



# Modeling, validation and analysis of mechanical stress generation and dimension changes of a pouch type high power Li-ion battery

Rujian Fu\*, Meng Xiao, Song-Yul Choe

Mechanical Engineering, Auburn University, 1418 Wiggins Hall, Auburn, AL 36830, USA

## HIGHLIGHTS

- ▶ An electrochemical, thermal and mechanical model for Li ion battery is developed.
- ▶ The model is validated against experiment data.
- ▶ The battery thickness is a function of SOC.
- ▶ Stress in anode is higher than that in cathode particles.
- ▶ The highest stress is generated in the electrode particles near the separator.

## ARTICLE INFO

### Article history:

Received 26 June 2012  
 Received in revised form  
 21 September 2012  
 Accepted 23 September 2012  
 Available online 4 October 2012

### Keywords:

Li ion polymer battery  
 Electrochemical  
 Thermal and mechanical model  
 Stress modeling  
 Volume change

## ABSTRACT

Mechanical stress is generated in electrode particles of a Lithium ion Polymer Battery (LiPB) during charge and discharge. The stress can cause cracks and fractures in the solid particles over time when cells are cycled, which leads to a disorder and a fracture of the electrodes. In order to understand the mechanism, a stress model for a pouch type high power LiPB is developed based on electrochemical and thermal model, where the stress induced by the ion concentration in the electrode particles is considered. The stress in the particles causes changes in the electrode volumes and leads to changes in the thickness of a battery cell, which is measured using a device designed with two linear voltage displacement transducers (LVDT). This model is validated against experimental data obtained from a pouch cell. Analysis shows that the magnitude of stress depends upon locations and C rate, while the thickness of a single cell is mainly affected by the state of charge (SOC), but not C rate.

© 2012 Elsevier B.V. All rights reserved.

## 1. Introduction

LiPB is mostly preferred as an energy storage device in hybrid and electric vehicles because of its high power and energy density as well as its high coulombic efficiency. However, the behavior of internal physical variables of a cell is not well known. Thus, there have been attempts to describe the battery mathematically using principles of electrochemical kinetics, potential theory, mass transports, energy balance and elasticity.

The first electrochemical model proposed by Doyle et al. [1] assumed that a cell is made of several thin-film layers. The working mechanism is described with electrochemical principles. Fuller et al. [2] extended the model by considering other cathode materials like  $\text{LiCoO}_2$ ,  $\text{LiMn}_2\text{O}_4$  and used this model to investigate the effects of material property parameters on the performance of

a cell. After that, the model was included with transference number [3], activity coefficient in electrolyte [4], diffusion coefficient in  $\text{LiPF}_6$  electrolyte [5], and particle size distributions on the discharge capacity [6].

On the other hand, the material property, related to ion transport and intercalation/de-intercalation mechanism, is strongly affected by heat generation and mechanical stress that take place at charging and discharging. This relationship is depicted in Fig. 1, where the electrochemical kinetics and mass transport are coupling with thermal and mechanical behaviors. Song [7] and Smith [8] improved the electrochemical model by adding the energy equations considering various heat generation terms. Chen and Evans [9] then included the behavior of heat transfer to the electrochemical model. The typical heat generations considered are from different sources including the entropy heating, the Joule heating and the heat of mixing.

In addition, mechanical stress is generally generated by change of ion concentration in particles, so that electrodes expands or

\* Corresponding author. Tel.: +1 334 750 7274; fax: +1 334 844 3307.  
 E-mail address: [rzf0007@auburn.edu](mailto:rzf0007@auburn.edu) (R. Fu).

