Virtual design of thick electrodes for Li-ion batteries

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Li-ion batteries are commonly used in portable electronic devices due to their outstanding energy and power density. However, in order to reach the requirements of the automotive industry for next-generation electric vehicles regarding safety, life-time, energy density, and rate capability further developments are inevitable. Additionally, a reduction of material and production costs is needed to improve the competitiveness of electric vehicles. Recently, novel attractive battery concepts based on thick electrodes were suggested in the literature [Hopkins; Delattre; Singh]. These concepts provide a high theoretical capacity with only a few electrode layers which additionally has the potential to reduce production time and cost. However, increasing the active material loading can cause transport limitations of the shuttling lithium ions which also reduce the rate capability and practical capacity of the cell [Singh; Danner].
In this contribution we will present a methodology for the virtual design of electrodes for Li-ion batteries based on 3D stochastic microstructure generators [Westhoff] and 3D microstructure-resolved electrochemical simulations within the thermodynamically consistent simulation framework BEST [Latz]. It is shown that this simulation-based approach can be a powerful and efficient tool for the analysis and design of porous electrodes for Li-ion batteries [Hein].
State-of-the-art NMC positive electrodes with different thickness and density were prepared and characterized electrochemically in collaboration with our partners [Tran]. In a next step reconstructions of the electrodes were created with the help of synchrotron tomography and a 3D stochastic microstructure generator [Westhoff; Hein]. The resulting microstructures are then input to microstructure-resolved electrochemical simulations and good qualitative agreement between the simulations and experimental data can be reported. Based on these results different design concepts such as laser perforation and/or porosity gradients were evaluated regarding their performance improvements at high C-rates. For this purpose multiple realizations of virtual electrode microstructures were generated and characterized using the simulation framework described above. This virtual screening of different configurations provides material-structure-function relationships which are a helpful tool for the development of improved functional materials and electrochemical devices.

Acknowledgement
This work has been funded by the 'Bundesministerium für Bildung und Forschung' within the project HighEnergy under the reference numbers 03XP0073D and 03XP0073E.

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