Modelling Aqueous Zinc-Ion Batteries with a Novel Multi-Process Description of MnO_2-based Cathodes

Niklas J. Herrmann[1,2], Birger Horstmann[1,2,3]
[1]*German Aerospace Agency (DLR), Insitute of Engineering Thermodynamics*
[2]*Helmholtz Institute Ulm (HIU)*
[3]*University of Ulm, Institute of Electrochemistry*
Helmholtzstraße 11, DE-89081 Ulm
niklas.borchers@dlr.de

Amid the energy transition, the highly fluctuating supply from renewable energies prevents a rapid shift away from fossil fuels. It increases energy prices, further fuelled by geopolitical instabilities in gas supply. This situation emphasises the urgency of powerful and affordable electrochemical energy storage systems for a successful energy transition. Next-generation storage technologies are in a tight race competing in energy density, environmental safety, and cost per capacity. For several decades, zinc-based anodes have been commercially successful, though no production-ready zinc-insertion cathode exists yet [1]. Manganese dioxide cathodes, widely used in alkaline cells, present a reversible zinc storage capacity in mild aqueous electrolytes. This finding increased the research interest in zinc-ion batteries in the last decade, and many successful systems were proposed [2].

A series of challenges are facing aqueous metal batteries. The limited electrochemical stability of the electrolyte, the dynamic electrolyte composition and sensitivity to variations in local pH heavily influence performance. Additionally, a single redox couple rarely describes the cells cycling behaviour. This contribution presents a thermodynamically consistent dynamic cell model, which considers the electrolyte's complex formation and coupled transport properties [3]. Building on this, we implement a multi-process model for the manganese oxide cathode, reflecting the most reported side reactions in literature [4], manganese dissolution, and proton co-insertion. We use this to identify experimental characteristics, describe pinholes, and identify optimisation potential for next-generation zinc batteries.

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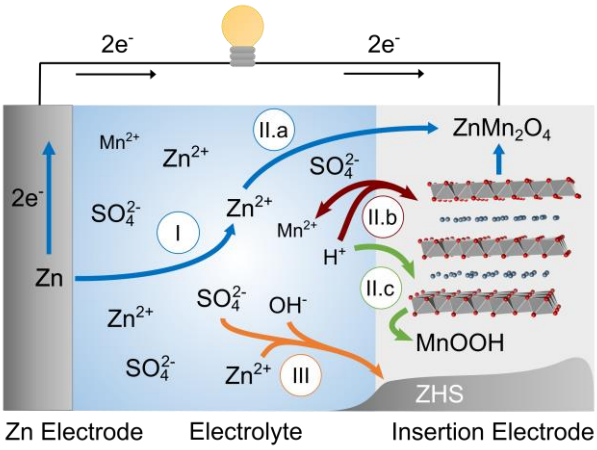

Figure 1: Schematic of the modelled aqueous Zn-MnO_2 battery showing the redox-processes modelled in this contribution. Adapted from [2]

References:

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