Probing the origins of electrochemical properties in electrodes for lithium ion batteries through *in operando* diffraction

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In operando diffraction methods are widely employed to qualitatively follow the reaction progression in operating battery electrodes. However, performing thorough structural analysis with the aim of understanding the origins of battery performance during electrochemical cycling is significantly less common. There exists a unique opportunity to further exploit *in operando* diffraction to extract detailed information on the dynamic changes taking place to the electrode materials during battery operation. With careful experimental design, *in operando* methods provide a unique perspective on understanding the electrochemical processes in electrode materials. Tracking the rate of phase conversion throughout a battery electrode, for example, provides insight into the competing sources of resistance in an electrode under different cycling conditions. Further, subtleties in the electrochemical reaction of battery electrodes, such as differences in structural changes between lithium insertion and extraction from a host material, can be identified.

By changing the focus from simple phase identification towards more detailed structural analyses, *in operando* neutron diffraction becomes increasingly attractive. While there has been rapidly growing interest in performing *in operando* neutron diffraction experiments for lithium ion batteries, it remains a relatively inaccessible technique due to the difficulty of preparing custom cells with adequate electrochemical performance. Multiple custom cells inspired by commercial cell designs have been investigated within our group with the aim of fine tuning the electrochemical performance while maintaining high quality diffraction data for Rietveld analysis.

Using $LiFePO_4$, $LiNi_{0.5}Mn_{1.5}O_4$ and $LiFeSO_4F$ as case study materials, this contribution will focus on investigations of electrochemical properties of battery electrodes using the dynamic structural response taking place during cell operation.

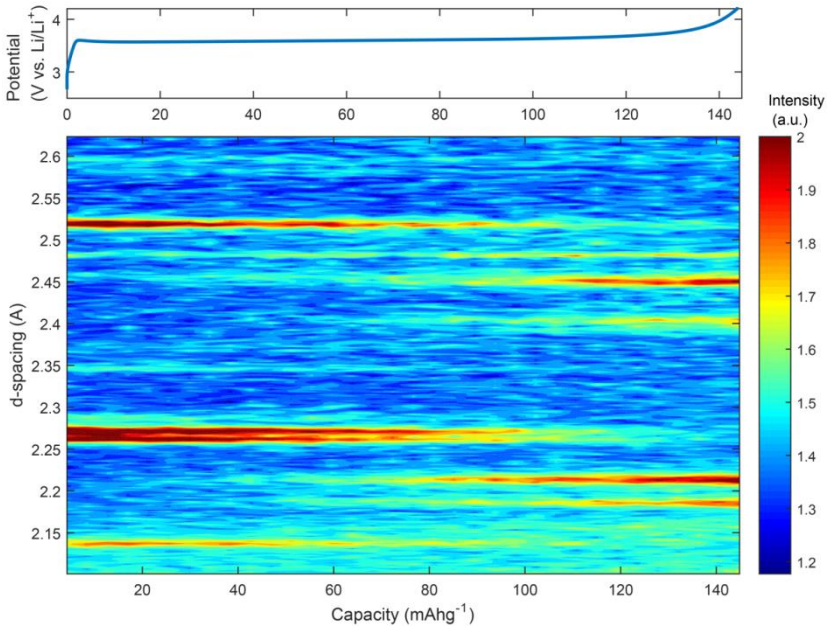

Figure 1: Contour plot of the first discharge of $LiFePO_4$ in a coin cell showing the two phase conversion reaction.