Electro-optical in-situ measurements of Li-intercalation in graphite anodes

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Graphite is mostly used as anode material in Lithiumion batteries. Depending on material parameters it allows both high energy and power densities. By tuning the design of the anode it is possible to reduce losses occurring during Lithium intercalation. In literature several electrochemical models (1-4) are proposed for a better understanding and simulation of this process.

The challenge is to parameterize and validate those models unambiguously. Therefore electrochemical investigations e.g. electrochemical impedance spectroscopy (EIS) in half cell setups under variation of boundary conditions as state of charge (SOC) or temperature are required (5). However it is difficult to get enough information for parameterization especially that some parameters as electrical and ionic conductivity show similar dependencies in their physical equations.

Besides a decreasing electrical electrode potential Lithium intercalation causes a change of the diffusive reflectance due to SOC dependent photo-molecular interactions like intraband transitions (6). In this work we conduct the dynamic behavior of the macroscopic anode's surface reflectance. To combine this behavior with electrochemical models some requirements must be fulfilled. Therefore a new half-cell setup with a Lithium ring reference electrode and a glass window has been developed allowing simultaneously optical and electrical in-situ measurements (Fig. 1).

Furthermore the influence through geometric deviation from ideal face to face setups on EIS measurements was modeled by a transmission line model considering the graphite impedance. This model, in turn, was validated with cell arrangements of different geometries by EIS.

In a next step optical measurements are performed under steady-state conditions and varied electrical excitations using reflected-light microscopy and ultraviolet-visible spectroscopy of the anode's surface. Thus optical information therein can either be used for precise SOC determination or as an additional quantity for electrochemical model validation.

References

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Fig. 1: Measurement and half-cell setup for combined electro-optical measurements. The reflected light from the electrode is either conducted by an ultraviolet-visible spectrometer or a light microscope.