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Structure and Morphology Study of Co-Precipitated $LiNi_{0.65-x}Co_{0.24+x}Ti_{0.1}Al_{0.01}O_2$ (x = 0.0 , 0.1 , 0.2) Materials

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Structured Abstract

Background: Lithium-ion batteries are widely used due to their high energy density, long cycle life, and efficiency. Enhancing their performance relies heavily on selecting stable and high-capacity cathode materials. Ni-rich layered oxides such as $LiNi_{0.65}Co_{0.24}Ti_{0.1}Al_{0.01}O_2$ (NCTA) offer strong potential, with stoichiometry crucial for controlling cation ordering and reducing Ni^{2+}/Li^{+} mixing. Proper element ratios stabilize the layered structure, limit phase transitions, and improve cycling durability. Thus, optimized NCTA compositions enhance structural integrity and overall battery performance.

Methods: The synthesis was conducted via co-precipitation, in which all precursors were thoroughly homogenized by continuous stirring for 4 hours. The mixture was then filtered and repeatedly washed with deionized water to remove residual impurities. After filtration, the sample was dried overnight and subsequently pre-sintered at 480 °C for 5 hours. This was followed by high-temperature annealing at 700 °C for 15 hours. After annealing, the product was washed for 15 minutes and dried again overnight in a vacuum oven. The final powder was characterized using X-ray Diffraction (XRD) to determine its crystal structure and Field Emission Scanning Electron Microscopy (FESEM) equipped with Energy Dispersive X-ray Spectroscopy (EDX) to analyze its morphology and elemental composition.

Results: XRD results confirmed a single-phase layered α-$NaFeO_2$ structure ($R\bar{3}m$) with no impurities. Among the samples, $LiNi_{0.65}Co_{0.24}Ti_{0.1}Al_{0.01}O$ showed the highest RIR value (1.09), indicating lower cation mixing and better structural stability compared to $LiNi_{0.75}Co_{0.14}Ti_{0.1}Al_{0.01}O_2$ and $LiNi_{0.85}Co_{0.04}Ti_{0.1}Al_{0.01}O_2$ (0.96 and 0.92). FESEM revealed smaller, more uniform crystallites for $LiNi_{0.65}Co_{0.24}Ti_{0.1}Al_{0.01}O_2$, while EDX confirmed a homogeneous distribution of Ni, Co, Ti, and Al consistent with the target composition. The measured atomic ratios were Ni (64.03–65.20 at.%), Co (24.09–24.51 at.%), Ti (9.36–10.05 at.%), and Al (1.29–1.72 at.%). These results show that stoichiometry strongly affects structural quality.

Conclusion: The findings indicate that modifying the stoichiometry of Ni-rich cathode materials significantly influences their structural stability and morphological characteristics. The $LiNi_{0.65}Co_{0.24}Ti_{0.1}Al_{0.01}O_2$ material demonstrated superior crystallinity, reduced cation mixing, and enhanced morphology, making it a more promising candidate for lithium-ion battery applications.

Keywords: Lithium-ion batteries, co-precipitation method, XRD, Pumping system, NCTA

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