Microstructure-resolved Modelling and Simulation of Cathode Active Material Particles

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For the advancement of lithium-ion battery (LIB) technology, the improvement of cathode active materials (AM) plays a key role as they are decisive for the energy density on cell level. Furthermore, these AM particles have a complex inner structure, which can be revealed with advanced imaging and measurement techniques. This particle micro structure has a direct effect on cell performance while also being challenging to access experimentally. Therefore, increasing efforts have been made to link influences of the production process on resulting AM particle properties such as internal porosities, grain structures and boundaries. In order to rigorously investigate degradation and transport processes on this so-called particle scale, advanced transport models can help by elucidating the interior particle dynamics. This can then be used to deduce relations between chemical and structural properties and particle performance.

As part of our investigations, we extended a thermodynamic-consistent transport theory [1]. Consequently, this well-established continuum modelling approach for battery simulations can be applied to conduct 3D-microstructure resolved simulations of AM particles [2]. We incorporate 3D microstructural particle information and combine it with electrochemical data to investigate interior particle dynamics. Additionally, by resolving the structure of the current collector (CC), the influence of electronic conductivities and contact to the CC can be investigated. In our contribution we demonstrate the approach on a cobalt-free high-voltage spinel material.

References

[1] A. Latz, and J. Zausch, "Thermodynamic consistent transport theory of Li-ion batteries", Journal of Power Sources, vol. 196, no. 6, pp. 3296-3302, 2011
[2] BEST - Battery and Electrochemistry Simulation Tool, ITWM, https://itwm.fraunhofer.de/best, accessed: 2023-02-14.