Effects of microstructural features on the performance of a commercial Ni-rich NMC cathode

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Li-ion batteries are widely used in consumer electronics due to their high energy density and currently gain further importance with regards to future mobility and their application in electric vehicles. In order to reduce production cost and thereby establish a competitive battery production, a further optimization of the cell components is required. Since extensive testing is time-consuming and expensive, predictive simulation tools are needed that are able to evaluate the electrode performance based on a given electrode structure.
In this contribution, we will present 3D microstructure-resolved electrochemical continuum simulations conducted in the simulation framework BEST [1]. The governing equations are given by the mass and charge conservation in the active material and electrolyte. Discretization is done using a Finite Volume scheme which allows to directly use real tomographic data of the electrode microstructures as the simulation domain. Previous studies have shown the importance of microstructural simulations with regards to the battery operation [2,3] and contributed to a deeper insight into the observed electrode behavior [4].
In our work we analyze a commercial NMC811 cathode to reveal the influence of individual electrode features. The simulation domain is generated based on 3D-reconstructions of electrode samples generated by focused ion beam - scanning electron microscopy (FIB-SEM). The simulation results are then compared to experimental data in order to identify and isolate important design parameters. Here, the poor electronic conductivity of the electrode due to a low content of carbon-binder-domain (CBD) is identified to severely limit achievable cell capacity and increase the cell impedance. The developed method will also be used in order to identify critical microstructural parameters with regards to aging of NMC cathode materials in future work.

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