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Probing Thermal Degradation of Li-ion Battery Layered Oxide for NMC 333 Cathodes by Neutron Diffraction

Lithium-ion batteries employing $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC333) cathodes face critical safety challenges due to oxygen release and structural collapse at elevated temperatures. This study combines in-situ neutron total scattering (NOMAD beamline, SNS) and operando gas analysis to resolve atomic-scale structural dynamics and gas evolution during thermal degradation (25–550℃). This work aims to determine critical temperatures for layered oxide in NMC 333 cathode material during structure degradation, oxygen gas release, and structural phase transition. Results demonstrate that abnormal change in average bond length for Li-O and Me-O, changes in cell parameters a, c, and cell volume indicate temperatures at which "hidden"phase changes take place. Structural evolution correlates with changes in Ni occupancies at atomic sites, revealing phase transitions. Evolution of oxygen compliments information about temperature ranges with phase transitions. There are additional slope changes in cell parameters as function of temperature not explained with Rietveld analysis results. Beyond long-range order, PDF function provides information about short-range order in local atomic structure and reveals more complex mechanisms for structural evolution. These findings will enable targeted diagnostic metrics for early thermal runaway detection, and targeted suppression of oxygen release via Ni-site stabilization which can aid in design of cathode materials with improved thermal stability.

Topical Area

Hard matter: energy materials

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