in-situ and ex-situ characterization of lithium ion batteries using x-ray and neutron diffraction methods

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This talk will provide an overview of past, present, and ongoing research efforts at ORNL and elsewhere using x-ray and neutron scattering methods in support of lithium-ion battery research. Considerable effort continues around the world with the objective to develop safer, longer-lasting, higher capacity, and more efficient batteries for electrical energy storage. Battery designs are constrained by the intended application, with transportation-related batteries having to meet particularly challenging targets for storage density (to reduce size and weight), voltage fade and other degradation issues, recharging times, etc. For the case of lithium-ion batteries, understanding these changes in properties requires a detailed knowledge of the crystal structures, phase transformations, and interactions in the anode, cathode, and electrolyte materials, and characterization by diffraction is a powerful approach for obtaining essential quantitative data.

The experiments required to support research on these battery systems provide an excellent example of the complementary value of x-ray and neutron diffraction methods. X-rays are very well suited for ex-situ and in-situ studies on lithium ion batteries, as they are a good match to many of the common battery geometries (e.g., thin-films, coin cells, pouch cells). It is straightforward to build suitable sample holders to utilize laboratory XRD instruments for this purpose, though synchrotron XRD instruments provide both higher resolution and higher flux, resulting in several important benefits. Synchrotron and neutron sources can be accessed through “user programs” at numerous facilities around the world, though the value of laboratory-scale XRD should not be overlooked. Neutron diffraction is more sensitive to scattering from the lithium ions, and is therefore well suited to the study of these systems, and can also provide spatially-resolved in-situ data on working batteries, often without much (or any) modification of standard battery cells. Additional x-ray and neutron scattering techniques of value to battery research such as reflectometry and imaging/tomography will also be discussed.