



Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Study on microstructures of electrodes in lithium-ion batteries using variational multi-scale enrichment

Sangmin Lee ^a, Ann Marie Sastry ^b, Jonghyun Park ^{c,*}^a Mechanical & Aerospace Engineering Department, University of Notre Dame, Notre Dame, IN 46556, USA^b Sakti3, Ann Arbor, MI 48108, USA^c Department of Mechanical and Aerospace Engineering, Missouri University of Science and Technology, Rolla, MO 65401, USA

HIGHLIGHTS

- Develop an advanced microstructure model using enrichment approach.
- Model multiphysics phenomena among the particle aggregates in the electrode.
- Explore the impact of microstructures on battery performance.

ARTICLE INFO

Article history:

Received 4 November 2015

Received in revised form

17 February 2016

Accepted 28 February 2016

Keywords:

Variational approach

Microstructures

Multiscale modeling

Battery design

Tortuosity

Porosity

ABSTRACT

Performance and degradation of a Li-ion battery reflect the transport and kinetics of related species within the battery's electrode microstructures. The variational multi-scale principle is adapted to a Li-ion battery system in order to improve the predictions of battery performance by including multi-scale and multiphysics phenomena among the particle aggregates in the electrode; this physics cannot be addressed by conventional homogenized approaches. The developed model is verified through the direct numerical solutions and compared with the conventional pseudo-2D (P2D) model method. The developed model has revealed more dynamic battery behaviors related to the variation of the microstructure—such as particle shape, tortuosity, and material composition—while the corresponding result from P2D shows a monotonous change within different structures.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

One key solution for the challenges related to pollution and transportation energy costs is to replace conventional fuels with cost-competitive and domestically-produced alternatives, such as advanced batteries. The development of an advanced battery, with a corresponding reduction in its cost, requires optimal battery design and battery health management. The optimal battery design allows for minimizing unnecessary components that increase both weight and cost. Also, battery performance and life expectancy are quite dependent on how a battery is used, which means that optimal battery health management can significantly increase the life of a battery and reduce its cost. In particular, current battery systems are substantially oversized for meeting power and energy

performance requirements at the end-of-life, which indicates the importance of adequate battery health management.

Optimal battery design and health management via modeling is the most effective way in terms of processing time and cost, compared to experiments. However, modeling tools for these purposes must include appropriate design elements and must be accurate in prediction. In this light, current battery models are not sufficient because they suffer from an important drawback, a lack of detailed morphology of the internal structures of electrodes. Modern battery electrodes involve micro-/nano-composites of ionic storage materials and ionic/electronic conductors. Consequently, battery performance is determined by the local transport of ions and electrons through inhomogeneous internal structures and kinetic reactions at the interfaces among them. These spatial inhomogeneities generate localized fluxes and irregular gradients of species concentration, and eventually different cell voltage responses. Consequently, in order to achieve the best battery

* Corresponding author.

E-mail address: parkjonghy@mst.edu (J. Park).

performance, a battery designer must control and optimize the species transport path, interface surface area, and kinetic reaction rate. Therefore, a microstructural battery modeling tool is necessary.

Further, the degradation of battery performance is closely related to the composition and structure of the constituent particles in the electrode. Interfacial side reactions and kinetics, interfacial surface areas, mechanical particle networks, and transport phenomena are microphysical processes and therefore are affected by the characteristics of the involved microstructures in the electrodes. As a result, most of the proposed degradation mechanisms in Li-ion batteries—such as active materials dissolution, SEI (solid-electrolyte interphase) layer formation, and mechanical failure—are directly connected to the microstructure of the electrodes [1–4]. Consequently, it is essential to elucidate the microstructural effects on battery performance and to optimize the microscopic feature in the electrode materials of Li-ion batteries to fully understand the physics inside the cells, and eventually to resolve the given problems.

A Li-ion battery cell can be decomposed into scales of three different lengths: meso-, micro-, and nano-scale. The kinetics and transport phenomena at the micro- and nano-scales must be linked to the meso-scale perspective, including electrode geometry, porosity, and thermal behavior. Generally, the shape of particles in the electrode materials is assumed to be ideal—such as is the case with spheres and ellipsoids [8,9]. However, the real microstructure of the electrodes involves irregularly shaped particles as reported in Refs. [5–7]; as a result, the transport and kinetics are non-uniform throughout the entire electrode domain. Consequently, the simulation results using such a homogenized model cannot account for the uncertainty of the battery response coming from geometric irregularity at the particle scale.

