

Lithium-ion Migration in Layered $\text{Li}_{1.06}\text{Ni}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ Cathode Materials Synthesized at Different Temperatures

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We examined the effects of synthesis temperature on the structural and electrochemical properties of layered $\text{Li}_{1.06}\text{Ni}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ cathode materials synthesized by co-precipitation. Scanning electron microscopy showed that a higher synthesis temperature resulted in a bigger primary particle size. Rietveld refinement revealed that the content of nickel ions at the 3b site decreased from 0.041 to 0.038 and subsequently increased to 0.064 as synthesis temperature rose from 800 to 980 °C. The incircle/circumcircle radii of the tetrahedral sites providing space for lithium-ion migration increased gradually with synthesis temperature. The $\text{Li}_{1.06}\text{Ni}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ sample synthesized at 920 °C displayed the optimal electrochemical performance, delivering a discharge capacity of 181.6 mAhg⁻¹ and initial coulombic efficiency of 84.2% at 0.1C between 2.5 and 4.5 V. Our analysis indicates that the level of cation mixing and the incircle/circumcircle radii of tetrahedral sites in $\text{LiNi}_x\text{Co}_y\text{Mn}_z\text{O}_2$ are the main factors that affect its electrochemical performance rather than primary particle size.

Keywords: Layered cathode materials; Cation mixing; Tetrahedral for Li-ion migration.

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