Modeling the Multiphysics Processes in Lithium Ion Battery Cells within a Computational Homogenization Framework

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ABSTRACT

In recent contributions the computational homogenization technique was tailored to model the multi-physics processes that take place in Li-ion batteries. The formulation originally proposed in [1] has been recently extended [2] to take into account electroneutrality, quasi-static Maxwell equations, time dependent scale transitions, and scale separation in time.

The approach described here originates from the fundamental balance laws (of mass, force, charge) at both scales. The weak formulation derived preserves an energetical meaning which allows to extend the Hill-Mandel energy averaging theorem to the problem at hand.

This note details the microscale formulation. Balance laws are accompanied by constitutive assumptions that emanate from a rigorous thermodynamic setting. After spatial discretization of the weak form a Backward Euler time-advancing algorithm has been implemented by means of Abaqus User Element (UEL) scripts.

Several case studies have been simulated to validate the implemented formulation.
The first [3] concerns a one-dimensional application to ionic transport in Li-ion batteries electrolyte, inspired by [4]. The second case study [5] simulates the charge/discharge process of an all-solid-state Li-ion battery. The numerical results have been compared with the outcomes of one-dimensional characterization derived in [6]. Finally the proposed theoretical framework is applied to a two-dimensional problem, with the aim of investigating the behavior of a multi phases microstructure [3].

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