

Stress Analysis of the Separator in a Lithium-Ion Battery

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ABSTRACT

A separator is a membrane that prevents the physical contact between the positive and negative electrodes while enabling ionic transport. The integrity of the separator is vital to the performance and reliability of a battery. This paper presents finite element stress analysis for the separator in a lithium-ion battery using a macro-scale battery cell model. In this model, the porous electrodes were treated as homogenized media and represented with the effective properties estimated using the rule of mixtures. To compute the deformation due to lithium (Li) intercalation & deintercalation and temperature variation, the Li concentration distribution and temperature change due to electrochemical reactions must be known. These parameters were computed using a multi-physics model in COMSOL and mapped to the macro-scale model in ANSYS. Numerical simulations were conducted to identify the locations and magnitudes of the maximum strain and stress of the separator in the pouch cell. The effects of temperature change and the effective friction between separator and its surrounding electrodes were also investigated.

INTRODUCTION

Battery separators are porous membranes made of electrically insulating materials. In production, the separators are sandwiched between positive and negative electrodes and then spirally wound together in cylindrical or folded back and forth in prismatic configurations. The pores of the separators are filled with ionically conductive liquid electrolyte. Although separators do not participate in the electrochemical process, they perform the critical function of physically separating the positive and negative electrodes in order to

avoid internal short circuits. A short circuit due to separator failure can often lead to a thermal event [1,2].

The primary failure modes of separators are melting, degradation, fatigue and crack. Most of them related closely to the stress conditions, thus, stress analysis of the separator is very important to avoid the failure of the separators and the entire battery system. Stress in separators arises from multiple sources. In the battery assembly process, the separator is stretched and hence in a state of tension. In service, the volume changes in positive and negative electrodes during Li insertion and extraction induces stress in the separator. In addition, the differential thermal expansion between different battery components is another source of stress.

Not until recently, the mechanical problems inside a lithium-ion (Li-ion) battery have attracted much attention. Christensen and Newman studied the stress generated inside $\text{Li}_y\text{Mn}_2\text{O}_4$ [3] and carbon [4] electrodes. Zhang et al. [5] considered the stress effect on the Li diffusion and stress distribution inside one single $\text{Li}_y\text{Mn}_2\text{O}_4$ particle. Cheng and Verbrugge studied the effect of surface tension and modulus on the diffusion induced stress within spherical nonparticles [6], and compared the stress evolution processes under galvanostatic and potentiostatic operating conditions [7]. Verbrugge and Cheng [8] also examined the stress in spherical particles under periodic potential excitations. Renganathan et al. [9] considered the stress arising due to phase transformation. Golmon et al. [10] presented a multi-scale finite element approach to study the electrochemical-mechanical interaction phenomena at macro-, meso-, and micro-scales. Generally, these studies were focused on one

single particle or a 1-D (pseudo 2-D) model. There is one 2-D model developed by Garcia et al. [11]. However, this model didn't consider the real contact between different battery components and the real shape of the battery. As to the thermal issues, although several studies considered heat generation inside Li-ion batteries [12, 14], no previous research studied thermally induced stress.

To investigate the stress in a separator in operation, Xiao et al. [15] developed a multi-physics, multi-scale model for a Li-ion battery. Built upon the rechargeable Li-ion battery model in COMSOL [16], the multi-scale model took into account the reaction kinetics, Li diffusion and stress. This model was extended to include heat generation, heat transfer, and thermal stress [17]. The model employed a continuous mesh. The stress calculated by this approach may represent the condition in the center of a cell but not at the electrode edges.

The focus of this work is the stress in a separator at the edge area of a pouch cell. A pouch cell is manufactured by stacking up layers of electrodes separated by separator films. Figure 1 presents the schematic of a pouch cell [18]. The actual stacking and folding configuration in batteries may vary. It is expected that the stress in a separator is higher near the edge than in the center. To reveal the stress in this edge area, the contact between the separator and the electrodes needs to be represented in a finite element (FE) model. This can be accomplished by employing an FE package developed for structural analysis.

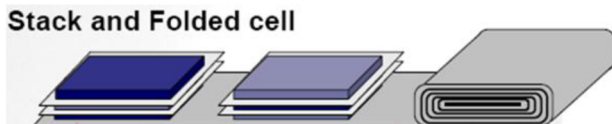


Figure 1. Schematic of a pouch cell [18].

This paper presents a macro-scale Li-ion battery model developed in ANSYS [19], and discusses the results of the parameter study carried out by using this model.

MODEL DEVELOPMENT

MODEL DESCRIPTION

As discussed above, the stress inside a separator is closely related to the actual stacking and folding configuration of the battery, materials properties, and the Li intercalation in the electrode materials. A representative macro-scale 1.5 cell model is shown in Figure 2. The components from the bottom to the top are anode current collector (Cu), anode, separator, cathode, cathode current collector (Al), and another cathode. The separator is wrapped around the anode and closely held by both the anode and the cathode. The shape of the separator in the transition corner is assumed to be a smooth circular arc.

