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AN EFFICIENT COMPUTATIONAL TOOL FOR FIBER-BASED LITHIUM-ION BATTERIES

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Fiber-based electrodes are receiving increasing attention for their possible applications in high-performance and structural batteries [1]. In the design of these battery cells, the electrolyte (either liquid or solid) accommodates fiber-type battery-functional components. Active materials are cast as high aspect ratio fibers. Active material fibers are characterized by a larger specific surface area compared to their particle-shaped counterpart [2], resulting in an enhanced lithium exchange with the electrolyte that improves the battery performance.

In this contribution we propose an efficient computational tool for the analysis of fiber-based battery cells. Considering a single battery cell, the field variables in the electrolyte, namely ionic concentrations and electrical potential, are coupled through the Nernst-Plank equation [3], and the electroneutrality condition is assumed to hold. To ease the generation of a finite element mesh for the fiber-based electrodes, a mesh-independent embedded fiber method [4] is used. With a discrete definition of fibers, local field variables are accurately described. This allows the introduction of appropriate interfacial conditions between the electrodes and the electrolyte, which is crucial for the battery cell model to function. In this work, the reaction kinetics across the active material-electrolyte interface is explicitly taken into account [2].

As a simplification to a reference solid finite element model and due to the fibers' high aspect ratio, fibers are reduced to mathematically equivalent one-dimensional objects in the numerical model. In the numerical simulations, results of the dimensionally-reduced model are validated against reference finite element solutions.

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