Abstract #551, 224th ECS Meeting, © 2013 The Electrochemical Society

The Origins of An Unsafe Li Battery: the Fundamentals of Oxygen Evolution From Cathodes Interrogated With *In Operando* Soft X-Ray Absorption Studies

Faisal M. Alamgir* and Cole Petersburg

School of Materials Science and Engineering
Georgia Institute of Technology

The danger inherent in lithium-ion batteries has been highlighted by recent high-profile thermal runaway incidents in aircraft. Since the batteries in these cases were largely destroyed before they could be analyzed for defects, these unfortunate incidents underscore the need for *in operando* characterization of the active materials. Research on cathode materials, which are often suspected to initiate thermal runaway reactions, are typically done ex-situ, hiding, therefore, the dynamic processes of species such as oxygen. In this work, a new *in operando* technique is used to delithiate powder-based cathode materials while performing soft X-ray spectroscopy.

Hard X-ray absorption near-edge spectroscopy (XANES) on LiMO2-based Li batteries reveals that although the charge compensation mechanism is based on TM ion oxidation, some of the reversible charge capacity cannot be explained: oxygen is suspected of oxidizing to compensate charge lost to delithiation. In order to probe the oxygen 2p and TM 3d orbitals in these cathodes, we have developed a new all solid state *in operando* cell that allows us make near-edge X-ray absorption fine structure (NEXAFS) using soft X-rays. The absence of a liquid electrolyte in this novel cell design allows studies of the cathode, anode and electrolyte surfaces and interfaces during battery charging. In $LiMO_2$ cathodes, oxidation of oxygen is revealed to proceed in series or in parallel with TM oxidation, thereby explaining the fundamental origins of oxygen evolution. Applications of this operando cell to further studies of gas exposure and gas evolution experiments will be discussed.