Continuum Modeling of Ca-based Batteries

Laura Femmer[1,2], Max Schammer[1,2], Birger Horstmann[1,2,3]

[1]*Institute of Engineering Thermodynamics, German Aerospace Center, Wilhelm-Runge-Straße 10, 89081 Ulm, Germany*
[2]*Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany*
[3]*Institute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany*

Calcium is a promising anode material because of its high natural abundance and improved safety compared to lithium, while only having a slightly lower electrochemical potential than lithium.[1]

We model Ca-based batteries to gain a better understanding of the processes inside the batteries. We do this using the 1D+1D model, which is based on porous electrodes and the concentrated solution theory. The model describes the one-dimensional transport of ions from the anode to the cathode on a macroscopic scale by means of a system of differential algebraic equations. The charge transfer reactions are modelled using Butler-Volmer kinetics.[2] We adapted this model to a battery with an anode primarily made of Ca-Sn alloy and a 1,4-polyanthraquinone cathode[3] and parametrized it.

In the context of the CaSino project, we model the Ca-S cell, which consists of a calcium metal anode and a sulfur cathode. Given that the anode is a metallic component, the cell is modeled as a half-cell, wherein the anode is considered in the boundary conditions. We suspect that the polysulfide shuttle occurs at the sulfur cathode. For each sulfide, a transport equation has been formulated, and the concentration or the porosity is described respectively.[4]

References

[1] K. See et al., Adv. Energy Mater., Vol. 3 (2013), 1056-1061.
[2] M. Schammer et al., J. Electrochem. Soc. 168 (2021), 026511.
[3] Z. Zhao-Karger et al., Nat Commun 13 (2022), 3849.
[4] T. Danner et al., Electrochimica Acta, Vol. 184 (2015), 124-133.