In Operando Strain Evolution in Sodium Chromium Oxide Cathode for Na-Ion Batteries during Battery Cycling

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Layer-structured Na intercalation compounds such as Na_xMO_2 (M=Co, Mn, Cr) have attracted much attention as cathode materials for sodium-ion batteries due to their high volumetric and gravimetric energy densities. Among them, $NaCrO_2$ with layered rock salt structure is one of the promising cathodes since $NaCrO_2$ has a desirable flat and smooth charge/discharge voltage plateau.[1] In addition, $NaCrO_2$ has the highest thermal stability at charged state which makes it a potentially safer cathode material.[2] The $NaCrO_2$ exhibits a reversible capacity of 110 mAh g^{-1} with good cycling performance.[3] However, the transition metal oxide (TMO) cathode materials in NIBs undergo severe chemo-mechanical deformations which leads to capacity fade and poor cycling and is the limiting factor of NIBs. The electrochemical characterization and examination of the electrode structure were the primary focus of several investigations. To improve the lifespan and performance of electrode materials for Na-ion batteries, it is vital to comprehend how Na ions impact the chemo-mechanical stability of the electrodes.

In this talk, we will discuss the driving forces behind the structural and interfacial deformations on $NaCrO_2$ cathodes. Digital image correlation measurements were conducted to probe strain evolution in the electrode during cycling. The free-standing composite $NaCrO_2$ electrode was used for stain measurements in custom-cell assembly. The battery was cycled against Na metal in 1 M $NaClO_4$ in PC. The first part of the study involves structural and interfacial deformations in the lower voltage range of 2.3 V to 3.5 V where $x<0.5$ in Na_xCrO_2. And the second part focuses on the structural and interfacial deformations in the voltage range of 2.3 V to 4.7 V where $x>0.5$ in Na_xCrO_2. In the preliminary studies, we observed that the initial insertion of Na ions leads to negative strain evolution (contraction) in the electrode, followed by expansions in the electrode at a higher state of discharge. Similar phenomena are also observed during charge cycles, where extraction of Na results in an initial contraction in the electrode, followed by expansion at a higher state of charge. Understanding the mechanisms behind chemo-mechanical deformations will allow to tune structure & material property for better electrochemical performance.

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