Modelling of Side Reactions in Nickel-Zinc Battery Cells

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Rechargeable nickel-zinc batteries (RNZB) are promising candidates for next-generation energy storage based on cheap, abundant and easily recyclable raw materials with low toxicity and the advantage of high stability, safety and robustness. Disadvantages of RNZBs are their moderate cycle life, which results from the interplay of undesired side reactions.

In this contribution, we model a rechargeable nickel-zinc cell with special focus of the side reactions. Our 1D+1D model describes transport and reactions between the electrodes in one dimension and the diffusion within the cathode particles along another radial dimension. In addition, we describe the gas evolving side reactions which lead to the loss of electrolyte in the cell. At the cathode, it is important to describe the intercalation process of protons and the evolution of oxygen; in the zinc anode, nucleation and growth of zinc oxide, the evolution of hydrogen, and the recombination of oxygen is modelled, in the headspace above the cell, pressure development due to gas evolution is taken into account. Within the macroscopic perspective, microscopic phenomena such as electrochemical reactions and precipitation are considered.

Zinc anode challenges such as dendrite growth and hydrogen evolution have been the subject of a lot of research in recent years and many advances have been made[1]. Characteristic for the nickel cathode is the occurrence of the oxygen evolution reaction (OER) at high cathode potentials. In our modelling, we investigate the OER, the hydrogen evolution reaction at the anode (HER) and the diffusive transport of oxygen through the cell. The developed oxygen is recombined to a certain extent at the zinc anode[2]. The recombination of oxygen depends on the availability of the developed hydrogen. Non-recombined gas leads to drying out of the cell due to water consumption. We derive consistent equations for modelling the anode including side reactions based on research on similar zinc-based battery systems such as zinc-air batteries[3,4]. For modelling the cathode-side electrochemistry, we build upon similar nickel-based batteries such as nickel-metal hydride[1]. We focus in particular on OER, HER and the recombination of oxygen and hydrogen to gain a better understanding of the physico-chemical processes in a nickel-zinc cell.

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Key word: nickel zinc battery, alkaline aqueous electrolyte, oxygen evolution reaction, side reaction

References:

(1) Albertus, P. , Christensen, J., Newman, J. *J. of The Electrochemical Society* **2008**, 155, A48-A60

(2) Parker, JF., Chervin, CN., Pala, IR., Machler, M., Long, JW., Rolison, DR. *Science* **2017**, 356, 415-418

(3) Stamm, J., Varzi, A., Latz, A., Horstmann, B. *J. Power Sources* **2017**, 360, 136–149.

(4) Borchers, N., Clark, S., Horstmann, B., Jayasayee, K., Juel, M., Stevens, P. *J. Power Sources* **2021**, 484, 229309