Complementary investigation of lithium-ion batteries on the particle scale via single-particle measurements and simulations

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Lithium-ion batteries (LIBs) play a key role in the current transformation of our global energy system. A typical LIB cell consists of two electrodes (an anode and a cathode) with a porous separator in between them and an electrolyte which conducts lithium ions. Most state-of-the-art electrodes consist of active material (AM) particles, conductive additives and binding agents which form a complex microstructure that is soaked with the liquid electrolyte. Together with other effects like degradation phenomena, this leads to a complex interplay over multiple length scales.

For LIB cathodes, the above-mentioned AM particles are typically micrometre sized and inherit a complex inner structure, which can be revealed by advanced imaging techniques. This inner structure is influenced by various parameters in the synthesis process. Understanding of limiting processes opens up an interesting route for advancing the technology in terms of performance and cycle life. But accessing the particle scale is experimentally challenging and therefore many common electrochemical measurement techniques operate on the electrode scale. Similarly, most battery models are designed for simulations on the electrode level or above and simplify the AM particles such that most information on their internal dynamics is lost.

We tackle these challenges by a complementary approach that combines simulations and experiments on the particle scale. Experimentally, an optimized single-particle measurement (SPM) setup allows electrochemical measurements on single AM particles including rate tests, electrochemical impedance spectroscopy (EIS), and galvanostatic intermittent titration technique (GITT). Thereby, information on electrochemical properties of the materials can be acquired without any influence of an electrode microstructure. The derived parameters can then be used as input for 3D electrochemical simulations on particle and electrode scale. For this, we extended a previously developed transport model, cf. [1], to allow its application to the particle scale. It uses a physics-based continuum modelling approach, which only uses physically interpretable parameters as input. For our simulations, we use an implementation in the simulation framework BEST [2], which allows the flexible connection to 3D microstructural information on the interior of the AM particles. Results of this collaborative workflow will be presented.

References

[1] A. Latz, J. Zausch, Journal of Power Sources, 2011, 196 (6), 3296-3302.
[2] BEST - Battery and Electrochemistry Simulation Tool, ITWM, https://itwm.fraunhofer.de/best, accessed: 2023-01-20.