



Contribution ID: 59

Type: Poster

Structural analysis of cation mixing in NCA-type battery cathodes

Friday 6 December 2024 13:45 (3 hours)

Lithium-ion batteries with high-nickel content $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ (NCA) cathodes and high-performance graphite are emerging as key components in electric vehicles, offering high energy and power densities at low costs [1, 2]. However, the efficiency of these batteries is hindered by the diffusivity of Li-ions, particularly in nickel-rich cathodes where $\text{Li}^+/\text{Ni}^{2+}$ cation mixing can block the 2D diffusion pathways, reducing the cell capacity and structural stability [3]. This study presents a systematic ex situ neutron powder diffraction analysis of NCA cathodes from real 18650-type cells, showing decreasing lithium concentration with higher charge states and the absence of cation mixing within the NCA structure during the electrochemical cycle, as revealed by Rietveld refinement.

[1] Zhao, G., et al., *iScience*, 25(2), 2022 (DOI: 10.1016/j.isci.2022.103744).

[2] Purwanto, A., et al., *Materials Research Express*, 5(12), 2018 (DOI: 10.1088/2053-1591/aae167)

[3] Dolotko, O., et al., *Journal of Power Sources*, 255, 2014 (DOI: 10.1016/j.jpowsour.2014.01.010)

Primary author: HÖLDERLE, Tobias

Co-authors: SENYSHYN, Anatoliy; MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien)

Presenter: HÖLDERLE, Tobias

Session Classification: Poster Session

Track Classification: Structure Research