

Operando XRD-CT investigation of a BiVO₄ anode

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Lithium ion batteries are today's most significant rechargeable battery technology. To further improve the technology, development of novel electrodes with higher gravimetric and/or volumetric capacity is required to enable lighter and smaller batteries. To do this, fundamental understanding of reactions and mechanisms in the electrodes during operation is crucial.

We have investigated the (de-)lithiation processes in BiVO₄ using X-ray diffraction computed tomography (XRD-CT). By this method using our purpose-built operando battery cell, we remove the signal from the electrolyte, current collectors, counter electrode and casing, allowing specific insight to the reactions at the electrode. Furthermore we analyse the diffraction data using both conventional crystallography and total scattering methods, pair distribution function analysis (PDF), allowing us to not only follow the crystalline phases, but also nano-crystalline species. Tomographic images of the anode can be reconstructed from either the XRD or PDF data.

In Figure 1, the 1st discharge (top left) with corresponding measurement times (marked with ■) with $G(r)$ as a function of radial distance (Å) (top right) and $I(q)$ as a function of $Q(\text{Å}^{-1})$ (middle). The descending plots goes from the pristine BiVO₄ to the fully lithiated material. We clearly see the loss of all long-range structure in BiVO₄ during the initial stages of lithiation. However, from the PDF we can still follow the local structure in the electrode. From our results it is possible to identify nanocrystalline intermediates Bi and LiBi, as well as the fully lithiated phase Li₃Bi, giving insight to the differing lithiation and delithiation mechanisms in the electrode.

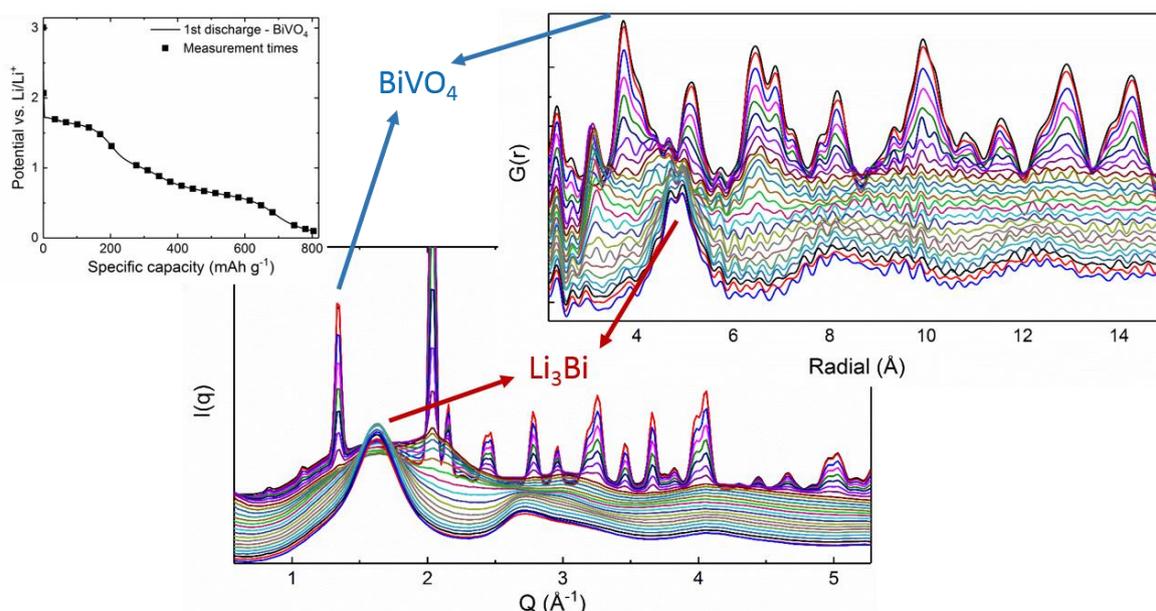


Figure 1: Discharge curve for BiVO₄ (top left), with $G(r)$ as a function of radial distance (Å) (top right) and $I(q)$ as a function of $Q(\text{Å}^{-1})$ (middle). Descending scans goes from the pristine BiVO₄ (top scan) to the fully lithiated material (bottom scan).