3D electrochemical simulations of experimental and virtual anodes in lithium-ion batteries

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Lithium-ion cells are widely used in many products like mobile phones or laptops. However, there are still many challenges for their application in other areas like electric vehicles. Especially the wide range of climatic conditions as well as the high energy and power densities have a major influence on the ageing behaviour of cells. It is well-known that the microstructure of the anode strongly influences the functionality of the cell.

Since experimental influence of the microstructure of electrodes is a great challenge, it is important to develop flexible modelling and simulation techniques for investigating the correlation between the microstructure of the electrodes and the performance of the battery. The stochastic model as proposed in [1] enables the generation of 3D microstructures, which are statistically similar in many structural parameters of experimentally produced microstructures. In this talk we extend this comparison by investigating the simulated electrochemical behaviour of experimental and virtual microstructures. This helps understanding which differences between virtual and experimental microstructures are negligible from an applicational point of view and which ones are not.

The simulations are performed using a finite volume discretization [2] of a thermodynamic consistent transport model [3]. The results of the electrochemical simulations are statistically analysed by investigating the spatial distribution of various physical performance parameters inside the anode microstructure such as current density distribution in the electrolyte and the local overpotentials at interfaces between electrolyte and anode particles. These parameters influence degradation mechanisms as e.g. lithium plating, SEI growth and heat generation.

Finally, we discuss qualitative and quantitative differences of the simulation results for experimental and virtual microstructures and it is shown that the experimental and virtual structures behave similar with respect to electrochemical simulations. Extensions of the stochastic microstructure model, which overcome small differences in electrochemical behaviour, are proposed.

***Keywords**:* 3D microstructure modeling, lithium-ion battery, thermodynamically consistent transport theory, virtual material testing, model validation

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