Effects of microstructure on electrode performance

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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 that is based on a thermodynamically consistent transport theory for mass and charge in the electrolyte and the active material [1]. Due to the finite volume implementation of the governing equations, real tomographic data of the electrode structure is used 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 measured electrode behavior [4].
In our work we analyze NMC/Graphite cells to reveal the influence of their geometrical, structural and chemical properties. This information is combined to develop a digital twin of the cell containing relevant information about the morphology, composition and tortuosity. As starting point for our analysis, the simulation domain is generated based on 3D-reconstructions of electrode samples generated by imaging techniques such as micro-computed tomography (µCT) or focused ion beam - scanning electron microscopy (FIB-SEM) and additional information of complimentary analytical characterization techniques will be included in future work. The electrochemical simulation results are then compared to experimental data in order to identify and isolate important design parameters. The developed method acts as a tool to gain a deeper understanding of the underlying electrochemical processes in the cell and reveals structure-performance correlations for future battery optimization.

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