Physically based modeling of impedance and discharge behavior of a $LiFePO_4$ battery

Christian Hellwig[1], Seniz Sörgel[1], Wolfgang G. Bessler[1,2]

[1] Deutsches Zentrum für Luft- und Raumfahrt, Institut für Technische Thermodynamik

Pfaffenwaldring 38-40, 70569 Stuttgart, Email: wolfgang.bessler@dlr.de

[2] Universität Stuttgart, Institut für Thermodynamik und Wärmetechnik

Lithium-ion batteries provide the highest energy density of all commercially relevant rechargeable battery types. Among the large number of different available materials systems, lithium-ion batteries based on lithium iron phosphate ($LiFePO_4$, LFP) positive electrodes are promising for electromobility applications due to their high power density, high lifetime, low material costs, and high operational safety. We present a detailed electrochemical model of a $LiFePO_4$ battery based on a multi-scale continuum description of chemistry and transport (Fig. 1). Chemical reaction kinetics of electron transfer and heterogeneous chemistry are modeled in the form of thermodynamically consistent elementary reaction kinetics. Chemistry is coupled to mass, charge and heat transport taking place on multiple scales (atoms and electrons inside the solid active materials, ions in the liquid electrolyte, electrons in the current collectors, heat within the full cell). The model is parameterized and validated using experimental impedance data and discharge curves obtained using commercial single cells. A very good agreement between model and experiments is observed along the complete range of investigated operating conditions (discharge rate, state of charge). We have thus achieved a model-based understanding of the complex physicochemical processes taking place in $LiFePO_4$-based lithium-ion batteries.

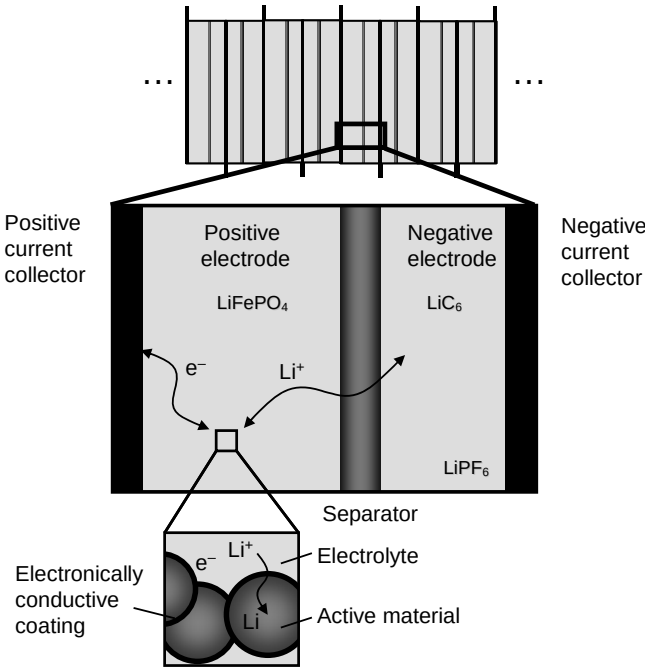

Fig. 1: Multi-scale model of $LiFePO_4$ cell