

Structural transformation in a $\text{Li}_{1.2}\text{Co}_{0.1}\text{Mn}_{0.55}\text{Ni}_{0.15}\text{O}_2$ lithium-ion battery cathode during high-voltage hold

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Supplementary information

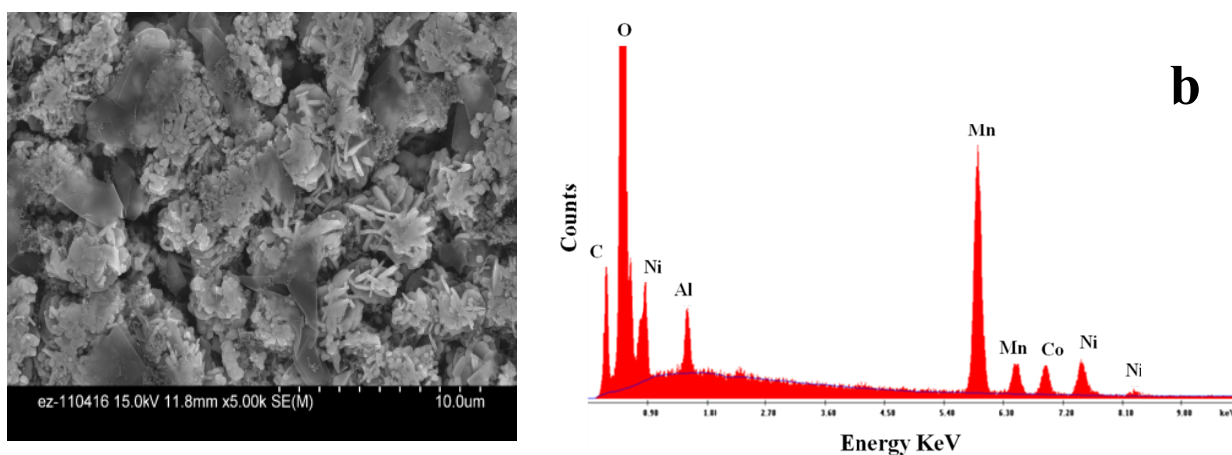


Figure S1: Scanning Electron micrograph of $\text{Li}_{1.2}\text{Co}_{0.1}\text{Mn}_{0.55}\text{Ni}_{0.15}\text{O}_2$ electrode (a) and collected energy dispersive x-ray (EDAX) (b) from the whole area. The EDAX shows the Co:Mn:Ni ratio as 0.11:0.54:0.15 which confirms the material composition as $\text{Li}_{1.2}\text{Co}_{0.1}\text{Mn}_{0.55}\text{Ni}_{0.15}\text{O}_2$.

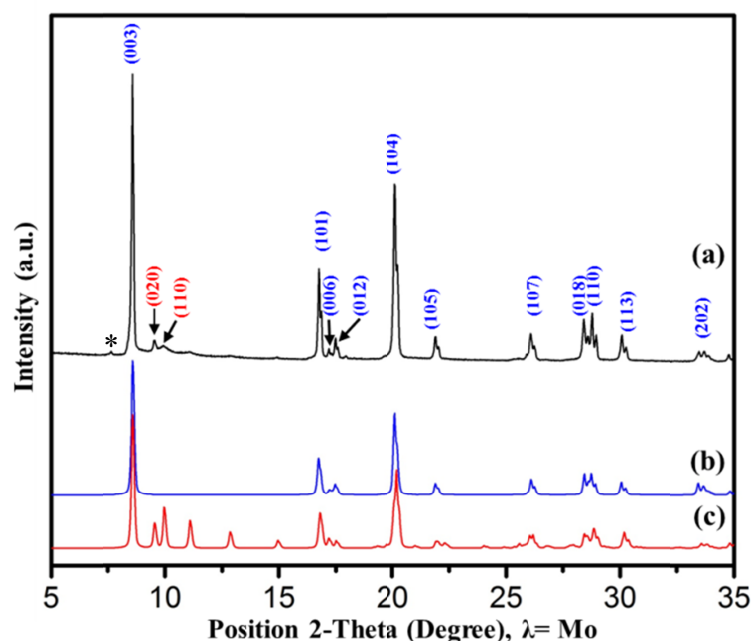


Figure S2: *Ex-situ* powder XRD of starting $\text{Li}_{1.2}\text{Co}_{0.1}\text{Mn}_{0.55}\text{Ni}_{0.15}\text{O}_2$ (a) along with the calculated patterns of rhombohedral (PDF # 00-056-0147) (b) and monoclinic (PDF # 04-011-3411) phase (c). The major reflections (marked as blue) in the experimental pattern are indexed with rhombohedra unit cell and (020) and (110) reflections (marked as red) confirms the cation- ordering in the transition metal layer
* represents the MoK β peak.