Several experimental studies have been conducted to investigate the effects of microstructure on battery performance. It has been reported that smaller particles showing larger areas of interface between the solid particle and the electrolyte can enhance capacity [10]. Volume fraction effects on capacity have been conducted by changing the temperature and pressure on the cell [11,12]. However, all of these studies were limited to reporting *only* the observation—without quantifying the microstructural features of battery performance. Moreover, those results are limited to specific materials, which is impractical for an application to battery systems with different materials and structures.

In the modeling and simulation work, the pseudo 2D (P2D) model [8] has been widely used in predicting battery performance. This model relies on the continuum-based porous electrode theory, in which active particles are modeled via a homogenized pseudo 2D approach. This model was extended to investigate different active material composition effects on power and energy performance [13], mechanical stress in the particles when the cell is subjected to a mechanical load [14], and gas evolution influence on battery cell degradation [13]. However, this method is limited to the study of the homogenized system, and therefore it cannot account for the effects of microscopic particle percolation and the geometry of the particle on battery cell performance. At the particle scale, the Li-ion diffusion process coupled with mechanical stress loading was simulated using thermal analogy volume expansion [9]. The developed electrochemical-mechanical model predicted that ellipsoidal particles with a smaller volume and a larger aspect ratio are desirable in terms of the stress level inside the particles. The intercalation-induced stress at the particle scale was further coupled to crack propagation problems with the following: different particle sizes and aspect ratios [15], stress distribution on the manganese oxide particle due to the phase transition [16], and the resistive heat generated by considering particle shape [17].

However, both Li-ion diffusion processes in the electrolyte and the interaction through the surface of the active particles are strongly dependent on microstructure geometric connectivity. To represent the microstructural particle network at the cell-scale, tortuosity is usually employed [18], and the effective properties based on tortuosity are used in the simulations [19,20]. Still, this approach cannot account for the local microscopic particle network.

Some efforts to study the microstructural effect have been made; these include coupling between measurement and modeling. Tomography data were used both to produce the 3D microstructure of a cathode electrode as well as to calibrate electrochemical properties from inhomogeneous cathode particles [21]. A set of 3D full cells with details of microscopic active materials, conductive additives, and electrolytes were used to predict microstructural parameter effects on discharge capacity in Refs. [22,23]. Such models are capable of introducing realistic electrode geometries and of investigating their structural effects on cell performance. However, these models are generally computationally expensive due to the fact that they require a full mesh of the system; they are therefore not feasible for parameter studies or optimizations for improving battery performance.

In order to include the microstructural effect in the Li-ion battery model, a multi-scale framework was established based on a homogenization approach and surrogate-based scale bridging [24]. Homogenization resulted in a micro/macro formulation for lithium batteries that was derived by employing a generalized Poisson-Nernst-Planck (PNP) equation set [25]. Wang and co-workers [26,27] used volume-averaged equations and a parabolic profile approximation for solid-phase concentration. This helped reduce the solid-phase partial differential equation to two differential algebraic equations. Nevertheless, an appropriate multi-scale method has not been introduced in the battery field, while fluid mechanics, ceramic matrix composites, heat transfer, and many other areas have successfully adopted macro/micro coupled multi-scale approaches. Generally, the scale-bridging between scales of different lengths using the homogenization approach is based on an assumption that the micro length scale is much smaller than the macro-scale; thus it is assumed that the micro-scale is at a steady state [28]. The Li-ion battery system is investigated using an asymptotic multi-scale model based on the assumption that the length scale is very different between macro and micro [29]. However, the steady state assumption is not applicable in the Li-ion battery system because the length of the electrode is generally several hundreds of micrometers, and microscopic active particle aggregation is several tens of micrometers [30]. Therefore, the microscopic particle aggregations cannot be assumed as a point in the cell-scale.

In this study, we adopted the variational multi-scale enrichment method, which is effectively applicable to the multi-scale study of the Li-ion battery system. Unlike conventional multi-scale approaches based on the homogenization method, this method can decompose the scales without assuming scale separation. Also, the transient phenomenon at the micro-scale can be included. Initially, the multi-scale variational formulation was developed in order to find detailed solutions that were missing in the general finite element approximation [31–33]. Independently, a similar multi-scale framework was developed for the advective-diffusive model as well as for the linearized compressible Navier-Stokes equations; these methods have been shown to stabilize numerical simulations by implementing bubble functions [34,35]. The approach has been extended to solve incompressible Navier-Stokes equations [36–38] and has been applied to solid and fluid systems combined with other numerical methods: mesh-free [39,40], x-FEM and level set [41], and adaptive FEM [42]. By employing the variational multi-scale approach, this paper presents the general procedure of

Download English Version:

<https://daneshyari.com/en/article/7728255>

Download Persian Version:

<https://daneshyari.com/article/7728255>

[Daneshyari.com](https://daneshyari.com)