Linking Battery Performance to Microstructural Properties of Active Material Particles

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For the transformation of our global energy system towards renewable energies, lithium-ion batteries (LIBs) continue to play a decisive role. A typical LIB consists of two electrodes (an anode and a cathode) with a porous separator in between 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. As the AM particles carry the device's energy, their mechanical and electrochemical properties are a significant factor for performance, capacity and endurance of the full battery cell. These particles are typically micrometre sized and inherit a complex inner structure, which can be revealed by advanced imaging techniques. For material research, it is therefore important to accurately and reliably quantify the properties of AM particles. However, their determination by conventional approaches involves the investigation of the composite electrode with many design variables and thus involves high uncertainties. Furthermore, understanding how microstructural features influence the performance of AM particles and linking them to design parameters in the material's production process, opens up an interesting pathway for the advancement of LIB technology.

In order to improve the development process of active materials, we employ 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. 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. We combine this with digital 3D twins of particles, generated by a stochastic microstructure-modelling approach [3]. By training the generator with data obtained by advanced imaging techniques, this approach can capture the microstructure of AMs realistically.

A combination of the above methods allows to investigate and quantify how different particle structures as well as the surrounding conditions of the experiment influence the accuracy of the SPM measurement setup. Furthermore, different particle properties can be linked to interior dynamics and, consequently, to particle performance by applying extended transport models to 3D particle microstructures. We present results of this collaborative workflow.

References

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