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In situ x-ray and neutron diffraction to investigate the solid-state synthesis reactions of battery materials

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In situ diffraction studies can capture transient crystalline phases forming during chemical reactions. Whether the reaction is a chemical solid-state synthesis, or an electrochemical intercalation process within typical layered compounds used as battery electrodes, proper sample environments can nowadays be developed to perform in situ diffraction experiments. Furthermore, operando studies, in the case of batteries, can be used to capture the materials´ evolution during the realistic functioning of the device.
In both cases, the time-resolved nature of the experiments allows to obtain a greatly increased amount of information. For example, in the synthesis of inorganic materials, reactions often yield non-equilibrium kinetic byproducts instead of the thermodynamic equilibrium phase [1]. To rationalize that, the competition between thermodynamics and kinetics occurring during the process need to be investigated in real time. Fully determining the reaction pathway potentially is a key requirement to achieve the rational synthesis of target materials [2, 3]. In this presentation, recent examples from our work applying in situ synchrotron and neutron diffraction to understand the synthesis of relevant industrial compounds such as LiNiO2 [4] and doped version thereof [5] will be reported and compared. The use of neutrons as possible probes with Li sensitivity for such reactions, targeting large sample amounts comparable to common laboratory furnaces, will be discussed in particular detail.

References:
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