

Estimating the Graphite Electrode Phase Evolution from Electrode Potential Measurements[★]

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Abstract:

Knowledge of the internal state of lithium-ion batteries (LIBs) is critical for enabling fast and safe charging. Graphite is commonly used as the negative electrode due to its high specific capacity and cycling stability. When such LIBs are charged, lithium intercalates into the layered carbon structure, and the electrode material transitions through a series of phases differentiated by the number of carbon layers between each lithium layer. Reaching the final phase increases the risk of severe degradation mechanisms such as lithium plating, making it interesting to track the phase evolution during fast charging. However, direct measurement of the phase composition requires spectroscopic techniques unsuitable for implementation in a battery management system (BMS), while estimation via incremental capacity analysis (ICA) loses reliability at higher charging currents.

In this work, we propose a novel method for estimating the graphite phase evolution from electrode potential measurements during constant-current charging. The key observation is that both the electrode potential and the phase evolution exhibit similar smoothing at higher currents due to increasing lithiation inhomogeneity. This observation is exploited by combining ICA-based phase identification at low currents with kernel smoothing, enabling phase estimation beyond the range where ICA is applicable.

The method is validated using physics-based simulations of multiphase electrode dynamics for charging rates up to C/5 (a 5 hour rate), achieving an average estimation error below one percentage point per phase. Application to experimental coin cell data shows strong agreement with simulations in the mid- to high-state-of-charge (SOC) range, where the risk of triggering lithium plating is highest, demonstrating the method's potential as a first step towards BMS-compatible phase tracking. In the low-SOC range, the estimates deviate from the simulations, as the simulated electrode potential does not match the experimental measurements well. This discrepancy may be explained by model simplifications at low SOC and the use of parameters fitted to different coin cells than those used in our experiments.

Keywords: Energy storage systems; Kernel density estimation; State estimation

REFERENCES

- (1) Borghed I., Bian X., Huang Y., Wik T., Estimating the graphite electrode phase evolution from electrode potential measurements, *Materials & Design* 266 (2026) 116218, doi: <https://doi.org/10.1016/j.matdes.2026.116218>.

[★] This work was funded by the Swedish Energy Agency under project No. P2023-00144, and the Chalmers Foundation through the Energy Area of Advance.