MS44 Crystallography in large scale facilities

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Battery materials and diagnostics using advanced operando techniques

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Since the commercialization of lithium-ion (Li-ion) batteries by Sony in 1991, researchers have been extensively working on increasing the specific energy of both negative and positive electrode materials by replacing, respectively, graphite and LiCoO2 used therein. Although the specific energy of Li-ion batteries can be slightly increased, this nearly 30-year-old intercalation-chemistry-based battery technology is approaching its limitations. Thus, other battery chemistries based on Na-ion chemistry or on solid electrolytes have received considerable attention. During electrochemical cycling, these battery systems exhibit several changes at the bulk and the interface/surface levels, the investigation and understanding of which require new characterization tools. There are two different approaches to understand the reaction mechanism of electroactive materials during cycling, namely using either *ex situ* or *in situ*/*operando* modes. For the latter approach, the development of reliable electrochemical cells is of a prime importance (Figure 1). This is never an easy task though, since the design of such cells has to be adequate to the technique of a choice and its individual requirements. Once a proper design is, however, found, the surface, the bulk, the interphases, and finally the combination of these can be studied and the reaction mechanisms can be better understood and/or elucidated, thus further improving the battery technology. Through this talk, we will focus on the analysis of the electrochemical reactions occurring during cycling of selected materials by combination of different *operando*/*in situ* studies like X-ray diffraction, neutron diffraction, neutron imaging and X-ray tomographic microscopy etc.

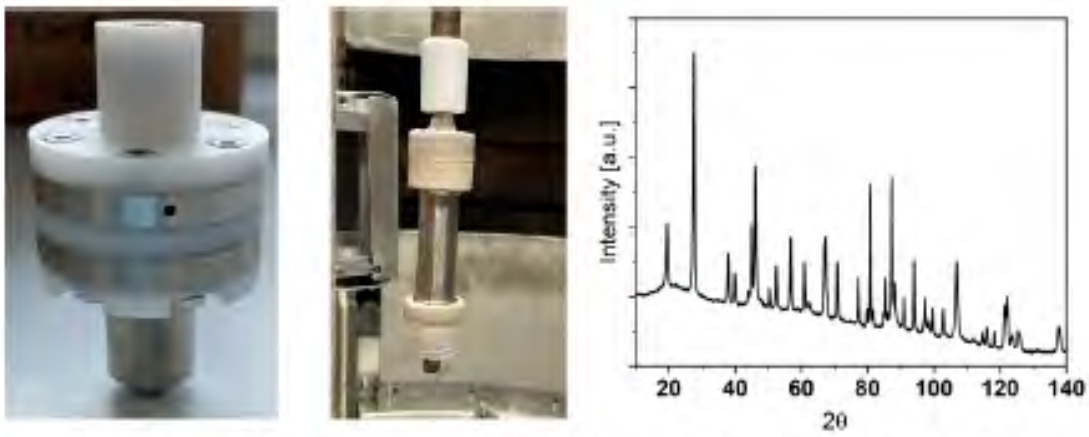

Figure 1, from left to right: Operando neutron diffraction cell for solid state batteries, operando neutron diffraction cell for liquid-based batteries, and the corresponding neutron diffraction pattern of a full cell composed of Li-rich NMC and graphite.