

## Structural characterization of $\text{NaNi}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$ cathode material for Rechargeable Sodium-Ion Batteries

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Layered sodium-ion battery cathode material, O3-type  $\text{NaNi}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$ , was systematically investigated by using Synchrotron-based X-ray techniques to characterize the structural behavior during electrochemical process. X-ray Absorption Spectroscopy (XAS) shows the reversible electronic structural changes during  $\text{Na}^+$  deintercalation/intercalation and that Ni and Fe are both active in  $\text{Na}_{1-x}\text{Ni}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$  cathode and redox couples of  $\text{Ni}^{2+}/\text{Ni}^{3+}/\text{Ni}^{4+}$  and  $\text{Fe}^{3+}/\text{Fe}^{4+}$  are responsible for the reaction mechanism. High Resolution Powder Diffraction (HRPD) results reveal that O3-type ( $R\bar{3}m$ ) phase transforms into a P3 ( $R3m$ ) structure coupled with  $\text{Na}^+$ /vacancy ordering during charge and further elucidate the final P3-OP2 of phase transformation on over-sodiated state. Moreover, internal Fe migration occurs from octahedral site into tetrahedral site, which is possible due to formed vacant space by highly deintercalation of Na ions and this atomic level of movement causes the layered structure to have structural distortions. An in-depth analysis of the structural behavior and reaction mechanism for  $\text{NaNi}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$  cathode material when the Na ions are used of the entire composition widens an electrochemical perspective and suggests a direction where we better understand the nature of structure which can be used as the cathode for the advanced rechargeable batteries with high energy density. More details will be discussed in the meeting.