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A three-dimensional, coupled model for fully resolved finite element simulations of all-solid-state lithium-ion cells

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Due to their potentially very high energy density, all-solid-state lithium-ion cells constitute a promising technology for future energy supply. Since comprehensive and in-depth experimental investigations are often unfeasible, computational tools have gained in importance. However, many current modeling and simulation approaches are based on a number of simplifications, especially geometric homogenization, and are therefore not always adequate for accurate analyses and reliable predictions. This is mainly due to the complexity of the physical phenomena, such as lithium and charge transport, interfacial charge transfer, and mechanical effects. These include volume changes of the active material, possibly leading to large strains and stresses, plasticity, or even to fracture.

Against this background, this work introduces a novel computational framework for all-solid-state lithium-ion cells. In particular, we present a three-dimensional, coupled finite element model resolving porous microstructures and local physical phenomena without homogenization. Unlike most existing approaches such as the one published in [2], our model is derived from nonlinear continuum mechanics and capable of capturing large deformations beyond linear elasticity. For this purpose, we solve an ALE formulation of all governing equations on moving meshes, taking diffusion-induced strains and stresses into account. Also, based on previous work presented in [1], we establish a novel interface coupling strategy by consistently solving the Butler–Volmer charge transfer kinetics, while considering mechanical contact and separation between the active material and the solid electrolyte. All governing equations are treated in a monolithic fashion to maximize computational robustness and efficiency. To this end, we also propose advanced, physics-oriented block preconditioning and solution techniques for the resulting linear systems of equations. Combined with the full MPI parallelization of our implementation, our model thus opens up new possibilities for large-scale, high-performance computations in settings with strict demands on accuracy.

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