



	Experiment title: Non-Resonant Inelastic X-ray Scattering Study of Li-ion Batteries	Experiment number: HE-1479
Beamline: ID16	Date of experiment: from: 03 Feb 2003 to: 10 Feb 2003	Date of report: 25 Feb 2004
Shifts: 18	Local contact(s): Dr. G. Vanko	<i>Received at ESRF:</i>
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Report:

Li-ion batteries have been in the focus of substantial interest as power sources for portable telecommunication and IT equipment as well for hybrid electric vehicles. In order to improve li-ion battery technology further, understanding the electronic structure of novel battery materials, such as LiNiO_2 , is of fundamental importance. There are conflicting reports regarding the redox chemistry of Ni and the role of oxygen during battery cycling in LiNiO_2 based cathode materials. In some experiments the hole doping following lithium removal from the cathode is observed to happen mostly on oxygen sites while in other experiments the charge compensation is observed to occur through oxidation of the transition metal ions.

This experiment aimed to answer these discrepancies by measuring the evolution of Non-Resonant Inelastic X-ray Scattering (NRIXS) spectra of O in a series of $\text{Li}_x\text{Ni}_{0.85}\text{Co}_{0.15}\text{O}_2$ samples with a varying degree of lithium content x . In NRIXS, by tuning the energy transfer over the core electron binding energies, an equivalent of conventional inner shell absorption spectrum can be measured. In this experiment we tuned the energy transfer over oxygen 1s binding energy and thus we were able to measure the O K-edge absorption spectra using hard x-rays, making this a bulk sensitive experiment. Most previous experiments have been done using surface sensitive techniques. As Li_xNiO_2 surface layer easily degrades in ambient atmosphere, the use of hard x-rays circumvented the problem.

We measured the O K-edge spectrum of $\text{Li}_x\text{Ni}_{0.85}\text{Co}_{0.15}\text{O}_2$ ($x = 1, 0.75, 0.65, 0.50, 0.25, 0.00$) and a series of standards (LiNiO_2 , LiCoO_2). The spectra obtained from LiNiO_2 , LiCoO_2 and $\text{Li}_1\text{Ni}_{0.85}\text{Co}_{0.15}\text{O}_2$, shown in figure 1., clearly demonstrates the high quality of the data obtainable at the beamline ID16 with the NRIXS technique. The differences in the pre-peak at 0.53 keV energy transfer at the O K-edge caused by the Co doping of LiNiO_2 is clearly observed.

In the series of $\text{Li}_x\text{Ni}_{0.85}\text{Co}_{0.15}\text{O}_2$ samples we observed no change in the relative intensities of the 0.53 keV peak, indicating the passivity of O during the Li extraction. Computational work is underway to analyze the spectra in a more quantitative manner.

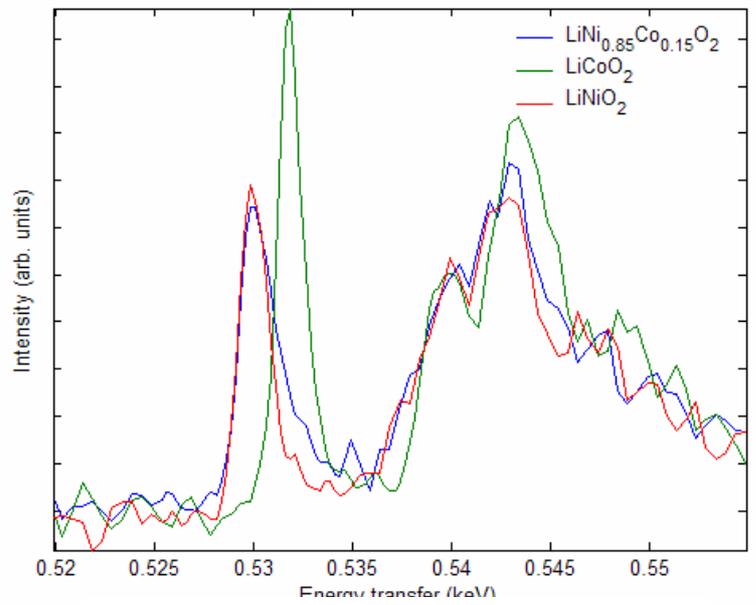


Figure 1. Non-resonant inelastic x-ray scattering from the O K-edge.