using the sample #1 as the cathode material, and operated it. The charge-discharge condition was controlled and the voltage was measured by the apparatuses (see Fig. 2). We collected the diffraction data in the charge-discharge cycle similar to that in the conventional button cell. We will analyze the data after the measurement of background of the in-situ cell.</p>

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

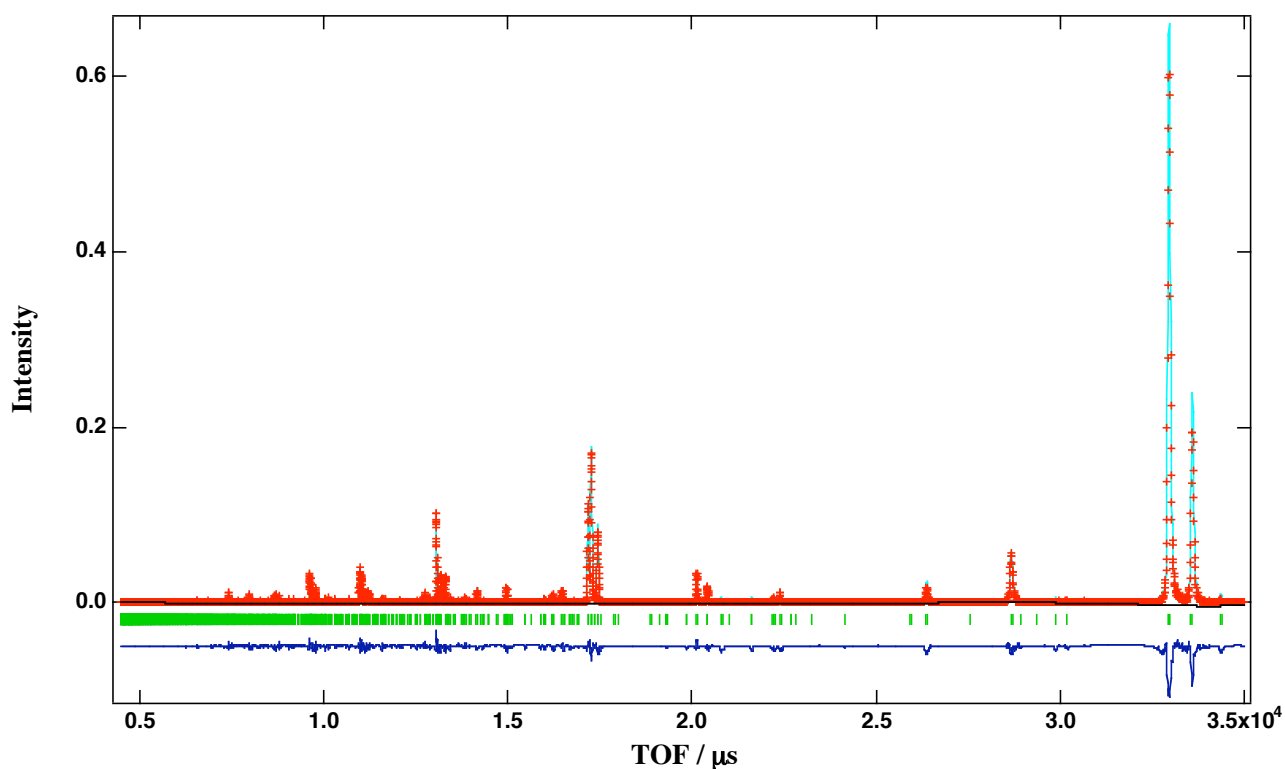


Figure 1. Rietveld refinement pattern for the sample #1.

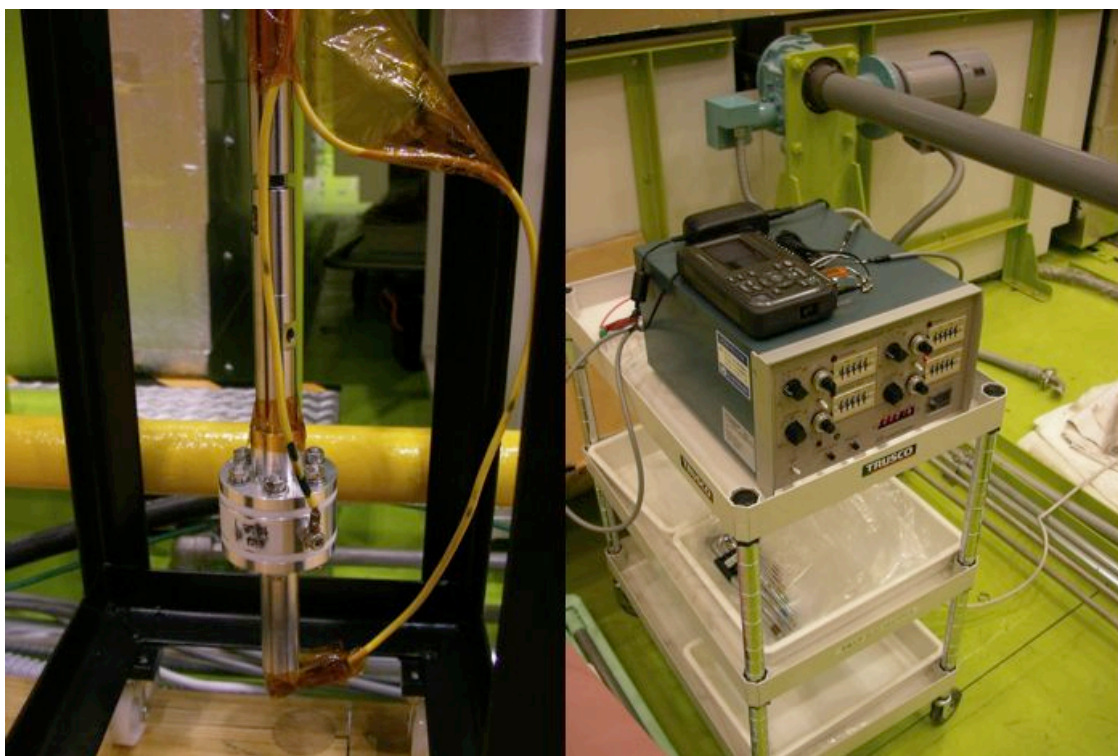


Figure 2. The cell for in-situ measurement (left), charge-discharge control unit and data logger (right).