Extending porous electrode models for Lithium-ion battery electrodes to particle size distributions

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An important factor for the power capability of lithium-ion cells is their chemical characteristic which is pre-determined by the choice of the active materials. Another deciding impact on the cell performance is given by the microstructure of the cell components, especially of the electrodes.

The microstructure of the electrodes can be obtained from focused ion beam tomography or by micro x-ray tomography. Even though, these reconstructions provide an excellent basis to analyze and characterize electrode microstructures [1], it is difficult to use these highly complex structures directly for electrode simulations. Nevertheless, it is possible to use the information from the reconstructions to parameterize homogenized models (e.g. the Newman model [2]). By doing so, a lot of information about the microstructure is discarded, such as the particle size distribution.

As can be seen in simulations of the charge/discharge curves of a graphite anode (figure 1), a homogenized electrode model with only one particle diameter preserves the steps between the different graphite stages also at higher charge and discharge currents. If instead of using one particle diameter, the model is extended to two particle diameters (figure 1), the steps between the voltage plateaus split into two smaller steps.

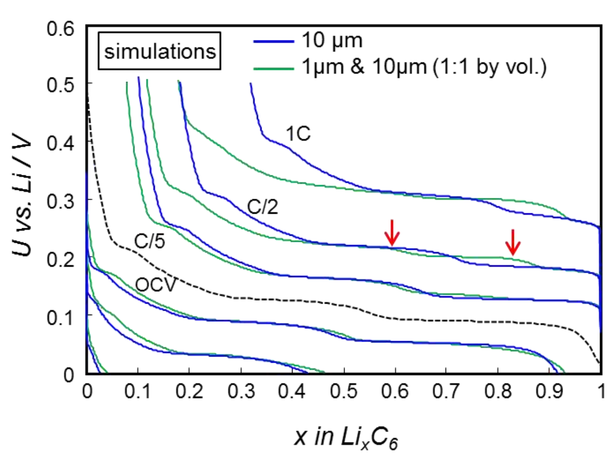

Figure 1: comparison between the charge-/discharge-simulations of a graphite anode using one particle diameter and two particle diameters. In the latter case, the steps between the voltage plateaus split into two smaller steps.

This work introduces an extended homogenized porous-electrode model which includes particles of various diameters (figure 2). For such a particle size distribution, the steps between the potential plateaus are smoothed out at higher currents. Of course, the model can be used for the simulation of both, anodes and cathodes, and can also be included in full cell models.

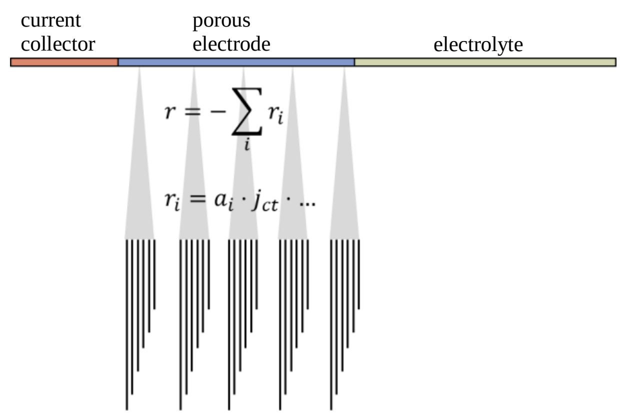

Figure 2: Schematic setup of the homogenized electrode model including a particle size distribution. This means, that every point within the electrode is coupled to a number of spherical particles with different diameters.

A comparison to the commonly known homogenized porous electrode model based on one size of spherical particles will be given, as well as a comparison to measurements.

References

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[2] M. Doyle, J. Newman, A. S. Gozdz, C. N. Schmutz, and J. M. Tarascon, J. Electrochem. Soc., **143**(6), p. 1890 (1996).