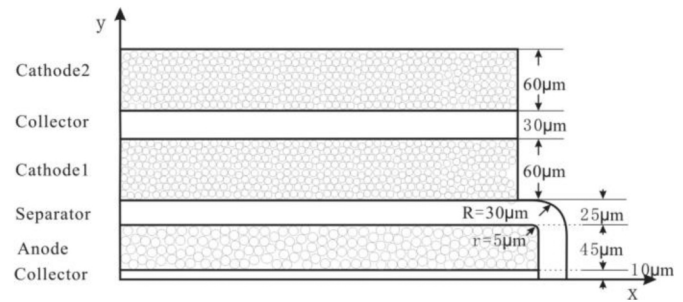


Figure 2. Schematic of the 1.5 cell model

EFFECTIVE PROPERTY

This study is focused on the stress in the separator. Since the influence due to the local differences is relatively small from the macroscopic point of view, the electrodes can be assumed to be homogeneous media with effective properties. This is a reasonable assumption due to the fact that as long as the same equivalent macroscopic strain and stress are generated, the final estimated stress in the separator would closely approximate the real conditions.

Limited by the availability of material properties, a Cu/Li_xC6/PP/Li_yMn₂O₄/Al cell has been selected in this investigation.

1. Diffusion induced expansion coefficient

Porous electrodes were modeled as homogeneous solids. The electrolyte was considered to be compressible, but its volume variation due to Li concentration change was assumed to be negligible. In the electrodes, we assume only the volume occupied by the electrode particles experiences volume changes due to intercalation and deintercalation of Li. To account for this effect, an effective diffusion expansion coefficient was estimated. Porous electrodes were considered as composites of active particles and pores. The diffusion induced expansion coefficient was estimated by the rule of mixtures similar to composite systems [20]:

$$\alpha_{eff} = \sum_i \alpha_i V_i \quad (1)$$

where α_{eff} is the effective diffusion expansion coefficient of the composite, α_i , and V_i are the diffusion induced expansion coefficient and the volume fraction of the i^{th} phase, respectively. Omitting the contribution of the electrolyte phase, the expression can be reduced to

$$\alpha_{eff} = \alpha_p V_p \quad (2)$$

where α_p and V_p are the diffusion induced expansion coefficient and the volume fraction of the active particles, respectively.

With an effective diffusion expansion coefficient, the macroscopic equivalent strain of an electrode due to Li insertion and extraction can be obtained. The effective thermal expansion coefficient of the electrode was estimated in the same way.

2. Young's modulus

Similarly, the Young's modulus of a porous electrode is different from that of an electrode particle. The effective modulus of a composite consisting of particles dispersed in a matrix is found to fall between an upper bound,

$$E_{eff} = E_m V_m + E_p V_p \quad (3)$$

and a lower bound,

$$E_{eff} = \frac{E_m E_p}{V_m E_p + V_p E_m} \quad (4)$$

where E_{eff} is the effective Young's modulus of the composite, V_m and V_p are the volume fractions, and E_m and E_p are the Young's modulus of the matrix and particles, respectively [20, 21].

The mass fraction of the active materials in electrodes was assumed to be 0.8 [22]. From the mass fraction and densities of battery components, the computed volume fractions of the active materials were 0.69 for the carbon anode and 0.53 for the LiMn₂O₄ cathode. At a high particle volume fraction, the upper bound estimation provides a closer approximation. Therefore, the prediction by Equation (3) was used in this work. The effective properties are listed in Table 1. With an effective Young's modulus, the macroscopic equivalent stress of an electrode can be computed.

COUPLING WITH BATTERY MODEL

1. Lithium concentration

The Li concentration distribution in the electrode was obtained using a pseudo 2-D battery model (available in COMSOL 3.5a [16]) based on a 1D model by Doyle et al. [23, 24]. The coupling between the macro-scale model and the pseudo 2-D model is illustrated in Figure 3. The pseudo 2-D model consists of a 1-D battery model and a 2-D spherical particle diffusion model. The details about this model can be found in reference 15 and 16.

In a previous study using a multi-scale model [15], it was observed that the stress inside the separator did not change

during the relaxation time in a charge-discharge cycle, when lithium ions inside the electrode were redistributed. In this work, to simplify the analysis, we assume that the lithium inside a particle is evenly distributed and the lithium concentration varies only in the thickness direction of the electrode.

The average Li concentration inside a particle is calculated by

$$c_{ave} = \frac{1}{\frac{4}{3}\pi r^3} \int_0^r 4\pi r^2 c_1 dr = \frac{3}{r^3} \int_0^r r^2 c_1 dr \quad (5)$$

2. Temperature rise

According to Wu et al. [17], the thermal stress imposed on the separator due to the self-heating of the battery is substantial. Therefore, to better understand the stress behavior of Li-ion battery, the self-heating of the battery must be considered. For just one Li-ion battery cell, the temperature over the whole field can be treated as the same, thus, a uniform temperature rise of 38.8°C was assumed in this work. All the material properties used in this work were considered to be independent of both the temperature and Li concentration.

SOLUTION PROCEDURE AND BOUNDARY CONDITIONS

The phenomena considered in the macro-scale model included the diffusion induced stress, thermal stress, and mechanical stress. The problem was solved by using ANSYS.

The boundary conditions for the macro-scale model are shown in Figure 4. There are two types of boundaries in this model: external and internal boundaries. For the external boundaries, a symmetric displacement boundary condition was prescribed at the left and bottom boundaries, a distributed normal pressure with a default value of 10 psi (unless specified otherwise) was prescribed at the top boundary, and the rest were defined as free boundaries. The boundaries between the components are internal boundaries. A contact relationship was prescribed at the boundaries between the separator and electrodes with an effective friction, the boundaries between the current collector and the electrode were modeled as to be continuous.

The Li concentration distribution is introduced by imposing a through-thickness profile in each electrode as shown in Figure 4. The Li profiles are obtained from the COMSOL battery models.

EFFECTIVE LENGTH

A pouch cell has a large length to thickness ratio. It is not feasible to build an FE model with the actual dimensions of