



Contribution ID: 33

Type: **Poster contribution**

## Structural investigations of $\text{Li}_2\text{MnO}_3 \cdot \text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$ – Neutron diffraction, in situ X-ray diffraction, and in situ Raman spectroscopy

*Thursday, 5 July 2012 10:30 (1h 30m)*

$\text{LiCoO}_2$  is today's standard cathode material for Li-ion batteries.  $\text{Li}_2\text{MnO}_3 \cdot \text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$  (NCM) is a very promising candidate to replace  $\text{LiCoO}_2$  since it shows an approx. 2 times higher specific charge and is less expensive. We investigated the structural changes of NCM upon charge and discharge with ex situ neutron diffraction, in situ X-ray diffraction, and in situ Raman spectroscopy.

The in situ XRD measurements were performed at SLS (X04) in a "coffee bag" cell using an automatic sample changer. The neutron diffraction was performed at SINQ (HRPT). The in situ Raman spectroscopic measurements were performed on a LabRAM HR (HoribaJovinYvon SA), using a He-Ne laser as excitation source (632.8 nm, 18 mW) in a cell which allows for recording of Raman spectra from the backside of the electrode.

Data from the diffraction techniques showed the phase transitions during galvanostatic cycling. NCM showed an expansion of the c axis during charging and proved a release of oxygen at 4.5 V which was also detected with Differential Electrochemical Mass Spectrometry (DEMS). NCM also showed changes in Raman spectroscopy according to the processes visible in the galvanostatic curve. The new set of peaks cannot yet be ascribed to a phase and two hypotheses are under investigation: An NCM layer without lithium or  $\text{MnO}_2$  created by  $\text{Li}_2\text{MnO}_3$  activation, which means release of oxygen.

In short, the combination of these techniques gave the opportunity to understand the reaction mechanism of NCM.

**Primary author:** Mr BLEITH, Peter (Paul-Scherrer-Institute)

**Co-authors:** Dr VILLEVIEILLE, Claire (Paul-Scherrer-Institute); Mr LANZ, Patrick (Paul-Scherrer-Institute); Prof. NOVÁK, Petr (Paul-Scherrer-Institute)

**Presenter:** Mr BLEITH, Peter (Paul-Scherrer-Institute)

**Session Classification:** Poster Session

**Track Classification:** Materials / Nanomaterials