Analysis of limiting factors for Li-Ion battery performance and life-time: Micro-structure resolved simulations with BEST

In our presentation we will show examples of micro-structure resolved simulations in our battery simulation tool BEST (Battery and Electrochemistry Simulation Tool [1]). BEST was originally developed for the simulation of Li-Ion batteries in the former group of one of the authors (AL) at the Fraunhofer ITWM Kaiserslautern. The governing equations are derived in a rigorous approach from fundamental non-equilibrium thermodynamics and are implemented based on the CoRheos framework for complex and granular flow. DLR/HIU and Fraunhofer ITWM are collaborating to develop models for additional physical and chemical processes as well as new battery chemistries and to implement them in the software package. BEST is under constant active development and gives insights to fundamental physical processes as well as the latest developments for state-of-the-art battery materials.
Li-Ion batteries are commonly used in portable electronic devices due to their outstanding energy and power density. Remaining issues which hinder a breakthrough e.g. for stationary storage applications or electric vehicles are high production costs as well as safety risks. Recently, new battery concepts with thicker electrodes (>300 µm) or solid electrolytes were suggested to resolve these issues [2]. In both cases mass and charge transport limitations can be severe at already small currents due to long transport pathways, small transport coefficients, or inhomogeneous material properties. This could be a trigger for degradation effects, such as Li plating at the graphite anode, and reduces the lifetime of the battery. A thorough understanding of relevant processes within the electrodes is urgently needed to avoid these problems.
The electrode micro-structures of our simulations are either taken from tomography data [3] or geometries generated in GeoDict. Our detailed 3D studies allow important insights on cell operation and reveal detrimental structural properties for battery performance. For instance, we are able to quantify the effect of an inhomogeneous distribution of conductive additive in the case of thick electrodes or imperfect impregnation of the electrodes with the solid electrolyte. Moreover, we investigate the occurrence of degradation processes, such as Li plating during battery charge. Our approach allows analyzing limiting processes and critical operation conditions and predicts possible optimization and operation strategies to improve the performance and life-time of Li-Ion batteries.

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[2] Hopkins, B. J.; Smith, K. C.; Slocum, A. H.; Chiang, Y.-M. J. Power Sources 2015, 293, 1032–1038.
[3] Ebner, M.; Geldmacher, F.; Marone, F.; Stampanoni, M.; Wood, V. Adv. Energy Mater. 2013, 3, 845–850.