Advanced Battery Power Conference 2022
Münster, Germany March 29-30, 2022

A Multi Scale Multi Domain Approach For The Modelling Of Large Format Lithium-Ion Battery Cells

Adrian Schmidt[1], André Weber[1], Marc Kamlah[2] and Ellen Ivers-Tiffée[1]

[1]*Institute for Applied Materials - Materials for Electrical and Electronic Engineering (IAM-WET),*
[2]*Institute for Applied Materials - Materials and Biomechanics (IAM-WBM)*
Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany

The increasing demand for electric mobility results in the growing relevance of large-format battery cells. Especially these cells have internally heterogeneously distributed potentials and temperatures, as shown in [1]. Multi scale multi domain (herein after referred as MSMD) models are widely used to calculate the electrochemistry on the microscale and simultaneously map e.g. the temperature distribution in the entire battery cell on the mesoscale. A particular problem is the high geometrical complexity due to the considerable number of electrochemically active layers in such large format cells. There are several models in the literature that use either simplified electrochemical models or reduced model couplings in order to handle the computational effort [1]–[6].

In this work a new homogenization approach for multi scale multi domain modelling is presented. This approach transfers the idea of volume averaging and homogenization of the commonly known Newman model [7] to the layer structure in large format battery cells. Thereby, the layer structure of the cell is taken into account by effective, anisotropic transport parameters without resolving it geometrically. The goal of this modeling approach is therefore an effective, fast computing MSMD model without simplifying the electrochemical model or the model coupling. The resulting model enables the calculation of a complete discharge of a large format cell in five minutes on conventional laptops, taking into account the local temperature and current density distribution. The schematic model structure and the correspondence to the Newman model are shown in the attached Figure 1.

The resulting multi scale multi domain model is parameterized for a battery cell consisting of graphite anode and NCA/LCO-blend cathode and will be applied to four different cooling conditions: no cooling, base plate cooling, tab cooling and side cooling. The full coupling of electrochemistry and temperature allows conclusions to be drawn not only about the occurring temperature profile in the cell, but also about the resulting local potential and current densities. Thus, it will be shown that locally inhomogeneous discharge rates in large format cells originate from the interaction of (i) voltage losses in the current collectors (ii) emerging and decaying SOC inhomogeneities (iii) the slope of the discharge curve and (iv) the temperature profile of the cell. For example, a local peak discharge rate of 2.8 C will be proven for base cooling during a 2C discharge, potentially connected with excessive aging of the cell. Even more important is the outcome, that the local distribution and the magnitude of excessive discharge rates develop counterintuitively, which underlines the necessity for fully coupled MSMD models.

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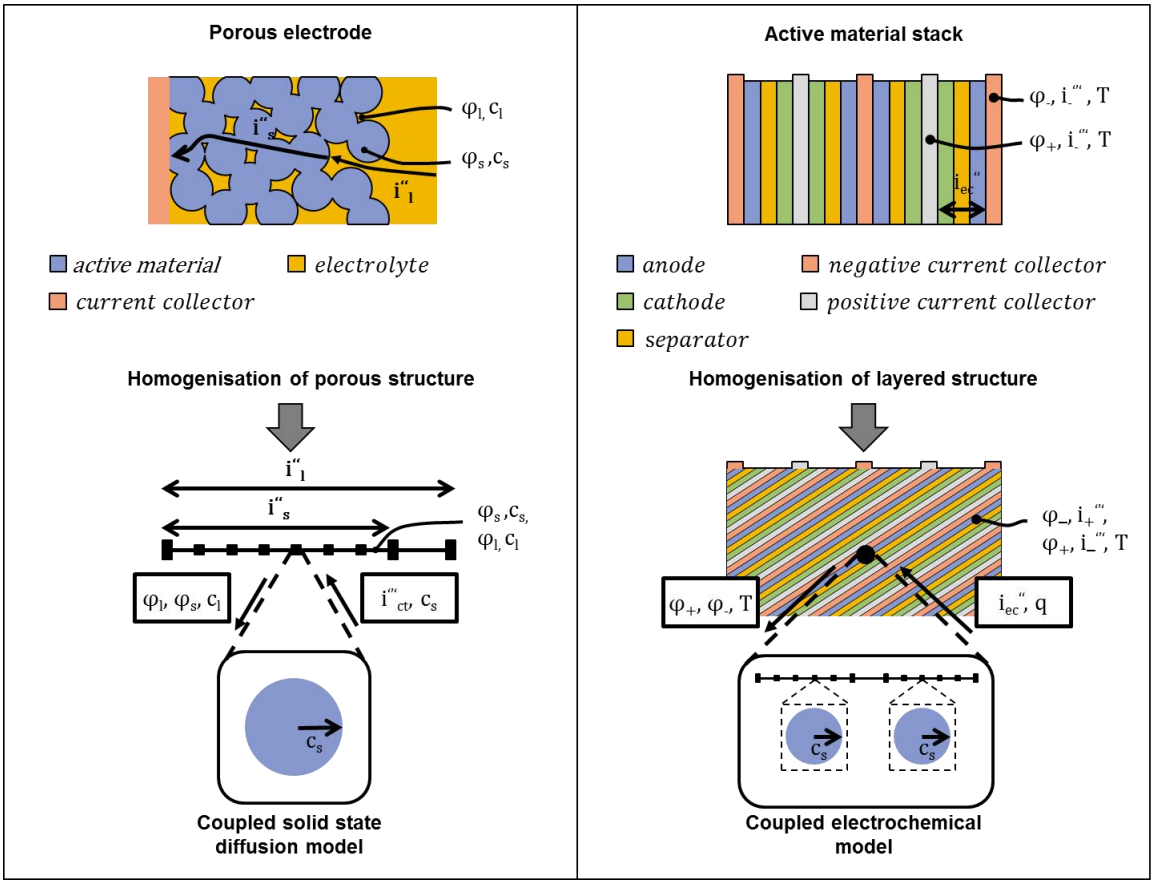

Figure 1: Illustration of the homogenization of (a) porous electrodes in the Newman model and (b) the internal layer structure in the MSMD approach.