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Synthesis, structural and Electrochemical Study of O3-NaMn_{0.4}Co_{0.2}Ni_{0.4}O₂ as cathode material for Na-ion Batteries

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Abstract

Hexagonal layered O3-NaNi_{0.4}Mn_{0.4}Co_{0.2}O₂ is prepared by mixed hydroxide solid state reaction method at an optimum temperature of 800 °C. Rietveld refined PXRD pattern reveals single phase formation with space group R-3m. Galvanostatic electrochemical studies reveal reversible sodium de-insertion/insertion with concomitant structural phase transitions. In the voltage window of 2.2 - 3.8 V, the first discharge capacities are 150 and 135 mAh g⁻¹ at C/20 and C/6.5 current rates, respectively. The capacity retention is 80% after 33 discharge cycle at C/20 rate and 78% after 40 discharge cycle at C/6.5 rate. When the voltage window is increased to 1.6 - 4.5 V, the initial discharge capacity is 173 mAh g⁻¹ at C/10 rate and a capacity retention of 63% is observed after 10 discharge cycle. The O3 phase undergoes a series of structural transformations from O3, O'3, P3, P'3 and P3" during charging and reverts to O3 phase upon de-insertion of Na during discharge. Structural stability is evident from ex-situ XRD studies even after 33 cycles, when cycled in the voltage window of 2.2 - 3.8 V at C/20 rate.

Keywords: Electrochemical study; Na -ion batteries; Layered metal oxides; NaNi_{0.4}Mn_{0.4}Co_{0.2}O₂