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# Investigating the Influence of Cyclic Ageing on the Structure of NCM Cathodes and Graphite Anodes in commercial 21700 Li Ion Batteries

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Li-ion batteries as energy storage devices play a significant role in the global agenda to mitigate emissions, move to sustainable energy sources, and fight climate change. In recent years, new battery formats have emerged with the intention of increasing energy. Moving from the conventional cylindrical 18650 design to the 21700 format can achieve higher energy content per cell.[1] These batteries are used in different scopes, such as electric vehicles in the automotive industry.

By scaling up the size of the battery, effects such as temperature and electrolyte distribution or inhomogeneities are gaining more influence on the cycling behaviour of the battery in comparison to smaller lab-size batteries.[2] Therefore, studying commercial cells to understand the lithiation and ageing mechanisms inside the electrodes is as essential.

Here, in-operando neutron diffraction experiments were conducted on 21700 cells with NCM as a cathode material and graphite as an anode material at the DMC instrument at the Paul Scherrer Institute (PSI). By comparing three different states of health, the influence of cyclic ageing on the electrodes could be investigated.

The loss of capacity can be seen in the electrochemical data and the structural change of the electrodes. The movement of the 113 NCM-peak is reduced for the aged cell, indicating that unit cell change is restricted due to the loss of Li. Simultaneously, the range in which the lattice parameters are moving during cycling is shifting to lower values for the aged cells suggesting that the cathode is pushed to higher potentials. For the anode, the amount of the LiC<sub>6</sub> phase is decreased for the aged cells, which confirms the loss of Li and is in accordance with the results from the cathodes.

[1] J. B. Quinn, T. Waldmann, K. Richter, M. Kasper, M. Wohlfahrt-Mehrens, J. Electrochem. Soc. 2018, 165, A3284-A3291.

[2] D. Beck, P. Dechent, M. Junker, D. U. Sauer, M. Dubarry, Energies 2021, 14, 3276.

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