Recent Development of Operando Neutron Diffraction and Its Application in Studying Energy Storage Materials

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Neutron scattering has unique advantages for battery research. Neutron scattering is very sensitive to light elements (e.g., H, Li, C, and O), which are the most important ingredients for rechargeable Li/Na-ion batteries. It can also distinguish adjacent transition metal (TM) cations (e.g., Mn, Fe, and Ni) in battery cathodes, especially when conducting isotope substitution experiments. This capability allows accurate investigation of how cation arrangements affect the electrochemistry performance of various rechargeable battery cathodes. Neutron scattering can also be used to probe dynamics, particularly ligand anion vibration/lattice dynamic and ionic diffusions, in both electrode and electrolyte materials.

Moreover, the strong penetration and nondestructive nature of neutron scattering makes it an ideal tool to characterize battery materials without damaging the sample or disturbing the electrochemical reactions, as often occurs with high-energy x-ray diffraction. Despite all these advantages, the use of neutron scattering (e.g., diffraction, quasi-elastic and inelastic scattering) for battery research has often been confined to ex situ studies of pristine or postmortem samples recovered from charged/discharged batteries. Although they may provide useful information about the functionality of individual components (e.g., cathode or anode), they often fail to provide key insights about what governs the battery performance. Furthermore, many charged or cycled materials are metastable, and recovered ex situ samples often differ from those under real operational conditions. Thus, developing operando neutron scattering capability for battery research, with the needed spatial/temporal resolution, is highly desired to fully unleash the unique advantages of neutron scattering. In this talk, I will present our recent efforts on developing neutron diffraction friendly in situ electrochemical cells, sample environments and related data reduction and analysis routines. Particularly, I will present the first high throughput operando neutron diffraction study of the conventional Li-ion batteries, and the recent breakthrough of operando neutron diffraction study of all solid-state batteries at NOMAD. Impacts of these recent developments and their applications in the field will also be discussed.