Journal of Power Sources 360 (2017) 360–372

Contents lists available at ScienceDirect

Journal of Power Sources

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

A battery model that fully couples mechanics and electrochemistry at both particle and electrode levels by incorporation of particle interaction

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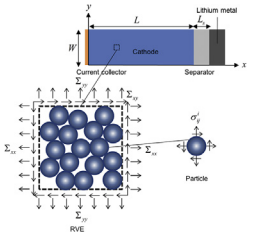
HIGHLIGHTS

- Fully coupled mechanics and electrochemistry at both particle and electrode levels.
- Particle interaction stress acts as loads on the particle surface.
- Stress affects electrochemical reaction rates by a stress-dependent over-potential.
- A small electrochemically inactive region can cause large stress in its vicinity.
- A strategy to reduce degradation by improving the homogeneity of the electrode.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 30 March 2017
Received in revised form
18 May 2017
Accepted 31 May 2017

Keywords:
Lithium
Particle
Fracture
Model
Multiscale
Mechanics

ABSTRACT

This paper develops a multi-scale mechanical-electrochemical model which enables fully coupled mechanics and electrochemistry at both particle and electrode levels. At the particle level, solid diffusion is modeled using a generalized chemical potential to capture the effects of mechanical stress and phase transformation. At the electrode level, the stress arising from particle interaction is incorporated in a continuum model. This particle interaction stress is in addition to the traditional concept of intercalation stress inside isolated particles. The particle and continuum electrode levels are linked by the particle interaction stress as loads on the particle surface, and by consideration of stress on the electrochemical reaction rate on the particle surface. The effect of mechanical stress on electrochemical reaction results in a stress-dependent over-potential between particle and electrolyte. Stress gradient in an electrode leads to inhomogeneous intercalation/deintercalation currents for particles depending on their interaction stress with neighbors, resulting in stress gradient induced inhomogeneous state of charge. Conversely, non-uniform intercalation/deintercalation currents in an electrode lead to stress between particles. With this model we have an important finding: an electrochemically inactive region in an electrode causes stress built-up. This model provides a powerful tool to address various problems such as fracture in-between particles.

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1. Introduction

Mechanical degradation is one of the main causes of capacity fade in lithium-ion batteries [1]. During lithium intercalation and

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http://dx.doi.org/10.1016/j.jpowsour.2017.05.115
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deintercalation, the active material particles of battery electrodes experience mechanical deformation, which induces stress inside particles and in-between particles. These stresses can lead to cracks and fractures of the electrode, such as cracks inside particles or in-between particles, causing isolation of active materials, disruption of the electrically conductive particle network and exposure of fresh surfaces for side reactions that result in capacity degradation [2].

Coupled electrochemical and mechanical modelling is essential to investigate stress generation and to evaluate its effect on battery performance. Prior models at the particle level mostly focused on a single, isolated particle [3–5]. Treating the intercalation-induced stress in analogy to thermal stress, a coupled electrochemical and mechanical model has been developed to study the stress and concentration field inside a particle [5]. This type of isolated particle model has been widely used and extended to address various problems [6–8], such as stress inside an agglomerate particle [9] and stress generation coupled with phase transition [10]. While these models are very useful to consider stress and fracture inside a particle, they cannot be used for problems such as fracture in-between particles since particle interaction is omitted. Mechanical stress can change the electrochemical potential of a solid and therefore (1) affects the diffusion in the solid, and (2) affects the electrochemical reaction between the solid and the electrolyte. Prior models mostly focused on stress-enhanced diffusion in a solid. For example, the developed stress gradient inside a $LiMn_2O_4$ particle is predicted to increase the effective solid diffusivity by up to 35% [5]. This is because both concentration gradient and stress gradient drive the diffusion flux, which is larger than the flux calculated from concentration gradient alone. Many models have followed the thermal stress analogy approach to couple the intercalation stress [8,11]. The effect of mechanical stress on the electrochemical reaction rate has not been included in most models, except in only few studies [7]. While the mechanical effect on electrochemical reaction rate may be negligible for an isolated particle, including this effect is necessary when modeling particle interaction since stress gradient in the electrode leads to spatial-dependent interaction stress between particles. It is necessary to account for different intercalation/deintercalation currents for particles under different stress states that are dependent on their interaction with neighbor particles.

