Abstract for oral presentation

3D Modelling and Simulation of Rechargeable Zinc-Air Cells

Tobias Schmitt*[1,2,3], Birger Horstmann[1,3], Arnulf Latz[1,2,3]
[1] German Aerospace Center (DLR), Institute of Technical Thermodynamics, Stuttgart, Germany
[2] Ulm University, Institute of Electrochemistry, Ulm, Germany
[3] Helmholtz Institute Ulm, Ulm, Germany
*Presenting author, email: tobias.schmitt@dlr.de, Tel.: +49 (0)731 5034 320

Metal-air batteries offer high energy densities and use abundant materials, which makes them attractive candidates for next-generation energy storage. Zinc-air batteries in particular are cheap to produce, non-toxic, and environmentally friendly. Potential applications lie in the fields of electro-mobility, portable electronics, and stationary grid storage. Up to now, only primary cells have been commercialized and further research is required to surpass lithium ion batteries on the rechargeable battery market.
In this contribution, we present three-dimensional modelling and simulation of rechargeable zinc-air batteries. Metal-air batteries are typically modelled along a single dimension connecting anode and cathode [1]. We develop a fully three-dimensional model of zinc-air batteries based on our one-dimensional model of primary zinc-air button cells [2]. Our model is capable of predicting full charge and discharge cycles. Local volume averaging is employed to describe nano-sized phase boundaries between gaseous, liquid, and solid phases and macro-sized battery cells in a single simulation [3]. Diffusion, migration and convection of all species are the relevant transport mechanisms; the electrolyte is locally electroneutral and incompressible [4]. We model thereby the reactions of zinc dissolution, zinc oxide precipitation and oxygen and carbon dioxide dissolution. Our numerical implementation is done in the software BEST [5]. It deploys a finite volume method with a non-equidistant Cartesian grid. We model an alkaline potassium hydroxide solution as electrolyte, which contains K^+, OH^-, $Zn(OH)_4^{2-}$,CO_3^{2-} and dissolved O_2. We focus on optimizing performance and cycle-life of the cells with a detailed study of distinct geometries and porosities of the electrodes. Our model is thereby validated by comparisons with recent and ongoing experiments with specially designed zinc anodes providing an exactly known geometry.

This work was supported by the Federal Ministry of Education and Research (BMBF) via the project “Zinc/Air Battery with Advanced Materials for Storage of Renewable Energies and Grid Balancing” (LUZI).

[1] B. Horstmann, T. Danner, W.G. Bessler, Precipitation in aqueous lithium-oxygen batteries: A model-based analysis. Energy & Environmental Science 6, 1299–1314 (2013).
[2] J. Stamm, A. Varzi, A. Latz, B. Horstmann, Nucleation and Growth of Zinc Oxide in Zinc-Air Button Cells, arxiv:1612.03464 (2016).
[3] Zhangxin, C., Large-Scale Averaging Analysis of Multiphase Flow in Fractured Reservoirs. IMA Preprint Series, 1229. (1994)
[4] A. Latz, J. Zausch. Thermodynamic consistent transport theory of Li-ion batteries. Journal of Power Sources 195(6), 3296–3302. (2010).
[5] Latz, A., 2010. BEST, ITWM, http://www.itwm.fraunhofer.de/en/departmen. Available at: ITWM, http://www.itwm.fraunhofer.de/en/departments/flow-and-material-simulation/complex-fluids/battery-simulation.html.