Analysis of Average and Electronic Structure and Nuclear Densities for $LiNi_{0.8}Co_{0.2}O_2$ during Charge Process Using Neutron and Synchrotron X-ray Diffractions

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Cathode material, $Li(Ni,Co)O_2$ system, of Li-ion battery has been attractive because of the advantage in low environmental load and in low Co content. However, detail structural changes during electrochemical processes are still ambiguous for site occupancy, local structures, and electronic structures [1]. This study revealed the crystal structures, electronic and nuclear densities, and local structures of $LiNi_{0.8}Co_{0.2}O_2$ during charge process using the quantum beam techniques such as neutron scattering.

The prepared $LiNi_{0.8}Co_{0.2}O_2$ was identified by powder XRD and ICP-OES. Four electrodes at different charge depths were prepared and investigated using the neutron diffraction (BL20, J-PARC) and the synchrotron X-ray diffraction (BL02B2, SPring-8). The data was analyzed with the Rietveld technique using Z-Rietveld and Rietan-FP, and by the MEM using the Dysnomia and Z-MEM programs.

The neutron diffraction patterns were measured for the cathode after several charge-discharge conditions as well as the pristine electrode (Fig. 1). It was demonstrated that the crystal structure analysis by ex-situ measurement could be successfully performed with a minor amount of about 10 mg. The nuclear density distributions of the electrodes were evaluated by Z-MEM to clarify the extraction process of Li with charge depths (Fig. 2). Therefore it was low cation mixing that the $LiNi_{0.8}Co_{0.2}O_2$ could reversibly extract and insert Li^+ ion from the host structure.

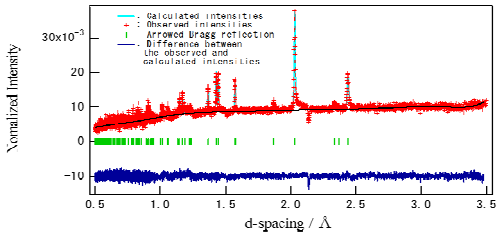

Fig. 1 Rietveld analysis for the electrode of $LiNi_{0.8}Co_{0.2}O_2$ after 2nd discharge

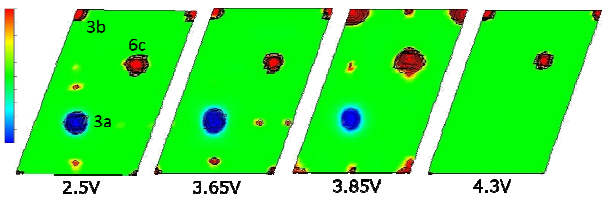

Fig. 2 The nuclear density distributions of the electrodes in each charge depths

References

[1] Y. Idemoto, Y. Tsukada, N. Kitamura, A. Hoshikawa, and T. Ishigaki, *Chem. Lett.*, **40**, 168 (2011).