MS20 Electric, opto-electronic and magnetic properties from elastic and inelastic scattering plus properties of materials from quantum crystallography

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Understanding the high-voltage crystallographic and electronic structure evolution in Li-ion battery cathodes through X-ray diffraction, scattering and spectroscopy

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Abstract

Increasing the nickel content of Li-M-O2 (M = transition metal) layered oxide cathodes in Li-ion batteries has led to the development of LiNi0.8Mn0.1Co0.1O2 (NMC811), which is touted to be a key player in the next-generation of electric vehicle batteries. NMC 811 is nearing industrial maturity when operated standard voltage window i.e. 3.0–4.2 V. Increasing the voltage window will further increase energy density by extracting more lithium ions but leads to rapid degradation associated with bulk structural and electronic changes together with surface oxygen loss. In the degradation regime, bulk O2- participate in the charge compensation but it remains unclear its role in driving degradation.

Here, we report on the latest in-house operando X-ray diffraction and the Ni K-edge X-ray absorption near-edge structure (XANES) studies of NMC811–Graphite LIB pouch cells built on the Battery Pilot Line at WMG (Warwick Uni.). This approach enables the synchronous tracking of the dynamic crystallographic and electronic structure changes in NMC811, specifically the collapse of the layered structure during delithiation and the associated changes in the Ni oxidation, over extended periods of cycling. We correlate the high voltage transformations with changes in the oxygen oxidation state using O K-edge resonant inelastic X-ray scattering in the regime where oxygen-loss induced degradation is pronounced.