Abs. 281, 206th Meeting, © 2004 The Electrochemical Society, Inc.

Performance of $LiNiCoO_2$ Based Materials for Advanced Lithium-Ion Batteries

Y. Itou and Y. Ukyo

Toyota Central R&D Labs., Inc.
Nagakute, Aichi 480-1192, Japan

Li-Ni based material such as $LiNiCoO_2$ is one of the most promising candidates for a cathode material of advanced lithium-ion battery because of its lower cost and higher capacity compared with $LiCoO_2$(1). The performance of $LiNiCoO_2$ materials for lithium-ion batteries have been studied by many authors (2). We also studied the performance of lithium-ion battery with $LiNiCoO_2$ as cathode materials at high temperature.

The capacity fading of lithium-ion battery with $LiNiCoO_2$ as cathode during cycling and storage at high temperature was analyzed from the standpoint of the change in the performance of cathode (especially structural change of $LiNiCoO_2$). For this purpose, *in situ* XAFS analysis seems to be very useful, because it will give the information on the local structure and the electronic structure (3-5). XAFS data for $LiNiCoO_2$ (the anode is graphite) were collected at various voltages before and after cycling and storage at high temperature by using the *in situ* coin cell newly developed in our laboratory for XAFS measurement (4). Ni and Co K-edge XAFS data were collected using beam line, No. BL16B2, in SPring 8. As an example, the Ni and Co K-edge XANES spectra at various states before cycling and storage are shown in Fig. 1(a), (b). The chemical shifts of the edge peak energy upon charging were found in both edges. Especially, the Ni scans show a steady progress of the entire pattern from lower to higher energy as a function of decreased Li content, indicating an increasing average Ni oxidation. The Fourier-transforms of Ni K-EXAFS spectra at various states before cycling and storage are shown in Fig. 2. The profile of Ni-O peak around 1.5Å indicates the symmetry of NiO_6 octahedron. These XAFS spectra after cycling and storage at high temperature were also collected and compared with the change in the performance of the cells to reveal the capacity fading of the batteries. A good relation between the range of chemical shift and the capacity of the cell was found. From analysis EXAFS data, capacity fading was found to be relation to Jahn-Teller distortion of the NiO_6 structure. In the presentation, the performance and capacity fading mechanism of the battery with $LiNiCoO_2$ based material as cathode will be discussed in detail by taking other information into account.

Acknowledgement
We thank 5004 Labs. and 6120 Labs in TCRDL for discussion and technical support.

References

[1] K. Sekai, H. Azuma, A. Omaru and S. Fujita., J. Power Sources, 43(1993)241-244.
[2] T. Ohzuk, A. Ueda and M. Nagayama, J. Electrochem. Soc., 140(1993)1862-1870
[3] L. Nakai, K. Takahashi, Y. Shiraishi, T. Nakagome, F. Izumi, Y. Ishii, F. Nishikawa and T. Konishi, J. Power Sources, 68(1997)536-539
[4] T. Nonaka, C. Okuda, Y. Ukyo and T. Okamoto, J. Synchrotron Rad., 8(2001)869-871.
[5] C.S. Johnson and A.J. Kropf, Electrochimica Acta 47(2002) 3187-3194

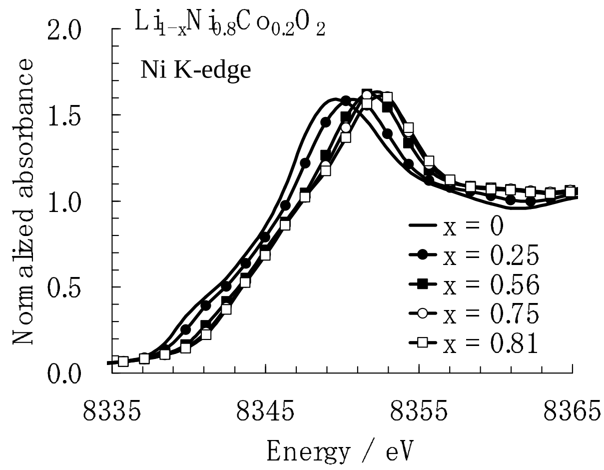

Fig.1(a) Ni K-edge XANES spectra of $LiNiCoO_2$ at various states.

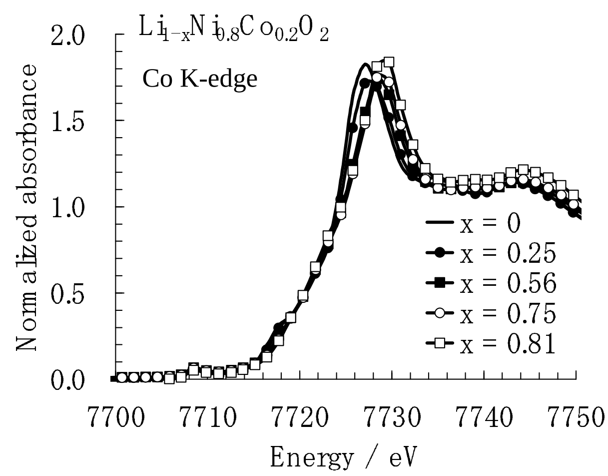

Fig.1(b) Co K-edge XANES spectra of $LiNiCoO_2$ at various states.

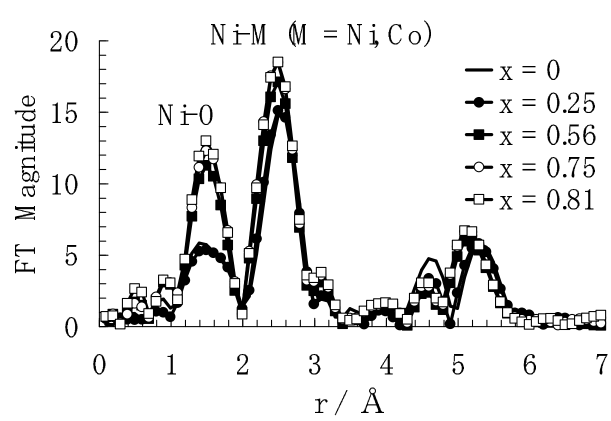

Fig.2 Fourier-transforms of Ni K-EXAFS spectra of $LiNiCoO_2$ at various states before cycling and storage.