Parameterization of a Physico-Chemical Model for Lithium-Ion Batteries

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Lithium-ion battery technology is promising for the application in hybrid- and electric vehicles, due to high power and energy density. They are also discussed for stationary applications. Today's challenges in lithium-ion battery technology are the lifetime, the low temperature performance and cost reduction, which requires further material and design development. In order to support material development and to minimize the experimental effort, simulation tools based on material properties are needed. Model approaches based on the work of Newman et al [1] exist, that reproduce the physical and chemical processes occurring in the battery, like diffusion, charge transfer,…Furthermore, degradation processes have been integrated using these models in order to investigate the influence of different material properties on aging [2]. The weakness of the physico-chemical models has always been and still is the large set of material parameters needed for parameterization that are hard to determine. Many parameter studies based on physico-chemical models exist, but there are hardly any attempts to parameterize and verify such a model using real existing systems [3]. In this work a physico-chemical model will be parameterized for a commercial high energy lithium-ion battery, based on Li(CoNiMn)O_2. After opening the cell, all necessary material and geometrical parameters will be measured in order to obtain an adequately description of the system.

Battery Model

The physico-chemical cell model used in this work is able to simulate the current-voltage behavior and spatially resolved potentials and lithium concentration distributions. The calculation of the current distribution is based on an electrical network consisting of lumped elements that describe physico-chemical processes in the cell. The electrical elements describe for example the charge transfer resistance, calculated using the Butler-Volmer equation, the local equilibrium voltage, resistances of current collectors, active material and electrolyte, as well as SEI resistance. For the calculation of the electrical elements, the lithium concentration distribution in the electrolyte as well as in the active material is needed. The calculation is based on the porous electrode model developed by Newman [1], where the active material is described by spherical particles, surrounded by electrolyte. The concentration model reproduces the diffusion processes in the electrolyte and the active material particles based on the finite-difference method. A simple thermal part is also incorporated in the model, in order to simulate the influence of temperature on the cell processes.

Parameterization

To parameterize the pysico-chemical model, material and geometrical parameters have to be determined. Therefore the cell was opened under argon atmosphere and material probes have been prepared for further investigations. Required parameters beside geometrical ones are the material properties of the active materials, e.g. open circuit voltage curves, diffusion coefficients, porosities, particle radii, conductivities,…Figure 1 shows exemlarily a mesurement that has been conducted on the cathode material using mercury porosimetry. With this method, porosity as well as particle radii have been determined.

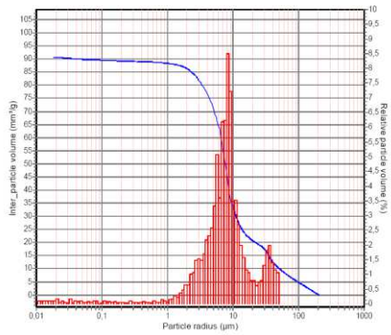

Figure 1: Mercury porosimetry of the Li(CoNiMn)O_2 material used in the cell. Relative particle volume of the sample (red) and inter-particle volume (blue) are shown over particle radius.

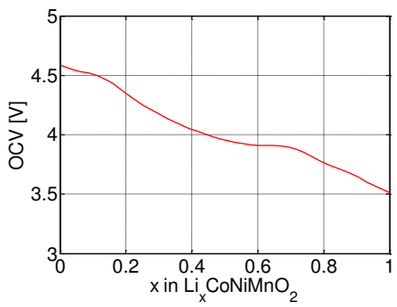

Figure 2: Open circuit voltage of Li(CoNiMn)O_2 vs . state of charge.

Figure 2 shows the results of the open circuit voltage measurements for the cathode using half cell measurements. Also the charge transfer kinetics have been determined using different electrochemical methods. Furthermore the material properties of the electrolyte as well as the separator have been measured and the temperatue dependencies of the different parameters have been examined.

The aim of this work is a fully parameterized physico-chemical model, that is able to to reproduce the cell behaviour in an adequate way.

References:
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