Oral presentation

Physically based impedance modeling for SOC diagnostics of a $LiFePO_4$ battery

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An important practical problem of lithium-ion batteries based on lithium iron phosphate ($LiFePO_4$, LFP) as positive active material is an inherent difficulty in determining the state of charge (SOC). This is due to two effects. Firstly, LFP shows a half-cell voltage that is independent of the SOC over a wide SOC range. This is due to the two-phase nature of the material [1]. Secondly, the cell voltage depends on cycling history. The origin of this behavior is subject of discussion; it has been interpreted in terms of tree-ring-type structures in the solid phases upon partial cycling [2], but also in terms of thermodynamic properties of multi-particle systems [3]. Both effects represent a challenge to SOC quantification in the battery management system (BMS).

Goal of the present study is to develop strategies for impedance-based SOC diagnostics of LFP cells using model-based impedance analysis. We present a multi-scale 1D+1D+1D electrochemical model of a single cell where governing processes are described by transport conservation equations with source terms due to electrochemical and chemical reactions, extending the type of models originally introduced by Newman [4]. Charge transport in the electrolyte is described by multi-component diffusion and migration for each dissolved species. Electrochemistry is based on a thermodynamically consistent description of active materials and Butler-Volmer kinetics [5]. The model uses a hierarchical representation of spatial scales: On the nanoscopic level, diffusive transport takes place in the active material particles. On the microscopic level, multi-component mass and charge transport as well as heat production is described in a single repeat unit (anode, separator, cathode, current collectors). On the macroscopic scale, the model describes heat transport in the radial direction of a cylindrical cell.

Electrochemical impedance spectra are obtained from the detailed model based on potential step and current relaxation simulations [6]: A small and fast potential step (1 mV, 10 ns) is applied to the battery at open circuit, and the current relaxation is simulated over 10^5 s. The resulting time traces of cell current and voltage are Fourier-transformed and the complex impedance is calculated in the frequency domain. Simulated impedance spectra show good agreement with experimental data over the complete SOC range.

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