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# Understanding Li/Ni disorder effects in NCA-type battery cathodes

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The replacement of combustion engines by battery-powered electric drivetrains is one of many important steps in order to reduce the emission of greenhouse gases on the way to a green future. Thus, the demand on Li-ion batteries with higher capacities, energy/power densities and cycling life is increasing. Based on these requirements different kinds, of commercial used mixed lithium transition metal oxide cathode materials have been developed. One of the most encouraging cathode material is high nickel content  $\text{Li}_{1-x}\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$  (NCA), crystallizing in a  $\text{NaCrS}_2$ -structure type and possessing high power/energy densities at lower costs and increased safety due to the minimized amounts of costly, rare and reactive cobalt [1, 2]. However, nickel-containing LIBs show poor thermal stability, capacity and power fading, as well as an efficiency loss due to the blocking of the 2D diffusion pathways of Li-ions caused by mixed occupations of Li/Ni (cation mixing) in the cathode. In order to address the problem of cation mixing ex situ neutron powder diffraction at the high-resolution powder diffractometer SPODI (FRM II) was applied on extracted NCA materials harvested from a series of 18650-type cells charged to different states. The collected structural data was modeled using full-profile Rietveld refinement and obtained results were discussed dependent on its electrochemical behavior. A decreasing character of lithium concentration upon cell charging along with charge-independent transition metal occupations revealed the absence of cation mixing in the NCA cathode during the discharge from 4.2 to 2.5 V in full cell configuration against the graphite negative electrode.

### References

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