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ABSTRACT:

Chemomechanics and Damage Simulation in Silicon during Lithiation

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For energy storage, computational approaches are transforming battery storage technologies. For understanding multiphysics processes, highly accurate and coupled solution algorithms are needed. Specifically for batteries, ions are moving due to chemical potential and thus also stress assisted flux is modeled.

Such a coupling between mechanics and diffusion makes numerical difficulties [1]. We discuss a possible framework for such simulations based on continuum mechanics simulations with monolithic methods by using energy based formulations. All computations are done by open-source packages with symbolic derivatives providing high accuracy at the coupling terms [2]. We give examples mimicking phenomena observed in tomography X-ray measurements for Si electrodes.

[1] Abali, B. E., & Isaksson, P., Damage Modeling in Batteries by Coupling Lithiation and Mechanics by Means of a Finite Element Method, In: Advances in Continuum Physics: In Memoriam Wolfgang Dreyer (pp. 317-334). Cham: Springer Nature Switzerland, 2025.

[2] Abali, B. E., Computational Reality, Solving Nonlinear and Coupled Problems in Continuum Mechanics, In: Advanced Structured Materials. Springer Nature, Singapore, 2017.