III Metal-air Batteries International Congress

Huesca
4th-7th June
2017

3D modelling and simulation of rechargeable zinc-air cells

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Abstract:

Metal-air batteries are attractive candidates for next-generation energy storage because they offer high energy densities and use abundant materials. Zinc-air batteries are particularly cheap as they are easily manufactured, and rely on abundant, non-toxic materials. Up to now, only primary cells have been commercialized and further research is required to enter the rechargeable battery market. We contribute to this goal with 3D cell level modeling of aqueous zinc-air batteries.

Most models of zinc-air batteries describe the cell dynamics along one dimension connecting anode and cathode [1,2]. They describe the temporal evolution of the concentrations of species, the volume fractions of phases, and the electric potentials. These transport equations are coupled with the (half-)cell reactions. This approach can qualitatively capture cell properties during discharge [1]. In this work, we want to understand local inhomogeneities inside the electrode structure as illuminated by Horn and Shao-Horn [3], and make quantitative predictions. To this aim, we develop a thermodynamically consistent [4] volume averaged 3D model. We focus on the correct description of transport taking into account electrolyte convection, zinc passivation, and multi-phase coexistence.

We perform simulations to understand the intimate connection between electrode structure, electrolyte composition, multi-phase coexistence, and zinc passivation. Our model is validated by comparisons with specially-designed recent and ongoing experiments on zinc anodes.

This work is 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).

Key words: Zinc-air battery, model, three dimensional

References:

[1] Stamm, J. Varzi, A. Latz, A. Horstmann, B. (2016). Nucleation and Growth of Zinc Oxide in Zinc-Air Button Cells, arxiv:1612.03464.
[2] Mao, Z., & White, R. E. (1992). Mathematical modeling of a primary zinc/air battery, Journal of the Electrochemical Society, 139(4), 1105–1114.
[3] Horn, Q. C. Shao-Horn, Y. (2003). Morphology and Spatial Distribution of ZnO Formed in Discharged Alkaline Zn/MnO_2 AA Cells. Journal of the Electrochemical Society, 150(5), A652.
[4] Latz, A. Zausch, J. (2010). Thermodynamic consistent transport theory of Li-ion batteries. Journal of Power Sources 195(6), 3296–3302.