Physics-based identification of degradation mechanisms in Li-ion batteries by using sample-efficient Bayesian methods

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Due to their outstanding performance and high versatility, lithium-ion batteries are considered as the pinnacle of electrochemical energy storage. Even though they are highly researched, the ongoing degradation taking place during storage and battery operation remains a major challenge for sustainability and long-lived high performance. In order to compete with the rising requirements for Li-ion batteries, a profound understanding of the degradation processes is inevitable. One main degradation mechanism taking place in Li-ion batteries is the formation of the Solid-Electrolyte Interphase (SEI), constantly consuming Li-ions and increasing the internal battery resistance.

The SEI is a thin passivating layer on the negative electrode, growing by ongoing decomposition of electrolyte. In the literature the SEI growth is considered to be limited by transport mechanisms of the different reactants. However, multiple transport mechanisms for electrons and solvent to the reaction location are proposed, leaving the real mechanism yet unclear. Nevertheless, we show that the automated parameterization of the proposed mechanisms by using Bayesian methods is indeed able to distinguish the different transport mechanisms and identify the best mechanism.

The results of our investigation emphasize the capability to combine automated machine learning (ML) and physics-based modeling. We show that sample efficient Bayesian algorithms [1] are able to obtain valid parameterizations and uncertainty quantifications of physics-based models, needing orders of magnitude less simulated samples than common algorithms. Further, the automated inverse analysis of experimental data with physics-based models is able to give insights on the physical background of the SEI formation. In case of multiple possible models, we show that Bayesian methods [2] can operate as a mathematically consistent model selection criterion, identifying Electron Diffusion [3] as the best model to describe SEI growth during storage. Moreover, the use of Bayesian methods yields physical reliable correlations in the overall parameterization and in feature specific perspectives. We show that a suitable selection of features for the inverse modeling has huge impact on the number of needed samples, the obtained parameterization and uncertainty, and the correct identification of the relevant physical mechanisms [4].

In conclusion, we use ML-based techniques to parameterize physics-based models of SEI growth in Li-ion batteries and present a model selection criterion to identify the responsible mechanism. We discuss the possibilities to capture correct physical features needing only a minimum of simulated samples. This automatable method finds wide application in the analysis of battery data, model development and can therefore accelerate battery research.

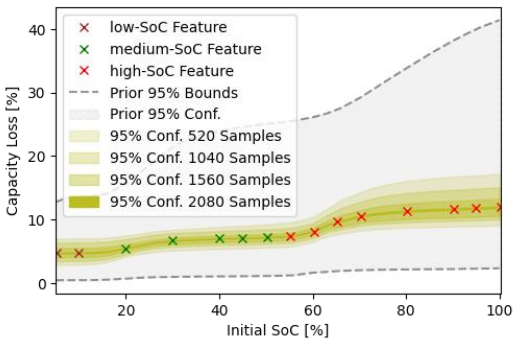

Fig. 1: Consecutive convergence of parameterization for storage data [4]

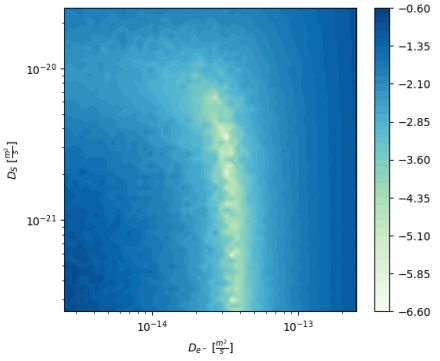

Fig. 2: Loss function of specific feature choices in parameter space considering noise [4]

1. Y. Kuhn, H. Wolf, A. Latz, B. Horstmann, Batteries & Supercaps. 2023, DOI: 10.1002/batt.202200374.
2. M. Adachi et al., IFAC-PapersOnLine 2023, DOI: 10.1016/j.ifacol.2023.10.1073.
3. L. Köbbing, A. Latz, B. Horstmann, J. Power Sources 2023, DOI: 10.1016/j.jpowsour.2023.232651.
4. M. Philipp, Y. Kuhn, A. Latz, B. Horstmann, *in prep.*