In comparison to single particle level, the electrode level model coupling electrochemistry and mechanics are lacking. There have been several attempts [7,11–13] to couple the mechanical model of isolated particles [5] with the porous electrode model [14] to analyze the distribution of intercalation stresses inside different particles across the electrode. In those attempts, however, the particles are considered isolated with no interaction between them. Particle interaction can result in stress level comparable to the stress generated from the concentration gradient. In addition, the gradient from a distribution of interaction stress can lead to highly inhomogeneous interaction/deintercalation currents for particles at different locations. Several experimental works have measured the stress and strain at the electrode level and highlighted the importance of mechanical stress [15–17]. A model that is capable of capturing the stress caused by particle interaction, and fully couples electrochemistry and mechanics at both particle level and continuum electrode level, is highly demanded. In addition to more accurate prediction of battery performance, such a model is necessary to predicting inter-particle phenomena such as fracture propagation between particles.

Recently electrode microstructures constructed from focused ion beam scanning electron microscope (FIB/SEM) [18] or X-ray tomography [19] have been directly modeled using finite element methods (FEM) to investigate the microscopic electrochemical and mechanical behaviors. Researchers have found considerable stress arising from the contact between particles [20,21], which highlights the importance to consider the interaction between particles. However, these direct numerical modeling of microstructures often incur high experimental and computational costs related to microstructure characterization and simulation. The requirement of a sufficiently large representative volume containing many microstructures to be statistically representative poses challenges on the size and the time scale of an electrode that can be practically simulated. Therefore a model that integrates electrochemistry and mechanics, and integrates the particle level and the continuum electrode level without introducing undue complexity is highly desirable to identify and interpret the mechanisms that affect battery performance, to allow for efficient parametric studies, and to guide electrode design.

The objective of this work is to develop a multi-scale and multi-physics model that integrates electrochemical and mechanical behaviors at both particle level and continuum electrode level with incorporation of particle interaction. As demonstration, we have used the model to simulate a $LiMn_2O_4$ half-cell, which revealed rich behaviors resulting from particle interaction and coupled electrochemistry and mechanics, and how the interaction between electrochemistry and mechanics manifests and interconnects across the two levels. We chose $LiMn_2O_4$ as a demonstration material system because its material parameters are available in the literature and because it exhibits phase transition during lithiation which allows us to demonstrate the capability of our model to capture the effect of phase transition. Our model is general and can be applied to various other materials, including anode materials. With this model we have found for the first time that an electrochemically inactive region in an electrode can cause significant stress built-up. The finding provides an important insight to reduce the degradation by increasing homogeneity of the electrode. This model provides a tool to study various problems related to inter-particle behaviors that cannot be addressed by the isolated particle model, such as defect growth and crack evolution in-between particles, electrode deformation and yielding, detachment of active material, or delamination of electrode from the current collector.

2. Model development

Fig. 1 illustrates the concept to model particle interaction and to link the particle level and the continuum electrode level. Each spatial point in the continuum level corresponds to a particle level representative volume element (RVE) consisting of many particles and porous volume occupied by the electrolyte. Individual particles are not visible in the continuum level. The mechanical stress in a particle comes from two sources: (1) stress induced by lithium concentration gradient inside the particle, denoted as σ_{ij}^c, and (2) stress induced by particle interaction, denoted as σ_{ij}^i. The stress σ_{ij}^c can be calculated by the lithium concentration distribution inside the particle. The expansion of a particle due to lithium intercalation is constrained by its surrounding particles. The interaction stress, σ_{ij}^i, depends on the expansion of the particle relative to that of its neighbors, as well as any macroscopic loading applied to the overall electrode. The stress in a particle is given by $\sigma_{ij}^c + \sigma_{ij}^i$. In the following sections, we first tackle diffusion in the solid and the associated σ_{ij}^c inside a particle in section 2.1. The interaction stress, σ_{ij}^i, is formulated in section 2.2.

2.1. Particle level

2.1.1. Stress

We first consider an isolated particle, where the stress arises

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