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Finding the lost lithium with neutron diffraction and physico-chemical modelling

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Capacity fade in NMC/C 18650-type cells, cycled 1000 times at a 1C charge/discharge rate, has been characterized by in situ neutron diffraction and electrochemical analysis. Neutron diffraction of the cells show a cyclable lithium loss corresponding to a capacity fade of about 23% in both electrodes of the cycled cell, which is validated by electrochemistry. The cycled cell suffers an anode stoichiometry shift from x = 0.84 to x = 0.65 in LixC6 (0⩽x⩽1) in its fully charged state and a cathode stoichiometry shift from y = 0.89 to y = 0.81 in Liy(Ni0.33Mn0.33Co0.33)O2 (0 < y⩽1.05) in its fully discharged state. Anode (x = 0) as well as cathode stoichiometries (y = 0.54) remain practically unchanged in the cell's fully discharged and charged states, respectively. These experimental results have been validated by a physico-chemical aging model, which attributes capacity fade to loss of cyclable Li ions into the formation and growth of a continuous SEI film on the anode. The stoichiometry shifts extracted from neutron diffraction match well with those derived from the model, and both neutron diffraction and model are in good agreement to the electrically determined capacity fade of 21%. In fact, cyclable lithium losses slightly exceed this value. Thus, capacity fade in these cells is mainly due to loss of cyclable lithium into the continuous growth of a SEI film on the anode surface.
N. Paul, J. Keil, F. M. Kindermann, S. Schebesta, O. Dolotko, M. J. Mühlbauer, L. Kraft, S. V. Erhard, A. Jossen, R. Gilles, Journal of Energy Storage 17 (2018) 383-394.

Authors: PAUL, Neelima; Mr KEIL, Jonas; Mr KINDERMANN, Frank M.; Dr SCHEBESTA, Sebastian; DOLOTKO, Oleksandr (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München (TUM),); MUEHLBAUER, Martin; Mr KRAFT, Ludwig; Dr ERHARD, Simon V.; Prof. JOSSEN, Andreas; GILLES, Ralph

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