3D electrochemical simulation of lithium plating

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Most lithium-ion batteries experience the degradation process “lithium plating” during low temperature cycling or high current charging. This process leads to a deposition of metallic lithium on the surface of the anode material. The presence of this pure lithium phase inside a lithium-ion battery can enhance the degradation processes, like decomposition of electrolyte, and lead to a loss of active lithium.

We present a new plating model, which enables the simulation of lithium plating and stripping in the 3D microstructure of a lithium-ion battery. The proposed model includes the lithium deposition reaction, additionally to the intercalation reaction, at all anode-electrolyte-interfaces. Lithium plating can take place as soon as it is thermodynamically possible. The local deposition of metallic lithium leads to a coverage of the local active surface and a thickness growth on this plated surface. The local intercalation from the electrolyte into the negative electrode is prevented, if the local surface is completely covered by plated lithium. At this position the current flux can then only drive further lithium thickness growth or dissolution.

The simulations are based on the framework BEST [1], which is a finite volume implementation of the thermodynamic transport model [2,3]. The implementation is extended by this new lithium plating model.

We will present the application of this extended model on realistic 3D anode microstructures. The influence of the deposition and dissolution process on different electrochemical quantities and the cell potential will be discussed.

***Keywords**:* Lithium battery, 3D simulation, thermodynamically consistent transport theory, lithium plating, lithium stripping.

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