Parameterization of physics-based degradation models in Li-ion batteries by using Bayesian methods

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Modeling physical processes inside a battery is an inevitable step in understanding and improving the lifetime of lithium-ion batteries (LIBs). The actual parameterization and validation of a specific degradation model is an intractable challenge due to the complex coupling of many processes, leaving the dominant degradation mechanism yet unclear [1].

To fully understand the measured degradation in LIBs, one has to model several degradation mechanisms and their coupling all-encompassing. Due to the lack of individual markers for each degradation effect, it is insurmountable to model all effects simultaneously. TherefDore, one has to analyze isolated effects first. In a first study, we investigate the responsible growth mechanism of the Solid-Electrolyte Interphase (SEI). The ongoing growth of the SEI is considered the main degradation mechanism during battery storage, and it also makes a significant contribution during battery operation [2]. To distinguish the proposed growth mechanisms, i.e., solvent diffusion, electron diffusion, and electron conduction, we inversely model degradation data with an automated parameterization routine based on Bayesian methods [3].

We emphasize that efficient Bayesian methods [3,4] are outstanding tools to parametrize physics-based models within reasonable sample numbers, operate as a consistent model selection criterion, and give reliable uncertainties and correlations in the overall and feature-specific parametrization [5]. We show that suitable feature selection can further improve the algorithmic performance and ensure the correct identification of the physical features. As a result, we identify electron diffusion [6] as the dominant growth mechanism of the SEI during battery storage. In conclusion, our inverse model routine helps to identify and parametrize degradation mechanisms of LIBs and is generalizable to include more mechanisms. This automatable method applies to analyzing battery data, model development, and validation and can, therefore, accelerate battery research.

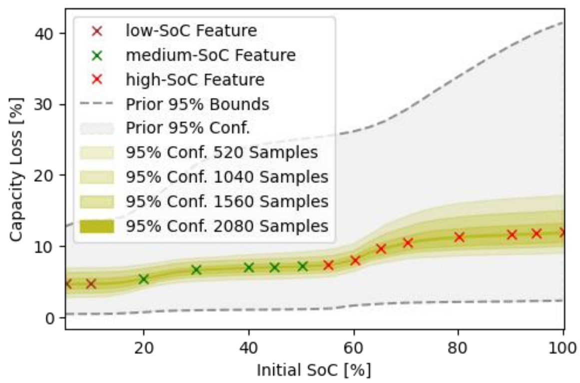

Fig. 1: Consecutive convergence of parameterization and uncertainty for storage data [5]

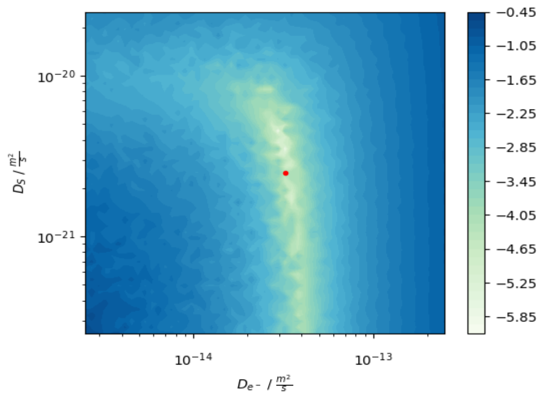

Fig. 2: Loss function of a specific feature choice in parameter space considering noisy data [5]

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