Nomenclature			
$A$	plate area of cell ( $\text{cm}^2$ )	$x_1$	coordinate along the width of single cell
$a_s$	specific surface area of electrode ( $\text{cm}^{-1}$ )	$x_2$	coordinate along the thickness of single cell
$c_s$	ion concentration in solid phase ( $\text{mol L}^{-1}$ )	$y$	stoichiometric number in cathode
$c_e$	ion concentration in electrolyte ( $\text{mol L}^{-1}$ )	$t_+^0$	initial transference number
$C_{\text{equi}}$	equivalent capacity of cell (A h)	<i>Greek symbols</i>	
$C_p$	heat capacity ( $\text{J kg}^{-1} \text{K}^{-1}$ )	$\alpha$	transfer coefficient for an electrode reaction
$D$	diffusion coefficient in electrode ( $\text{cm}^2 \text{s}^{-1}$ )	$\varepsilon$	strain or porosity of a porous medium
$E$	Young's modulus (MPa)	$\varepsilon_r$	radial strain in electrode particle
$E_{\text{chem}}$	electrochemical energy (J)	$\varepsilon_s$	volume fraction of solid phase in composite electrode
$F$	Faraday's constant ( $96,487 \text{ C mol}^{-1}$ ) or force (N)	$\varepsilon_t$	tangential strain in electrode particle
$g$	swelling coefficient	$\phi_e$	potential in electrolyte phase (V)
$h$	thickness of composite electrode mixed with electrolyte (cm)	$\phi_s$	potential in solid phase (V)
$h_{\text{cell}}$	thickness of the single cell (cm)	$\eta$	surface overpotential of electrode reaction (V)
$h_c$	convective heat transfer coefficient ( $\text{W K}^{-1}$ )	$\kappa$	ionic conductivity of electrolyte ( $\text{S cm}^{-1}$ )
$I$	current of the cell (A)	$\kappa_D$	concentration driven diffusion conductivity ( $\text{A cm}^{-1}$ )
$i_0$	reference exchange current density ( $\text{A cm}^{-2}$ )	$\nu$	Poisson's ratio
$J$	flux of ion diffusion ( $\text{mol cm}^{-2} \text{s}^{-1}$ )	$\rho$	density ( $\text{g cm}^{-3}$ )
$j$	transfer current density ( $\text{A cm}^{-3}$ )	$\sigma$	stress (MPa) or conductivity of solid active material ( $\text{S cm}^{-1}$ )
$L$	width of micro cell (cm)	$\sigma_r$	radial stress in electrode particle (MPa)
$l$	circumference of the packaging material (cm)	$\sigma_t$	tangential stress in electrode particle (MPa)
$N$	number of micro cells in the single cell	$\sigma_h$	hydrostatic stress in electrode particle (MPa)
$m$	mass of the single cell (kg)	$\Omega$	theoretical partial molar volume of Li-ion ( $\text{cm}^3 \text{mol}^{-1}$ )
$n$	amount of active electrode material (mol)	$\Omega_{\text{fitted}}$	fitted partial molar volume of Li-ion based on experimental data ( $\text{cm}^3 \text{mol}^{-1}$ )
OCV	open circuit voltage (V)	$\omega$	fractional expansivity of electrode material
$P_{\text{chem}}$	power contributing to the increase of chemical energy (W)	<i>Subscripts</i>	
$Q_{\text{rev}}$	reversible heat generation rate (W)	cell	the single cell
$Q_{\text{irr}}$	irreversible heat generation rate (W)	e	electrolyte phase
$Q_{\text{convect}}$	heat convection rate (W)	max	maximum
$R$	universal gas constant ( $8.3143 \text{ J mol}^{-1} \text{K}^{-1}$ )	pack	the packaging material
$R_s$	radius of spherical electrode particle (cm)	r	radial direction in electrode particle
$r$	radius (cm)	s	solid phase
SOC	state of charge	t	tangential direction in electrode particle
$T$	cell temperature (K)	0	without expansion caused by lithiation or initial state
$T_\infty$	ambient temperature (K)	0%	0% state of charge
$t$	time (s)	100%	100% state of charge
$U_{\text{equi}}$	equilibrium potential (V)	–	anode
$u$	radial displacement in electrode particle (cm)	+	cathode
$V$	volume of composite electrode mixed with electrolyte ( $\text{cm}^3$ )	<i>Superscripts</i>	
$V_T$	terminal voltage of cell (V)	eff	effective
$w$	width of the single cell (cm)	Li	Lithium ion
$x$	stoichiometric number in anode or coordinate along the width of micro cell		

contracts depending on charging and discharging. Fracture of the electrode materials is one of the durability issues, which is caused by ion-induced stress. During the diffusion process, inhomogeneous distribution of Li-ions in an electrode particle causes inhomogeneous localized volume expansions, which induces mechanical stress. When stress exceeds certain limits, the electrode would experience material failure, associated with cracking or fracture.

There have been several attempts to investigate the mechanism of stress generation and volume expansion using models. Christensen and Newman [10,11] first proposed a detailed model based on theories of transport and elasticity to predict stress in a single anode particle and a cathode particle. They found that high power application of Li-ion battery has an increased likelihood of particle

fracture, but reducing the size of particles can help to prevent such failure.

Another alternative method to describe the stress induced by the concentration gradient of solutes is proposed by Prussin [12], who first applied this method to describe stress generation during the inclusion of boron and phosphorus into silicon water. Yang [13] followed the same method and modeled chemical stress of solute in a thin plate. In 2007, Zhang [14] first applied this method to analyze the stress in a Li ion battery. Similar to thermal stress, a model for stress generation in a single cathode particle was proposed and the simulation result showed similar predictions as those in Christensen and Newman's work [11]. Zhang [15] then extended the model under a consideration of heat generation for ellipsoidal particles, and concluded that larger aspect ratios are

Download English Version:

<https://daneshyari.com/en/article/7741676>

Download Persian Version:

<https://daneshyari.com/article/7741676>

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