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Fachtagung „Kraftwerk Batterie“, 26.-27. April 2016

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Thema Numerical Simulation of Space-Charge Layer Formation in Solid Electrolytes

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Kurzfassung All-solid-state (ASS) batteries are a promising alternative to overcome the weaknesses of currently available battery technology. By the use of non-flammable solid electrolytes (SEs) instead of liquid electrolytes safety will be enhanced. However, ASS cells still have limitations such as low power densities. These limitations are traced back to processes at the interface between electrodes and electrolytes like space-charge layer formation and the concurring higher interface resistances.
To improve the performance of ASS cells a better understanding of these processes is essential. This will allow us not only to examine known SE materials but also to modify and optimize them.

In this contribution, we numerically simulate the process of space-charge layer formation in SEs sandwiched between two blocking electrodes. When electrodes and electrolyte are brought together, charge is redistributed until local equilibrium is reached. The system of partial differential equations (PDEs) is a non-linear, time-dependent drift-diffusion equation coupled with a Poisson equation and a quasi-static momentum equation. In contrast to classical generalized Nernst-Planck formulations, this model considers finite ion size and the local pressure in the electrolyte. It includes only one consistent ion flux. Space-charge layer formation is enforced by new time-dependent boundary conditions which ramp-up the quasi-static potential at the boundaries to open circuit potential.

The system of PDEs is discretized by a purely implicit finite volume scheme. The resulting algebraic equation system is solved by a Newton-type method. Computational results for different SE materials like $Li_{0.5}La_{0.5}Ti_{0.3}$ and $LiPO_3$ are presented and compared to experiments as well as known semi-analytical results. In accordance with theory, over time, equilibrium is established: The time dependent solution approaches the stationary one. Corresponding to semi-analytical results for a stationary 1D case, the width of the established space-charge layer is significantly bigger than in conventional liquid electrolytes. Furthermore, the observed space-charge layers are not symmetric. Both material modifications and thickness reduction decrease the arising electric fields at the boundaries and therefore reduce the interfacial resistance. These insights will give a useful perspective to improve ASS cells.