MS17. In situ and in operando crystallography

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MS17-O1 In-situ neutron scattering studies of Li-ion batteries

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The energy storage media based on Li-ion technology have received a broad use in different applications ranging from supplying of portable devices to large electric vehicles. Despite its overall advantages and popularity, the Li-ion technology possess numerous drawbacks, which cannot be overcome and require systematic and detailed research, e.g. on issues concerning safety, stability of electrode materials, capacity improvements, temperature, homogeneity etc.

Modern Li-ion batteries are sophisticated electrochemical devices, possessing numerous degrees of freedom along with complicated geometries of the electrode integration, which change their state immediately after opening. This calls for new dedicated experimental techniques capable to reveal the information about processes occurring inside the cell “live”. On the other hand the need for non-destructive battery testing eligible to minimize the risks for possible materials oxidation, electrolyte evaporation, cell charge changes *etc*. becomes of increasing importance in recent years.

In this sense neutron scattering has already been a well established tool for characterization of complex Li-containing systems [1], where the high penetration depths of thermal neutrons suits perfectly for non-destructive studies; the capability to localize light elements, e.g. hydrogen, lithium, provides excellent phase contrast; the neutron scattering lengths (not depending on sin(q)/l) give accurate structure factors leading to precise analysis of bond-length and Debye-Waller factor. In the current contribution the combination of two neutron-based experimental techniques, namely computed neutron tomography and neutron powder diffraction (both high-resolution and spatially-resolved), applied for studies on commercial Li-ion cells of the 18650-type (most common design with graphite and $LiCoO_2$ used as anode and cathode, respectively) will be presented. Different aspects of lithium-ion battery organization on different length scales vs. chemical composition, fatigue, state-of-charge, temperature will be presented and discussed in brief.

[1] H. Ehrenberg, A. Senyshyn, M. Hinterstein, H. Fuess (2012). In Situ Diffraction Measurements: Challenges, Instrumentation, and Examples. In E.J. Mittermeijer & U. Welzel (Eds.), Modern Diffraction Methods (528). Weinheim: Wiley-VCH.

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