Phase-field simulation of the phase separation and mechanical stresses in the composite lithium-ion battery electrodes with unfitted isogeometric discretizations

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ABSTRACT

In many phase-separating materials of lithium-ion battery electrodes, the phase separation can be damaging. In order to understand the phase separation and the mechanical stresses in the electrodes, we employ the Cahn–Hilliard equation, coupled with large deformations. The primal variational formulation of the fourth-order Cahn–Hilliard equation requires $\mathscr{C}^1$-continuous finite element discretizations in the context of isogeometric analysis. The additional essential boundary condition $\boldsymbol{\nabla} c = 0$ arises from the thermodynamic derivation of the Cahn–Hilliard equation and can not be fulfilled automatically in the weak formulation. In this presentation, we explore the variational imposition of this essential boundary condition based on the symmetric variant of Nitsche's method. Our formulation does not introduce additional degrees of freedom and is shown to be variationally consistent. In contrast to strong enforcement, the new boundary condition formulation can be naturally applied to any mapped isogeometric parametrization of any polynomial degree. Unfitted Cartesian B-spline meshes constitute an effective alternative to boundary-fitted isogeometric parametrizations for constructing $\mathscr{C}^1$-continuous discretizations, in particular for complex geometries. We combine our variational boundary condition formulation with unfitted Cartesian B-spline meshes and the finite cell method to simulate chemical phase segregation in a composite electrode during non-equilibrium lithiation. It involves the coupling of chemical properties with mechanical stresses on complex domains, as well as the coupling of different materials across complex interfaces, which demonstrates the flexibility of variational boundary conditions in the context of higher-order unfitted isogeometric discretizations.

Keywords: Cahn–Hilliard equation, the Nitsche method, the Finite Cell Method, lithium-ion battery, large deformations

REFERENCES

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