

***In operando / situ* data collection and advanced data analysis of a commercial Li-Ion battery during charge/discharge cycles on a XRPD laboratory diffractometer**

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In situ / Operando data collection of XRPD data of commercial Li-Ion batteries is typically carried out on Synchrotron beam lines. This is due to the higher flux as well as the option to use high-energy radiation, both factors can be used to optimize the measurement conditions.

In this presentation we will show however that Rietveld quality data can be collected very quickly even on a XRPD laboratory diffractometer. We will discuss the used measurement geometry and instrumentation, which includes an X-ray tube with Silver anode and an area detector optimized for high energy X-rays, to rapidly collect high quality XRPD data during charge/discharge cycles.

Further we will show how to automatically extract valuable information from this huge amount of data, such as accurate phase quantities and crystallographic information. The data extraction is carried out using a complex fitting model consisting of Pawley phases to model the fixed components (Aluminum and Copper electrodes), Rietveld phases to model variable components, like $\text{Li}_{1-x}\text{CoO}_2$, LiC_6 , LiC_{12} + Carbon and Profile fit peaks to model the polymer separator.

In addition we will address how Cluster analysis can be used to group and pre-sort the huge amount of raw data that is generated during the experiment.