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Antisite Li\Ni disorder in the NCA-type battery cathode

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The electrochemical efficiency of Li-ion batteries is largely determined by the diffusivity of Li ions and the transport of electrons between electrode materials in the cell. In nickel-containing cathode materials the mixed Li/Ni occupations often occurs, leading to structural disorder, blocking of the 2D diffusion pathways of Li^+ by Ni^{2+} , as well as the reduction of the capacity and structure stability. Mixed transition metal batteries like Li(Ni,Co,Al)O₂ and high nickel content Li(Ni,Mn,Co)O₂ are considered to be promising cathode materials showing better cycling stabilities, lower toxicity, lower costs etc. and are therefore of particular interest from the viewpoint of Li/Ni disorder [1, 2]. In literature, the studies and understanding of factors causing cation mixing is still controversial and are poorly presented. In the current contribution structural parameters of selected nickel-containing cathodes, obtained by neutron powder diffraction with the instrument SPODI at FRM II will be discussed together with their electrochemical characteristics.

[1] J. Zheng, Y. Ye, T. Liu, Y. Xiao, C. Wang, F. Wang and F. Pan, Ni/Li Disordering in Layered Transition Metal Oxides: Electrochemical Impact, Origin, and Control, Acc. Chem. Res. 52, 2201-2209 (2019).

[2] O. Dolotko, A. Senyshyn, M. J. Mühlbauer, K. Nikolowski and H. Ehrenberg, Understanding structural changes in NMC Li-ion cells by in situ neutron diffraction, Journal of Power Sources 225, 197-203 (2014).

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