

Preparation and Characterization of $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ Cathode Materials by Pechini Method

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X-ray absorption near-edge structures (XANES) spectroscopy was used to investigate the valence states of Cu in the single crystals of the solid solutions of $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ grown. The XRD measurements are sensitive to the electronic states and the structural symmetry of the sites of the absorbing atoms. Our investigations show that Cu is incorporated into these crystals in mixed valence electronic states during crystal growth which in turn influences their magnetic and superconducting properties. The threshold of the absorption feature of the Cu K-edge shifts to higher energy side on annealing the crystals at 1420°C in an atmosphere of $\text{O}_2:\text{Ar}$ which is attributed to a changes in the Cu d-orbitals. The X-ray absorption measurements on the Cu, Ru K-edge were carried out with synchrotron radiation at the 17C beam line.

The in-situ XANES of the $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ cathodes quasi-equilibrated at voltage range of 2.8 to 4.6 V were estimated from the energies of centre of the jump with NiO and LiNiO_2 as references are shown in Fig. 4-17. The estimated valences of Ni are increased from 2.1 to 3.6 with voltage increased from 2.5 to 4.8 V in 1st cyclic charge/discharge. The result is the same with the cyclic voltammogram test which are shown in Fig.1. The oxidation and reduction peaks at 4.63 and 4.30 V may be caused by the redox reaction of $\text{Ni}^{3+}/\text{Ni}^{4+}$ couple can be proved.

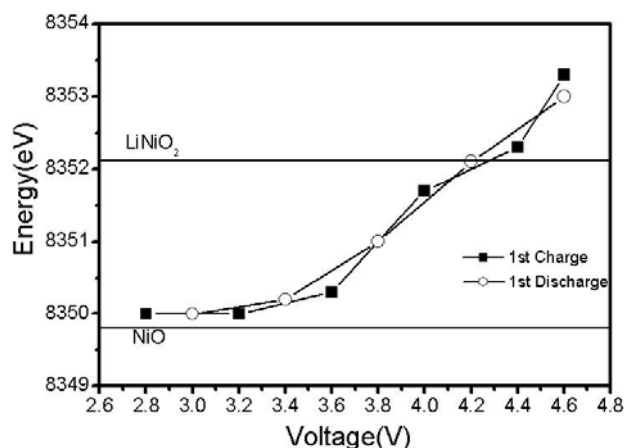


Fig. 1: The in-situ XANES of the $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ cathodes quasi-equilibrated at voltage range of 2.8 to 4.6 V were estimated from the energies of centre of the jump with NiO and LiNiO_2 as references.