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TRI-TRANSITION METAL OXIDE CATHODE MATERIALS WITH CHEAPER ALKALINE METAL ADDITIVES FOR LITHIUM-ION RECHARGEABLE BATTERIES

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ABSTRACT

Layered tri-transition metal oxides, specially LiNi1/3Co1/3Mn1/3O2 (NMC 333), have become a promising cathode electrode material in the rechargeable Lithium-Ion Battery (LIB). The electrochemical performances of NMC 333, mainly depend on its crystallographic structural properties including lattice parameters, dislocation density(δ), and lattice strain. In this study, the Pechini method, which is a low-cost wet chemical technique, was used for synthesizing K+ doped Li1−xKxNi1/3Mn1/3Co1/3O2, (x = 0, 0.04, 0.08) materials. The crystallographic structural properties of the synthesized materials were characterized using X-ray diffraction (XRD). In the refinement of XRD data, the reliability factor of $\chi 2$ and Rwp were found to be less than 3 with weighted factors of less than 10%, confirming an acceptable refinement. XRD confirmed the formation of a single-phase layered hexagonal α-NaFeO2 structure (R-3m space group) without any impurity phase for all prepared materials. Li0.96K0.04Ni1/3Mn1/3Co1/3O2 showed the optimum crystallographic properties with a better splitting of the (006)/(102) and (108)/(110) peaks. The crystallite size of Li1−xKxNi1/3Mn1/3Co1/3O2, (%) materials were 77.4 nm, 128.38 nm, and 122.6 nm for x = 0.00, 0.04, and 0.08 nm respectively. Scanning Electron Microscopy of synthesized materials showed sponge-like agglomerates, with well-defined compact and larger primary particles. The peaks observed at 479 and 596 cm−1 in Raman spectroscopy could be assigned to Raman-active species Eg and A1g modes for Li1−xKxNi1/3Mn1/3Co1/3O2, (x = 0, 0.04, 0.08) materials. Altogether, this study reveals that the addition of K+ by substituting Li+ improves the structural stability hence the potentiality of NMC 333 materials for the cathode of LIB.

Keywords: NMC materials, Na doping, K doping, Li-ion battery, Pechini method