The Numerical Simulation of Intercalation Processes in Lithium Ion Batteries

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Lithium ion batteries are key technologies for mobile power devices, as for example in smartphones, laptops or electric vehicles. For the better understanding of the electrode materials we investigate the temporal evolution of the lithium concentration and stresses in a single particle of the electrode material during the (dis-)charge process. A phase-field model coupling chemical and mechanical processes resulting in a fourth-order PDE is used, see (Huttin and Kamlah., 2012).

In our talk we focus on the efficient numerical solution of this time-dependent PDE. The main challenges arise from the high nonlinear character and the spatial as well as the temporal properties of this equation, which includes the handling of an almost sharp moving phase boundary and processes on different time scales.

To solve the arising system numerically we employ a higher order standard finite element method together with an adaptive time integrator. However, a full resolution of three-dimensional particles, respecting the very thin interface zone, generates a huge amount of degrees of freedom. We therefore developed a fully parallelizable, highly efficient solver, which totally avoids the necessity of storing matrices. The implementation was done with the matrix-free framework within the open-source finite element library deal.II (Bangerth et al., 2007).