Continuum Modelling and 3D Simulations of Ni/Zn Cells

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The growing demand for electric energy and role of renewable energy sources calls for inexpensive, reliable and sustainable storage technologies, such as novel zinc-based batteries. A key advantage is the use of widely available and low-cost resources, eco-friendly and recyclable materials and non-combustible components.[1,2]

A promising representative of this battery type, the nickel-zinc (Ni/Zn) cell, has good prerequisites for the use as a stationary energy storage, for example. However, many physicochemical processes during cycling are still insufficiently understood so that sustainable and reliable operation is not yet consistently possible, e.g. with regard to cycle stability. Relevant effects governing cell performance and degradation are shape change of the Zn electrode, compacting the zinc and reducing pore space, and gas formation affecting the electrolyte level.

Based on models for lithium-ion cells,[3] a 3D+1D continuum model based on thermodynamics and volume averages is implemented. This model is used for cycling simulations of a Ni/Zn cell, which allows the study of transport processes and electrochemical reactions during operation. In particular, the three-dimensional simulations allow to observe the spatial redistribution of phases (e.g. of zinc, see Figure 1) and chemical species in the battery cell.[4] The extra dimension captures solid diffusion on the particle scale. Results are compared to experimental findings, and the model then may be used to optimise e.g. the cell compostion and geometry to improve the cell performance and cycle life as well as to slow down degradation processes.

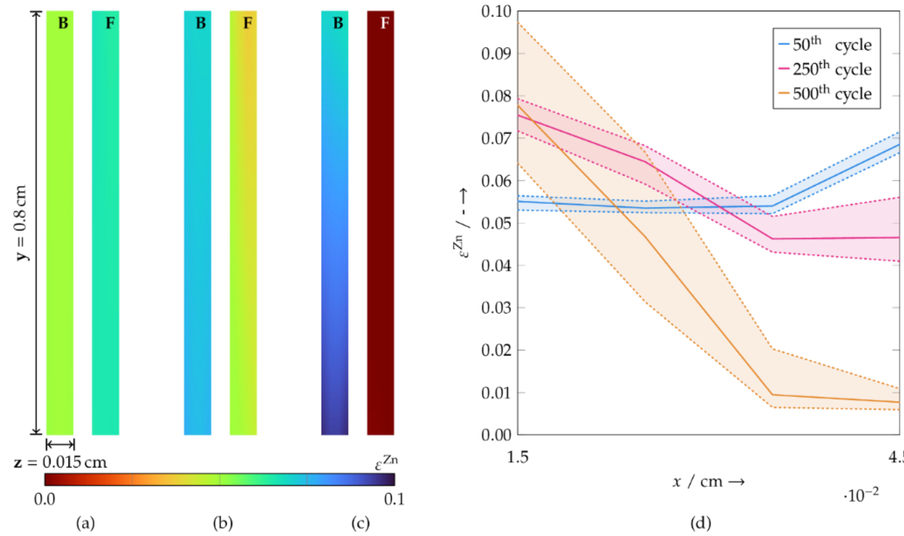

Figure 1: Evolution of the zinc distribution in x-direction (thickness) in the anode, fully discharged. In (a) - (c) the local distribution of Zn in the back (B) and front (F) of the anode is shown for cycles 50, 250 and 500. Over time, zinc shifts from the electrode's front to its back. In (d), for the same cycle numbers, the development inside the anode is made visible (cross-sectional average is used).

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