Electro-Chemical Modelling of Laser Structured Electrodes

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A simulation study performed in the scope of the project RealLi! is presented. One of the project's main goals is to improve NMC811 and graphite electrode cycling capacities at high C-rates.

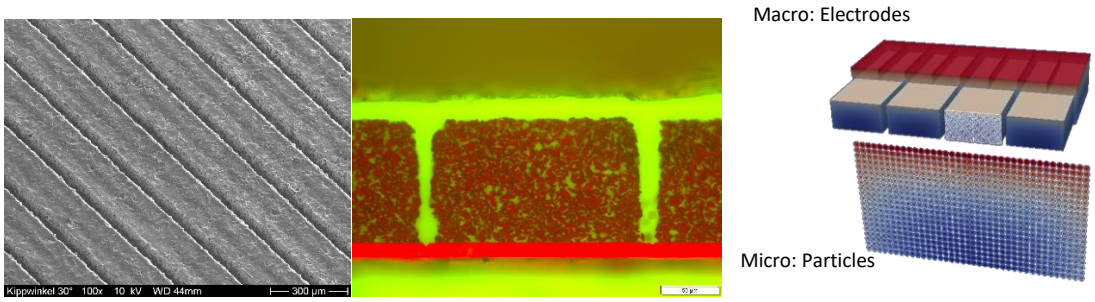
The rapid charging and discharging capability of batteries is improved using laser ablation to introduce structures into the surface of the electrode composite layers. Due to improved transport kinetics, this not only improves the electrochemical properties in the high-current range, but also homogenizes and accelerates the electrolyte wetting during production as a side effect. This is particularly advantageous in thick-film electrodes for providing high energy densities.

This study supports the laser structuring process of battery electrodes [1][2] via a virtual optimisation, based on electro-chemical battery models. The electrodes are structured by ultrafast laser ablation, with parallel channels being introduced along the electrode surface. This modification enables an easier electrolyte penetration, a reduced charge transfer resistance, and shortened lithium-ion transport pathways which finally leads to a reduced diffusion overpotential at high C-rates. The geometrical parameters of this process (distance, width, and shape of channels) and their impact on cell performance are virtually optimised by simulations.

The simulations are based on a homogenised multi-scale model, applied in 2D/3D macroscopic cuts, coupled with 1D microscopic particle cuts. The 2D/3D macroscopic electrolyte transport equations are common concentrated electrolyte equations. The microscopic particle transport equations are either a set of non-linear Fick's Diffusion equations [3] that are used to describe spherical symmetric NMC materials or a set of Cahn-Hilliard equations [4], that consistently describe the phase separating nature of graphite anodes in cylindrically symmetric particles.

The underlying numerical method is an implicit-multi-scale finite-element-method [2], that allows for a flexible implementation of such models. The first results of this ongoing project will be presented along with the overall structure of the method and its implementation. The results include geometrical as well as electro-chemical parameter variations and their respective sensitivity analysis.

Furthermore, in the discussed electrode geometry the possible anisotropic structure of an electrode (due to particle shape and distribution) has a bigger impact than in unstructured electrodes. The improved transport pathways along the channels, therefore, imply the necessity of a more thorough homogenisation than it is usually done, for example in a Newman-Model approach. A long-term goal of this work is to enable a significant increase in areal energy density, i.e., the use of thicker electrode films and the use of advanced high energy materials in battery electrodes.



Left: laser structured NMC electrode (©KIT); Middle: cut through laser structured graphite (©KIT) electrode; Right**:** preliminary simulation result (©VIF)

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