The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

Efficient Numerical Computation of Chemical-Mechanical Coupled Contact Problems for Battery Active Particles

R. Schoof[1], **G.F. Castelli**[2] **and W. Dörfler**[1]

[1] KIT - Institute of Applied and Numerical Mathematics, 76131 Karlsruhe, Germany
[2] KIT - Institute of Thermal Process Engineering, 76131 Karlsruhe, Germany

Corresponding author e-mail: raphael.schoof@kit.edu

Keywords: *Lithium-Ion Battery (LIB), Phase-Field Model, Mechanics, Contact Problem, Numerical Simulation, Finite Element Method*

During battery operation of LIBs, mechanical degradation is a crucial aging mechanism. This is important for phase separating electrode materials, where an inhomogeneous lithium concentration profile can lead to large mechanical stresses, which can induce particle fracture. Another example is the large volume change up to 300 % for lithium silicon (LiSi) [3]. However, the increase in mechanical stresses must not be neglected if the swelling of the particle is restricted, e.g., due to the current collector.

The used particle model couples lithium diffusion, large deformations and phase separation based on a thermodynamically consistent transport theory [1]. A solid solution model describes the diffusion and a finite strain theory models the deformations. A phase-field model is used to deal with the phase separation. In the end, a common free energy density connects all different phenomena. To incorporate the restricted swelling, the model is extended by an obstacle contact [2].

The resulting Cahn–Hilliard-type phase-field model approach is computationally expensive to solve. Therefore, a highly efficient adaptive numerical solution algorithm in space and time is used [1]. The particle contact is treated with the concept of the primal-dual active set algorithm. Physical and numerical aspects for an electrode particle of lithium iron phosphate (LFP) and of LiSi are investigated and compared: influence of phase separation, mechanics and different shaped obstacles. The efficiency of the solving algorithm as well as the parallel distributed memory usage allow the further analysis of computationally demanding parameter regimes and also three-dimensional particle geometries.

REFERENCES

[1] G.F. Castelli, L. von Kolzenberg, B. Horstmann, A. Latz, and W. Dörfler: Efficient Simulation of Chemical-Mechanical Coupling in Battery Active Particles. *Energy Technol.*, 9(6):2000835, (2021), doi: 10.1002/ente.202000835.

[2] J. Frohne, T. Heister, and W. Bangerth: Efficient Numerical Methods for Large-Scale, Parallel Solution of Elastoplastic Contact Problems. *Int. J. Numer. Meth. Engng*, 105(6):416–439, (2016), doi: 10.1002/nme.4977.

[3] L. von Kolzenberg and A. Latz and B. Horstmann: Chemo-Mechanical Model of SEI Growth on Silicon Electrode Particles. *Batteries & Supercaps*, n/a, (2021), doi: 10.1002/batt.202100216.