Parameterizing physics-based degradation models in Li-ion batteries with 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). To assess the validity of a model, it has to be correctly parameterized by comparing it to experimental data. However, modeling the observed degradation is a persistent challenge due to the complex coupling of many different processes [1], leaving the dominant degradation mechanism yet unclear.

To fully understand the measured degradation in LIBs, one has to model several degradation mechanisms and their coupling all-encompassing. As the information about the degradation occurring in the battery is mainly encoded in the measured capacity loss only, disentangling the various mechanisms at once is insurmountable. To still obtain a valid degradation modeling, one must first analyze isolated effects. In a first study, we investigate the responsible growth mechanism of the Solid-Electrolyte Interphase (SEI), as this effect can be isolated for the most part by looking at storage experiments. The ongoing growth of the SEI is considered the primary degradation mechanism during battery storage, but it also makes a significant contribution during battery operation [2]. We inversely model degradation data with an automated parameterization routine based on Bayesian methods [3] to distinguish the proposed theoretical growth mechanisms, i.e., solvent diffusion, electron diffusion, and electron conduction. With a valid SEI growth model, we can analyze the impact and behavior of additional degradation mechanisms in a follow-up study.

We show that sample-efficient Bayesian methods [3,4] are outstanding tools to parametrize physics-based models within reasonable sample numbers, as they successfully tackle obstacles like consistent model selection, reliable uncertainties, and correlations in the parametrization [5]. 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. Then, we can investigate more complex degradation data and model further degradation mechanisms, such as loss of active material and particle or SEI cracking. 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.

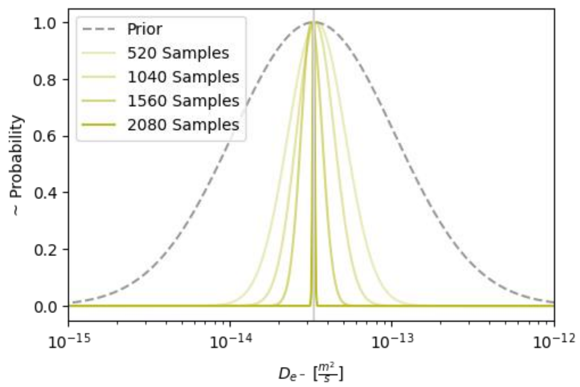

Fig. 1: Convergence of a prior belief about the parameter distribution with increasing knowledge [5]

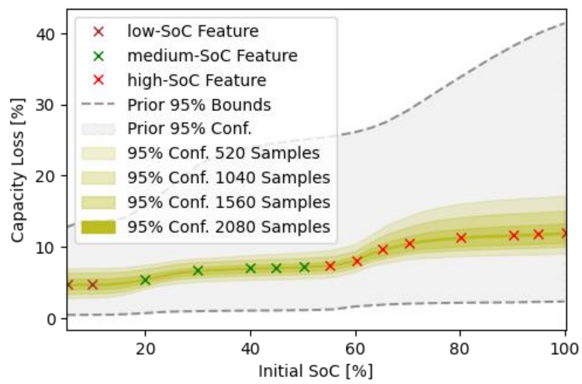

Fig. 2: Consecutive convergence of parameterization and uncertainty for storage data [5]

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