Physics-based inverse modeling of degradation in Li-ion batteries by using Bayesian methods

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Modelling at the cell level aims at improving and predicting the lifetime of Lithium-ion batteries (LIBs). To this aim, we want to understand and parameterize the degradation mechanisms. However, the different degradation mechanisms interplay and their origin are even debated in relevant cases [1].

As example, we consider the growth of the Solid-Electrolyte Interphase (SEI). It is the dominant degradation mechanisms during storage of LIBs and plays a significant role during battery operation [2]. To differentiate between various proposed growth mechanisms, i.e., solvent diffusion, electron diffusion and electron migration, we utilize an automated parameterization routine based on Bayesian methods that is able to distinguish the different mechanisms [3].

We show how efficient Bayesian methods [3,4] parametrize and quantify uncertainties of physics-based models, within reasonable sample numbers, operate as a consistent model selection criterion, and give reliable correlations in the overall and feature specific parametrization [5]. We discuss that feature selection has a huge impact on the algorithmic performance and the correct identification of the physical features. By applying this routine to real data, we find that electron diffusion [6] is the dominant growth mechanism of the SEI during storage. In conclusion, our inverse model routine can help to identify and parametrize degradation mechanisms of LIBs and is generalizable to include more mechanisms. This automatable method is applicable to the analysis of battery data, model development and validation and can therefore accelerate battery research.

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10-21



Fig. 1: Consecutive convergence of parameterization and uncertainty for noisy cycling data [5]

Fig. 2: Loss function of a specific feature choice in parameter space considering noisy data [5]

 $D_{e} - \left[\frac{m^{2}}{5}\right]$

10-14

10-13

0.60

-1.35

-2 10

.2 85

-3 60

-4.35

-5.10

-5.85

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