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Structural response of electrochemically cycled $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ ($0 < x < 1$) battery cathodes

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In view of increasing greenhouse gas emissions, the demand for renewable energies is rising in parallel with the demand for energy storage materials. Thus, the development of lithium ion batteries with high nickel content paves the way towards better cycling stability, higher energy and power densities at lower costs. One of them is the commercially available state-of-the-art 18650-type battery of $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ (NCA) and graphite chemistry, also used in the Tesla Model S of 1st generation [1,2]. The overall cell performance to large extent is limited by the diffusivity of Li-ions in the NCA structure, which becomes important in the context of the on-going discussion about occurrence of antisite disorder in nickel rich cathode materials, where the exchange of Ni^{2+} and Li^+ leads to the blocking the diffusion pathways of Li-ions. Such processes typically result in the rapid degradation of the cell capacity as well as in structure instabilities of various kinds [3,4]. Especially for NCA materials, presence of antisite defects at different lithiation levels is often controversial and studied poor in literature. Therefore, in the present contribution the structural response of delithiated NCA electrode materials obtained from commercial 18650-type lithium-ion batteries was investigated by a systematic ex-situ powder diffraction study on the instrument SPODI at the FRM II reactor in Garching. The structural parameters were modeled by full-profile Rietveld refinement. During electrochemical cycling, the lithium occupancy was found to decrease linearly with higher charge states, which was confirmed by chemical ICP-OES measurements, that agree well with the on-going delithiation. The remaining transition metal occupancies showed consistent behavior during electrochemical cycling, demonstrating the absence of Li/Ni antisite defects in the structure of NCA materials.

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