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A New Measuring Cell for Operando Neutron Diffraction on Li-Ion Battery Cathode Materials

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The use of operando diffraction has taken a major step forward, in no small part due to the increase in flux at large scale facilities such as synchrotrons and neutron spallation sources. While the X-rays are absorbed by the battery casing which necessitates special cells with windows, neutrons have a penetration depth large enough to probe the entirety of cell. This has allowed measurements directly on commercial batteries, giving unique insights into the evolution of cell parameters and composition of the cathode and anode phase, but also showing Li-consumption by decomposition of the electrolyte and plating of lithium metal.
When measuring on commercial cells, contributions from all parts of the cell are observed which complicates the analysis of the diffraction data. A desire also exists to measure on non-commercial electrode materials prepared in the lab. Thus, there exists an incentive to develop a measuring cell which allows easy measurement on a variety of different cathode materials, either commercial or synthesized.

In this work, we present a new operando neutron diffraction battery cell, especially designed for the new beamline ErwiN at the FRM-2 research reactor outside of Munich, Germany. The cell uses a Zr/Ti-alloy with negligible scattering strength to eliminate contributions from the casing. We present data on the commercial cathode materials LiFePO4 and LiNi1/3Mn1/3Co1/3O2 to demonstrate the capabilities of the cell, as well as on the non-commercial cathode material Li3V2(PO4)3. Li3V2(PO4)3 is interesting, as it has the highest gravimetric capacity among the known phosphates (197 mAh g-1). The material displays a complex series of phase transformations during charge and discharge, and interestingly, these transformations are very dependent on the number of Li-ions extracted during charging. The material has been investigated using operando synchrotron X-ray diffraction, but operando neutron diffraction is important to uncover the exact nature of the Li-ion dynamics.

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