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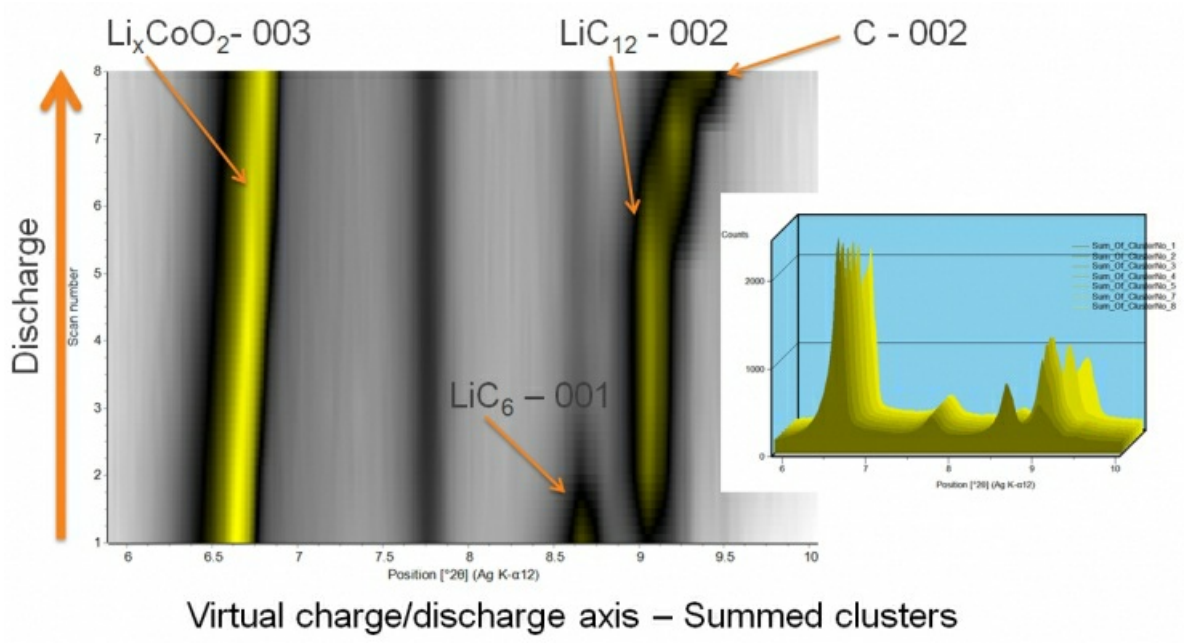
In operando data of Li-Ion batteries from XRPD laboratory diffractometers

Thomas Degen[1], Milen Gateshki[1], Mustapha Sadki[1], Detlef Beckers[1]
[1]*Development, PANalytical B.V., Almelo, Netherlands*
E-mail: thomas.degen@panalytical.com

Typically in operando / situ X-ray diffraction experiments of commercial Lithium-Ion batteries are carried out on synchrotron beam lines
due to the high brilliance sources and the possibility to use high-energy radiation. In this presentation however we will cover how to quickly collect high (Rietveld) quality XRPD data of commercial Lithium-Ion batteries during charge/discharge cycles on a laboratory XRPD diffractometer equipped with an X-ray tube with Silver anode and an area detector optimized for high energy X-rays. Further, we will discuss how to extract accurate phase quantities as well as crystallographic information automatically from multiple scans by using complex fitting model consisting of Pawley phases to model the fixed components (Aluminum and Copper electrodes), Rietveld phases to model variable components like Li1-xCoO2 , LiC6, LiC12 + Carbon and Profile fit peaks to model the polymer separator. Additionally 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. Cluster analysis can also be used for example to sort all scans of one or many experiments along a virtual charge/discharge axis.



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