An enhanced Li-ion Single Particle Model including Diffusion-Induced Stress, Volume Expansion and Electrolyte Dynamics, and its Numerical Solution

Pedro Ascencio[a] and W. D. Widanage[b]

[a,b] University of Warwick. WMG. United Kingdom. CV4 7AL.

[a] p.ascencio-ormeno@warwick.ac.uk, [b] Dhammika.Widanalage@warwick.ac.uk

Abstract

The use of new materials in lithium-ion batteries, such as silicon [1], have brought up the modelling of well-known phenomena [2] which traditionally have been neglected in Electrochemical-based models, in part by its complexity and/or marginal model contribution for standard materials [3]. Indeed, these models do not commonly include deformation dynamics for the particles [4], in spite of the significant evidence that the intercalation process lead to this effect, the extreme example of which is the colossal volume changes in silicon particles [1]. For instance, the typical computational tractable approaches, such as the pseudo two-dimensional (P2D) or Single Particle model (SPM), in general do not consider the effects of the mechanical change of the particles on the diffusivity process [5].

To investigate the operation of a lithium-ion silicon-based battery under transient current profiles, which lead to reach the limits of the battery capacity and emphasize the diffusion-induced stress dynamic, an enhanced SPM is formulated. The aim of this model is to keep its simplicity of its mathematical structure in order to facilitate the understanding of primary phenomena, which play a relevant role in this scenario. Thus, the traditional SPM is extended to include (i) diffusion-induced stress, under linear-isotropic elastic behavior [2], so that the effects of a symmetric volume change in the anode particles are identified, in terms of the output voltage response and concentration profile, with respect to standard fixed particles. In addition, this model includes (ii) electrolyte dynamics [6] (potential and concentration) in order to identify their contribution on the voltage response for low C-rates.

To solve the diffusion-induced stress dynamic (non-linear PDE) in the particle, a novel numerical method is presented [7]. It is based on a notable result from Real Algebraic Geometry: the Positivstellensatz, where the differential problem is recast as polynomial inequalities which are relaxed via their Sum-of-Squares (SOS) decomposition, leading to a convex optimisation problem, implementable via semidefinite programming.

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