Electrochimica Acta 256 (2017) 172–184

Contents lists available at ScienceDirect

Electrochimica Acta

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

Research Paper

# Multiphysics computational framework for cylindrical lithium-ion batteries under mechanical abusive loading

Binghe Liu[a,b], Hui Zhao[c,d], Huili Yu[c,d], Jie Li[c,d], Jun Xu[a,b,e,*]

[a] Department of Automotive Engineering, School of Transportation Science and Engineering, Beihang University, Beijing, 100191, China
[b] Advanced Vehicle Research Center (AVRC), Beihang University, Beijing, 100191, China
[c] Chongqing Changan Automobile Co. Ltd., Chongqing, 400023, China
[d] State Key Laboratory of Vehicle NVH and Safety Technology, Chongqing, 401120, China
[e] State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing, 100081, China

ARTICLE INFO

*Article history:*
Received 7 August 2017
Received in revised form 29 September 2017
Accepted 6 October 2017
Available online 7 October 2017

ABSTRACT

Lithium-ion batteries (LIBs) are now widely applied to electric vehicles, such that the inevitable mechanical abuse safety problem during possible vehicle accidents has become a prominent barrier. This study initially proposes a multiphysics computational framework model that couples mechanical, thermal, and electrochemical models to describe the complete process for a single 18650 LIB cell subjected to abusive mechanical loading from initial deformation to the final thermal runaway. The designed experiments reveal the proposed model's suitable agreement with the established multiphysics model. Parametric studies in terms of governing factors, such as state of charge, loading speed, and deformation displacement, are conducted and discussed. These studies reveal the underlying mechanism for the mechanical abuse safety of LIBs. This model can lay a solid foundation to understand the electrochemical and mechanical integrity of LIBs, as well as provide critical guidance for battery safety designs.

© 2017 Elsevier Ltd. All rights reserved.

## 1. Introduction

Lithium-ion batteries (LIBs) have been regarded as one of the most promising alternative energy sources in the automotive industry [1–3]. Extreme conditions, such as mechanical abuse [4,5], thermal abuse [6,7], and charging/discharging abuse, [8–10] can lead to irreversible and catastrophic consequences (e.g., fires or explosions) [11]. Thus, LIB safety has received extensive attention, particularly in terms of hazardous consequences caused by mechanical abusive loading during inevitable vehicle accidents [12,13].

Given the complicated multiphysics nature of LIBs, modeling LIB behavior under mechanical abusive loading is considered difficult. Therefore, models for mechanical abuse conditions have been gradually developed in the past several years. From the mechanical aspect, macroscopically homogeneous and detailed models are both employed to describe the mechanical behavior of LIBs under mechanical loading. Greve and Fehrenbach [14] first utilized the isotropic model to predict the mechanical behavior of LIBs under compression. However, although these pioneering models can predict compressive response correctly, they exhibit a large discrepancy in bending and indentation conditions. Xu et al. [15] developed an anisotropic model coupled with state of charge (SOC) and dynamic effects to predict complex loading conditions and overcome the said problem effectively. Wang et al. [16] established a finite element model based on clay-like mechanical properties. Zhang et al. [17] and Mehdi and Avdeev [18] built a detailed model by modeling each component (e.g., cathode, anode, and separator) separately. Moreover, Liu et al. [4] combined the concept of homogeneous and detailed models to describe the penetration damage in LIBs; they utilized the detailed model within the vicinity of the penetrator and adopted the homogeneous model in other parts.

From the electrochemistry aspect, the 1D battery model was first proposed by Newman et al. [19]. This model has since been developed in recent years [20–22]. The electrochemical properties of the anode [23–25], cathode [25–27], electrolyte [28], and separator [24,25] have been comprehensively studied to improve this battery model in recent years. The Arrhenius-type equation was modeled to reflect the relationship between chemical reaction rate and temperature [10,29]. The solid electrolyte interphase (SEI) decomposition [6,30,31], anode–electrolyte reaction [6,30,31],

* Corresponding author at: Department of Automotive Engineering, School of Transportation Science and Engineering, Beihang University, Beijing, 100191, China.
*E-mail address:* junxu@buaa.edu.cn (J. Xu).

https://doi.org/10.1016/j.electacta.2017.10.045
0013-4686/© 2017 Elsevier Ltd. All rights reserved.

