



Contribution ID: 307

Type: Poster

Li/Ni disorder of electrochemically cycled NCA-type battery cathodes

Monday, 20 March 2023 16:00 (2 hours)

The replacement of combustion engines with battery-powered electric drivetrains is one of many essential steps to reduce greenhouse gas emissions on the way to a green future, leading to an increasing demand on Li-ion batteries with higher capacities and energy/power densities. Thus, different kinds of mixed lithium transition metal oxide cathode materials have been developed, like high nickel content $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ (NCA), with high power/energy densities at lower costs and increased safety due to minimized amounts of costly and reactive Co[1]. However, Ni-containing LIBs show poor thermal stability, capacity/power fading and 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, actively discussed in literature[2]. Facing 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 Li 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 2.5V in full cell configuration against graphite negative electrode.

[1] A. Purwanto, C.S. Yudha, U. Ubaidillah, H. Widiyandari, T. Ogi and H. Haerudin, Materials Research Express, 2018

[2] O. Dolotko, A. Senyshyn, M.J. Mühlbauer, K. Nikolowski and H. Ehrenberg, Journal of Power Sources, 2014

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Presenter: HÖLDERLE, Tobias

Session Classification: Poster Session MONDAY

Track Classification: Chemistry of Materials (Structure and Spectroscopy)