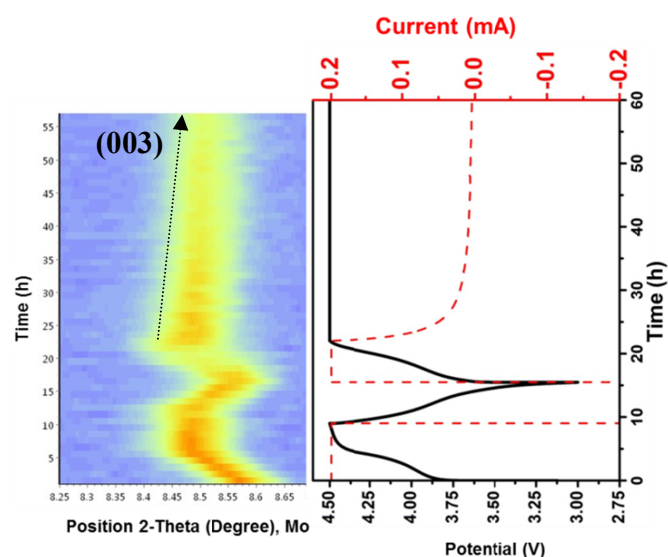


Figure S3: Isoplots of (003) peak of $\text{Li}_{1.2}\text{Co}_{0.1}\text{Mn}_{0.55}\text{Ni}_{0.15}\text{O}_2$ as a function of charge, discharge and high-voltage hold. During hold at 4.5 V, (003) peak shifts to the higher 2θ angle indicating decrease in c -lattice parameter.

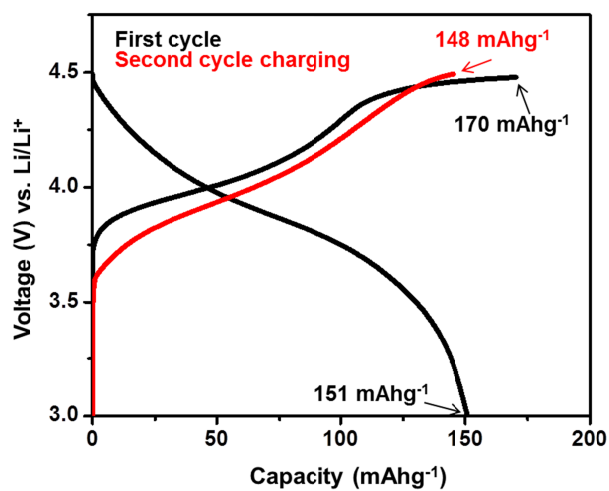


Figure S4: Voltage and capacity profile during first and second cycle

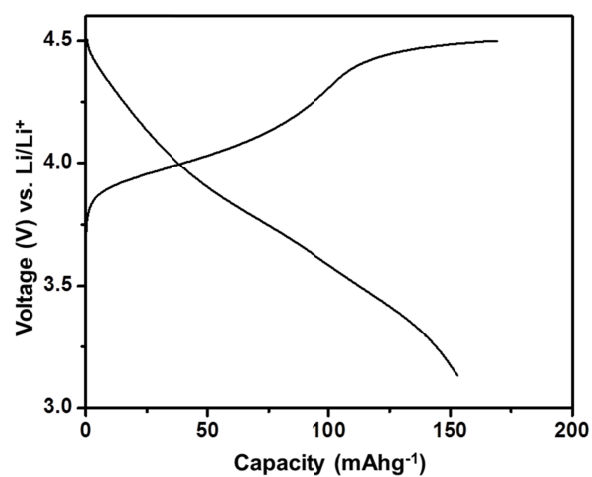


Figure S5: Electrochemical capacity curves from the ex-situ experiment by using regular coin cell (first cycle)