ESRF	**Experiment title:** Electronic density of $LiMO_2$ (M=Ni and Co), by Compton scattering	**Experiment number:** HE 388
Beamline: ID 15B	**Date of experiment:** from: 25 Mar 98 to: 02 Apr 98	**Date of report:** 28 Jul 98
Shifts: 18	**Local contact(s):** Abhay Shukla	*Received at ESRF.*

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Report:

Li_xMO_2 compounds are among the best candidates for new rechargeable batteries.

The aim of the experiment is to describe the changes in the d-states of Ni and the role played by the nature of the transition metal in Li_xMO_2.

Experiment on Li_xMO_2 has been performed using the scanning mode spectrometer of beamline ID 15B. The synchrotron radiation was monochromatized at 55.8 keV and the scattering angle fixed at $160°$.

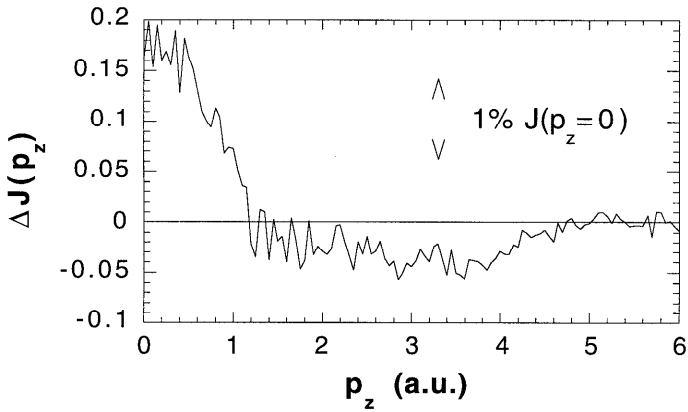
Two samples with different values of x (x = 1.05 and 0.63) in Li_xNiO_2, corresponding to different steps in the electrochemical cycling process, were measured, together with $LiCoO_2$.

The data sets have been corrected for energy dependent effects such as photoelectric absorption in sample, analyser and air as well as for multiple processes.

Valence Compton profiles were extracted from the total measured Compton profiles by substracting a QSCF core profile (in collaboration with A.Issolah, Algeria).

The difference between two valence Compton profiles measured for two lithium concentrations allows us to determine the importance of distorsion in the electronic density due to the de-intercalation of lithium. Moreover, such a procedure cancels out most of systematical errors.

The figure below shows the difference between $Li_{0.98}Ni_{1.02}O_2$ (stoechiometric $LiNiO_2$ not being synthetisable) and $Li_{0.63}Ni_{1.02}O_2$ valence profiles.



A surprinsingly high delocalisation in r-space in the region [0, 1 u.a.] is evidenced on the figure for valence electrons of $Li_{0.98}Ni_{1.02}O_2$ compared to $Li_{0.63}Ni_{1.02}O_2$ The reverse tendency is seen for larger p_z : the negative part is an evidence of a large electronic density distorsion.

We will be able to compare our experimental results with theoretical results calculated by Sohrab Rabii (University of Pennsylvania, USA) using an *ab initio* pseudopotential method. Wave functions have already been computed for the stoechiometric compounds ($LiNiO_2$ and $LiCoO_2$) by M.K.Aydinol et al. (Phys.Rev. **B56**,1354 (1997)) and will be provided to S.Rabii for Compton profile calculations.