Efficient Reformulation of Pressure Induced Solid Phase Diffusion in Coupled Electrochemical-Mechanical Models for Lithium Ion Batteries

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Electrochemical power sources are expected to play a significant role in the future in automobiles, power storage, military and space applications. Lithium-ion chemistry has been identified as a good candidate for high power/energy secondary batteries. Progress has been made towards modeling of such systems using physics-based models based on transport phenomena, electrochemistry and thermodynamics. These models are represented by coupled non-linear partial differential equations and are typically solved numerically and take minutes to hours to simulate [1-2].

Even if one-dimensional (x) transport is considered in the macro-scale, all of these continuum models require solid state diffusion to be solved in the pseudo second dimension (radius r) in the electrode particle. Lithium ions intercalate into and out of the solid electrode particles in the pseudo second dimension (r) and hence it is necessary to solve solid phase diffusion within the particle in addition to the macro-scale equations. This diffusion in micro-scale is typically modeled using Fick's law of diffusion. But for high power/energy applications of future, we need high energy capacity materials like silicon, germanium etc. which show significant stress development during lithium intercalation leading to volume and density changes. Therefore, to capture these phenomena, pressure induced diffusion must be included when solving for solid phase diffusion in the pseudo dimension (r) [3-4] which introduces complexities like moving boundaries, etc. in the model.. But inclusion of such physics in electrochemical engineering models not only adds to the complexity but also to the computational time/cost. Traditional discretization approaches like finite difference (FD) when used for solid phase diffusion in the second pseudo dimension (r) increase the number of equations by many folds thereby making the simulation of the system slower and complex.

This talk will discuss and compare efficient reformulation techniques for simulation of pressure induced solid phase diffusion during lithium intercalation into the electrode particles. Polynomial approximation and and a mixed order finite difference reformulation method with optimal node spacing [5] will be presented to reduce the computational cost/time. Finally, use of these reformulation techniques for representing solid phase concentration within active material particles for the real-time simulation of full order electrochemical-mechanical coupled models for lithium ion battery will be demonstrated which is important for determination of capacity fade due to stress development.

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