**Nomenclature**

| | |
|---|---|
| $A$ | Arrhenius constants (1) |
| $A_a$ | area ($mm^2$) |
| $b$ | weighing coefficient |
| $c$ | concentration ($mol/m^3$) |
| $c_{sei}$ | dimensionless amount of lithium-containing metastable species in the solid electrolyte interphase (SEI) (1) |
| $c_{sei\mathbf{O}}$ | initial value of the dimensionless amount of lithium-containing metastable species in the SEI (1) |
| $c_a$ | dimensionless amount of lithium intercalated within carbon (1) |
| $c_{a\mathbf{O}}$ | initial value of the dimensionless amount of lithium intercalated within carbon (1) |
| $c_e$ | dimensionless concentration of electrolytes (1) |
| $c_{e\mathbf{O}}$ | initial value of the dimensionless concentration of electrolytes (1) |
| $C_p$ | heat capacity (J/(kg·K)) |
| $d_z$ | thickness of 2D model/LIB length (mm) |
| $D$ | diffusion coefficient ($m^2/s$) |
| $D_{eff}$ | modified diffusion coefficient ($m^2/s$) |
| $E$ | Young's modulus (MPa) |
| $E_a$ | experimental activation energy (J/mol) |
| $F$ | Faraday's constant ($9.64853 \times 10^4$ C/mol) |
| $F_V$ | body force (N) |
| $F_L$ | deformation gradient |
| $H$ | volume-specific carbon content ($g/m^3$) |
| $h$ | heat transfer coefficient ($W/(m^2 \cdot K)$) |
| $I$ | current (A) |
| $i$ | current density ($A/m^2$) |
| $\vec{j}$ | current density ($A/m^2$) |
| $k$ | thermal conductivity (W/(m·K)) |
| $L$ | length (mm) |
| $S$ | Piola–Kirchhoff stress tensor |
| $S_{st}$ | short-circuit area ($mm^2$) |
| $S^*_{st}$ | normalized short-circuit area ($mm^2$) |
| $SOC$ | state of charge value |
| $t$ | time (s) |
| $t_+$ | transfer data |
| $\boldsymbol{u}$ | displacement field |
| $v$ | velocity field |
| $W_c$ | volume-specific carbon content ($g/m^3$) |
| $W_p$ | volume-specific positive active content ($g/m^3$) |
| $W_e$ | volume-specific electrolyte content in the jellyroll ($g/m^3$) |
| $\boldsymbol{X}$ | material coordinate |
| $\boldsymbol{x}$ | spatial coordinate |
| $z$ | dimensionless measure of the SEI layer thickness (1) |
| $z_0$ | reference dimensionless measure of the SEI layer thickness (1) |
| $Q$ | heat sources ($W/m^3$) |
| $Q_s$ | additional heat sources ($W/m^3$) |
| $Q_a$ | reaction heat ($W/m^3$) |
| $Q_j$ | joule heat ($W/m^3$) |
| $Q_r$ | resistance heat from current collectors ($W/m^3$) |
| $Q_i$ | irreversible heat ($W/m^3$) |
| $Q_{1D}$ | heat for 1D battery model ($W/m^3$) |
| $Q_{st}$ | heat from the short-circuit model ($W/m^3$) |
| $Q_{tr}$ | heat from the thermal runaway model ($W/m^3$) |
| $QTOT$ | total heat rate (W) |
| $\boldsymbol{q}$ | heat flux ($W/m^2$) |
| $\boldsymbol{q}_{fl}$ | heat flux by conduction ($W/m^2$) |
| $\boldsymbol{q}_{df}$ | heat flux by radiation ($W/m^2$) |
| $R$ | radius (mm) |
| $R_g$ | gas constant |
| $R_r$ | resistance ($\Omega$) |
| $t_+$ | transfer data |
| $T$ | temperature (K) |
| $\boldsymbol{T}$ | temperature field |
| $T_{amb}$ | external temperature (K) |
| $\alpha$ | conversion degree (1) |
| $\alpha_0$ | initial value of the conversion degree (1) |
| $\alpha_m$ | ratio of tension and compression (1) |
| $\rho_0$ | initial density ($kg/m^3$) |
| $\rho$ | density ($kg/m^3$) |
| $\sigma_{B-D}$ | Stefan–Boltzmann constant ($5.67 \times 10^{-8}$ $W/(m^2 \times K^4)$) |
| $\sigma_0$ | yield stress (MPa) |
| $\sigma_p$ | flow stress (MPa) |
| $\sigma_1$ | maximum principal stress (MPa) |
| $\sigma_2$ | middle principal stress (MPa) |
| $\sigma_3$ | minimum principal stress (MPa) |
| $\sigma^{eq}_{Unified}$ | equivalent stress of unified strength theory (MPa) |
| $\varepsilon_p$ | plastic strain (1) |
| $\delta$ | thickness (mm) |
| $\varepsilon$ | volume fraction |
| $\varepsilon$ | strain (1) |
| $\varepsilon_{Df}$ | surface emissivity (1) |
| $\kappa$ | electrical conductivity (S/m) |
| $\kappa_{eff}$ | modified electrical conductivity (S/m) |
| $\nu$ | Poisson's ratio |
| $\phi$ | potential (V) |
| $1 + \frac{d\ln f}{d\ln c^l}$ | molar activity coefficient |
| $\Omega(t)$ | area of the 2D model (LIB's section) with time ($mm^2$) |

Subscripts

| | |
|---|---|
| *eff* | modified |
| *eq* | equilibrium |

Superscripts

| | |
|---|---|
| *a* | anode |
| *a–e* | anode–electrolyte reaction |
| *c–e* | cathode–electrolyte reaction |
| *c* | cathode |
| *Cc* | Current collector |
| *e* | electrolyte decomposition |
| *D* | diffusion |
| *LB* | lithium-ion battery |
| *l* | electrolyte |
| *Me* | mechanical model |
| *nc* | negative collector |
| *ng* | negative electrode |
| *nl* | penetration nail |
| *pc* | positive collector |
| *ps* | positive electrode |
| *sei* | SEI decomposition reaction |
| *s* | electrode |
| *se* | separator |
| *St* | short-circuit model |
| *Tm* | thermal model |
| *1D* | 1D battery model |

cathode–electrolyte reaction [6,30,31], electrolyte decomposition reaction [6,30,31], and electrochemistry reaction [30] have been discussed extensively and concluded in the thermal runaway model. Ohm's law is generally employed in the short-circuit model

Download English Version:

https://daneshyari.com/en/article/4766623

Download Persian Version:

https://daneshyari.com/article/4766623

Daneshyari.com