Modelling OER and HER in NiZn battery cells

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In view of the transition to renewable and environmentally friendly energy sources, zinc-based battery technologies have increasingly become the focus of research in recent years, as part of the development of next-generation energy storage technologies[1,2]. Nickel zinc batteries (NiZn) are a promising candidate for stationary applications. The theoretical, physicochemical-based description and simulation of specific battery systems contributes to a better understanding of the phenomena that occur and thus to an improvement in battery design and performance[1].

We have developed a thermodynamically based model to describe the electrochemical reactions shown in Figure 1 and the performance of a nickel-zinc cell. The 1D+1D continuum model describes the electrochemical reactions at the electrodes, transport in the electrolyte and resulting local concentration changes, as well as local volume changes of solid, liquid and gas fraction.

The lifetime of rechargeable nickel-zinc batteries is limited to a large extent by unwanted side reactions during cycling. In this contribution we focus on the gas evolving side reactions. At the nickel hydroxide cathode, especially at the end of charge, oxygen is evolved[3] (OER); and at the zinc anode hydrogen is evolved (HER). The gas evolution leads to a pressure increase inside the cell and to a loss of electrolyte. To mitigate the negative effects of the gas evolving side reactions, we additionally model the gas recombination at a catalyst in the head space of the battery cell.

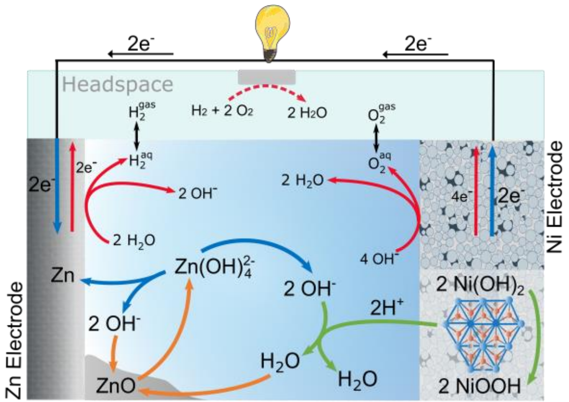

Figure 1: Modelling scheme for a nickel zinc battery cell during charge including zinc deposition (blue), zinc oxide dissolution (orange), deintercalation of protons (green), oxygen and hydrogen gas evolution (red, solid) and oxyhydrogen recombination reaction (red, dashed) at a catalyst

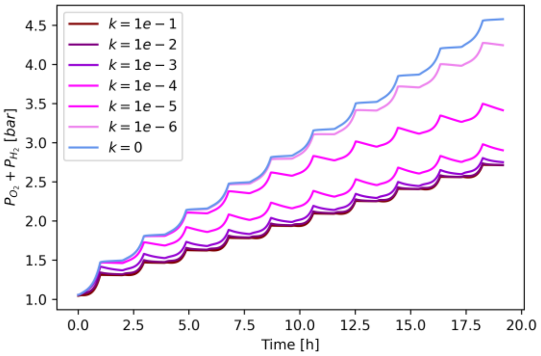

Figure 2**:** The increase in the summed partial pressure of oxygen and hydrogen on a catalyst as a function of time during cycling was modelled. The material-specific recombination rate was varied over seven orders of magnitude

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3. Albertus, P. , Christensen, J., Newman, J. *J. of The Electrochemical Society* **2008**, 155, A48-A60. DOI: 10.1149/1.2801381