Electrochemical Modeling and Simulation of Lithium Ion Batteries

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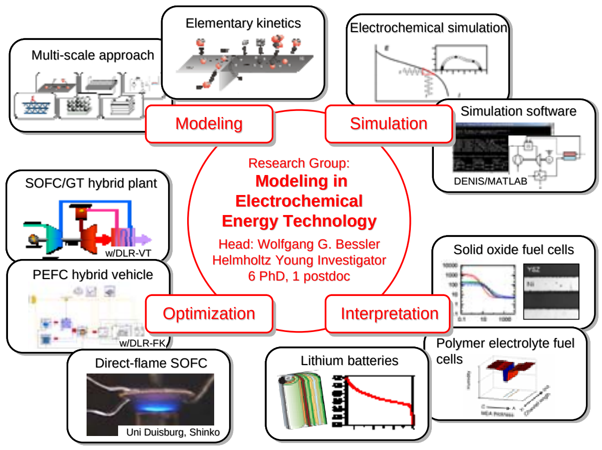
Motivation

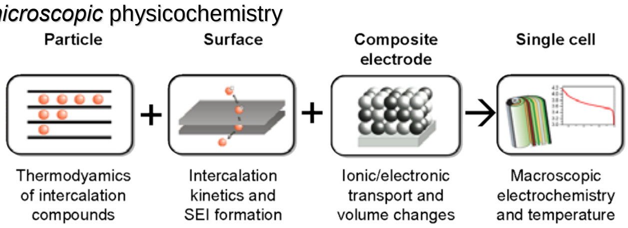
- Lithium-Ion batteries are recieving increased attention and importance for portable and mobile applications
- Fundamental processes on cell and electrode level are still not sufficiently understood
- Goal: Scientific understanding and model-based optimization of electrochemical and transport processes in lithium-ion batteries for supporting technological development
- Modeling framework [1] based on microscopic description of thermodynamics, kinetics, transport and structure to predict
  - Macroscopic electrochemical observables (discharge / charge behavior, capacity, SOC)
  - Ageing processes (SOH) and durability
  - Heat transport and hot spot formation

Research group



Modelling and simulation approach

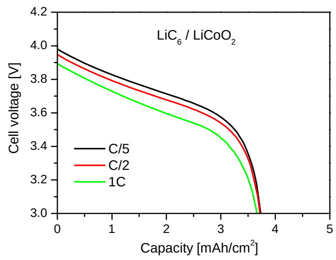
Multi-scale approach to understand *macroscopic* electrochemical behavior (capacity, power, SOC) and lifetime (SOH) from *microscopic* physicochemistry

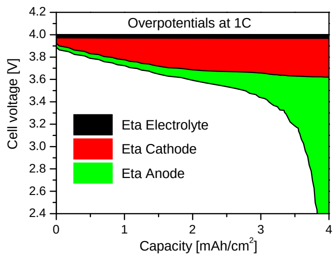


- Charge neutrality condition $\sum_i c_i z_i = 0$
- Nernst-Planck equation of ion transport $\frac{\partial c_i}{\partial t} = \nabla(D_i \nabla c_i) - \frac{z_i F}{RT} c_i \nabla(D_i \nabla \phi)$
- Arrhenius behavior of diffusion coefficients $D = D^0 \cdot \exp\left(-\frac{E^{act}}{RT}\right)$
- Butler-Volmer equation $i = i_0 \cdot \left(\exp\left(\frac{0.5 \cdot F \cdot \eta^{act}}{RT}\right) - \exp\left(-\frac{0.5 \cdot F \cdot \eta^{act}}{RT}\right)\right)$
- Stoichiometry of anode (x) and cathode (y) $x = \frac{\rho_{Li} M_{C_6}}{\rho_{C_6} M_{Li}}$ $y = \frac{\rho_{Li} M_{CoO_2}}{\rho_{CoO_2} M_{Li}}$
- Half-cell potential of anode and cathode from empirical polynomials [2,3]
- Parameters [2,3,4]: $D^0 = 1.07 \cdot 10^{-11}$ m²/s, $T = 298$ K, i^0 (Anode) = $3.6 \cdot 10^5$ A/m³, i^0 (Cathode) = $3.6 \cdot 10^5$ A/m³, ρ_{C6} = 1050 kg/m³, ρ_{CoO2} = 3225 kg/m³

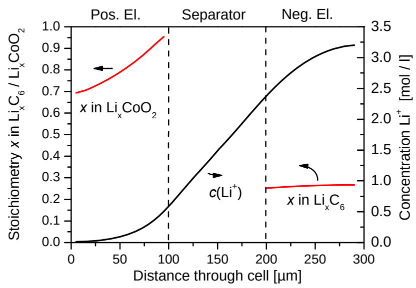
Results and discussion

- 1D model: Simulated discharge characteristics





- Simulation shows typical voltage behavior at low discharge rates



- Amount of intercalation of Li in electrodes depends on location of each particle and differs inside one electrode [3]
- Concentration of Li^+ in electrolyte shows good aggreement with other studies [4]

Conclusions

- Demonstrated multi-scale modeling and electrochemical simulation for physically-based prediction of cell behavior
- 1D simulations show typical discharge behavior. Distribution of loss processes can be quantified.
- Quantification of spatially resolved Li concentration in intercalation electrode and electrolyte

Outlook

- Half-cell potentials based on physical thermodynamic data in order to reduce empiricism
- Elementary kinetic models of side reactions such as SEI formation leading to ageing of cells
- Heat production and heat transport as well as its feedback on electrochemical behavior (e.g., hot spot formation)

[1] W. G. Bessler, S. Gewies, and M. Vogler, Electrochim. Acta 53, 1782-1800 (2007).
[2] G. Sikha, R. E. White, B. N. Popov, Journal of The Electrochemical Society 152, A1682-A1693 (2005)
[3] K. A. Smith, C. D. Rahn, C.-Y. Wang, Energy Conversion and Management 48, 2565-2578 (2007)
[4] D. Danilov, P. H. L. Notten, Electrochim. Acta 53, 5569-5578 (2008)