Phase Transformation and Chemomechanical Properties of Alkali Metal Ion Cathode Materials

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Chemical and mechanical properties interplay on the nanometric scale and collectively govern the performance of battery materials. Understanding the relationship between the two can inform the design of battery materials with optimal chemomechanical properties for long-life lithium and sodium batteries. The chemomechanical properties of cathode materials are associated with phase transformation behaviors and can promote the cathode–anode crosstalk in electrochemical cells, leading to the complication of the full cell electrochemistry. In this presentation, we will first discuss an integrative approach of mapping valence states and constructing chemical topographies to investigate the redox phase transformation in layered oxide cathode materials at the secondary particle level under thermal abuse conditions. Then, we will discuss a mechanism of nanoscale mechanical breakdown in layered oxide cathode materials, originating from oxygen release at high states of charge. Owing to the oxygen release, sporadic phase transformations from the layered structure to the spinel and/or rocksalt structures introduce local stress, which initiates microcracks along grain boundaries and ultimately leads to the detachment of primary particles. Finally, we will highlight some methods that we have developed to overcome chemomechanical breakdown.