The role of secondary particle information in microstructure-resolved simulations

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Lithium-ion batteries (LIBs) continue to play an important role in mobile applications like portable electronics and electric vehicles. Typical state-of-the-art cathodes in LIBs exhibit a complex porous microstructure, which consists of a mix of active material particles, conductive additives, and a polymer binder. Microstructure-resolved simulations facilitate the optimization of cell design as they allow assessing the influence of structural and electrochemical properties on the performance of battery cells.

Many current simulation models are based on a pseudo-2D-model developed by Newman and coworkers[1], which models the aforementioned active material particles as ideal homogeneous spherical particles. In contrast FIB-SEM-images reveal, that the internal microstructure of secondary particles is much more complex. Particles typically consist of primary particles with different shape and crystal orientation, as well as internal porosity which even evolves during cycling.

Furthermore, the search for cathode materials satisfying the needs for applications in the automotive sector (high energy density, rate capability, and low cost while retaining a reasonable cycling stability) has led to the development of novel material concepts. This has resulted in the emergence of specifically designed secondary particle structures, like core-shell materials, optimized micro-porosities and materials with full material gradients to name some examples. For these reasons, there is an increasing need for the inclusion of this information in current state of the art continuum models.

The application and extension of a thermodynamic consistent transport theory[2] allows full 3D microstructure-resolved electrochemical simulations with the additional secondary particle information included, extending the possibilities of state-of-the-art battery simulations. Results of this work-in-progress will be shown in our contribution providing insights into the impact of the secondary particle micro-structure on battery performance.

References:

1. Simulation and Optimization of the Dual Lithium Ion Insertion Cell, Fuller T. et.al., *J. Electrochem. Soc.* **141** (1), 1-9.
2. Thermodynamic consistent transport theory of Li-ion batteries, Latz A. et.al., *J. Power Sources* **196** (6), 3296-3302.