

Supplementary information for Manuscript CP-ART-04-2012-041134

X-ray diffraction patterns of the LiCoO_2 (LCO) and $\text{LiNi}_{0.4}\text{Mn}_{0.4}\text{Co}_{0.2}\text{O}_2$ (LNMCO) samples

Experimental:

The X-ray powder diffraction experiments were performed using a STOE STADI/P powder diffractometer working in transmission mode. The used radiation was Mo $\text{K}\alpha_1$ ($\lambda = 0.07093$ nm), selected by a curved Ge (111) monochromator. The diffraction patterns were measured in the 2θ range $4\text{--}65^\circ$ and recorded using a linear position sensitive detector with a step width of 0.02° (2θ). Structure refinement was performed with the Rietveld method using the WinPlotR software package [1, 2].

Results:

The measured diffraction patterns of both samples are shown in figures 1 and 2, respectively. The pattern calculated using the Rietveld method, the difference plot and the reflection markers of the respective phases are also shown.

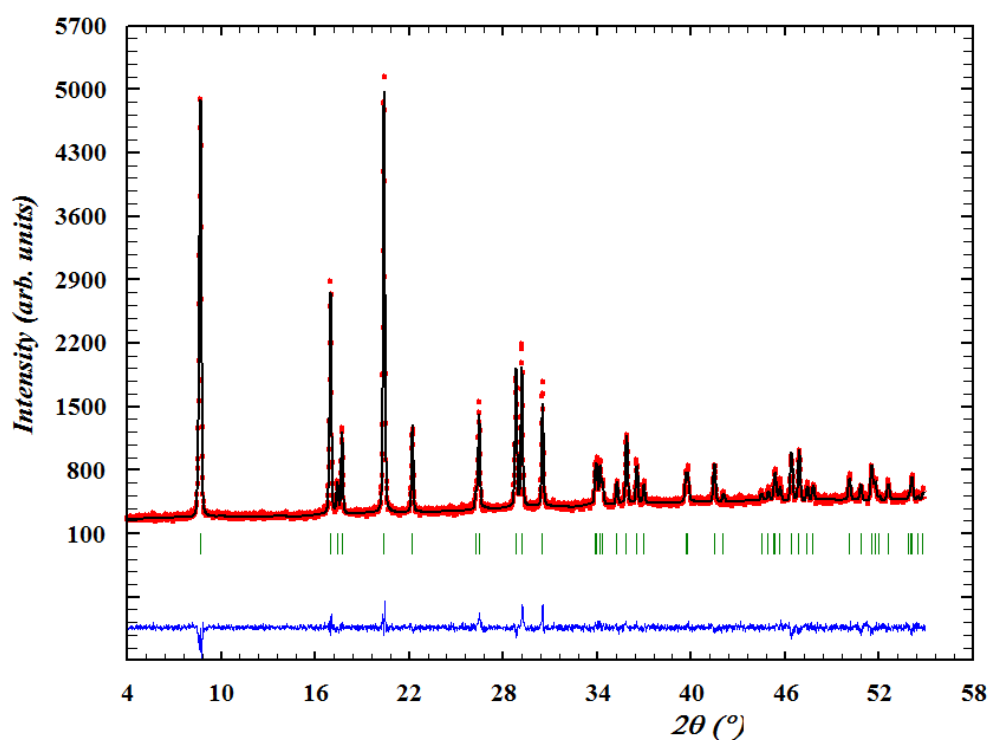


Figure 1: Calculated and measured diffraction pattern of LCO.

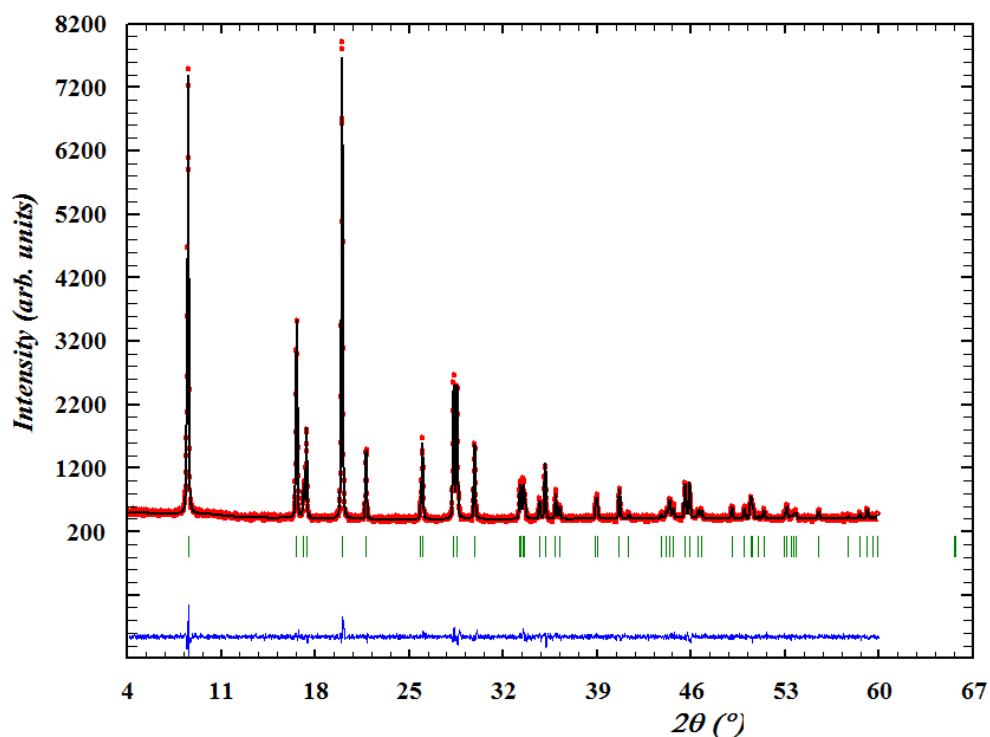


Figure 2: Calculated and measured diffraction pattern of LNMCO.

Both materials crystallize in the spacegroup R-3m (structure type α -NaFeO₂). The layered structure consists of Lithium ions on the 3b-sites, Cobalt (and Nickel and Manganese for LNMCO) on the 3a sites and oxygen on the 6c sites. Since for Nickel containing materials a slight cation mixing is reported [3], for the LNMCO sample an intermixing between Li on 3b and Ni on 3a was allowed during the refinement process. Both materials are single phase without additional phases detectable by XRD.

The results of the refinement are given in the following table:

Sample	a (Å)	c (Å)	Z _{Oxygen}	Ni on 3b	Chi ²	R _B	R _F
LCO	2.81650(6)	14.05926(49)	0.25816(36)	-	1.41	4.42	2.64
LNMCO	2.87620(5)	14.27692(42)	0.25809(42)	5.0(2)%	1.30	2.47	2.47

References

- [1] Roisnel, T. & Rodríguez-Carvajal, J. WinPLOTR: a Windows tool for powder diffraction patterns analysis. *Mater. Sci. Forum* **378-381**, 118-123 (2001).

- [2] Rodríguez-Carvajal, J. & Roisnel, T. FullProf.98 and WinPLOTR: New Windows 95/NT Applications for Diffraction. *Commission For Powder Diffraction, International Union for Crystallography Newsletter*, (Summer 1998)
- [3] Whittingham, M.S. Lithium Batteries and Cathode Materials. *Chem. Rev.* **104**, 4271-4301 (2004).