Journal of Energy Storage 11 (2017) 249–257

Contents lists available at ScienceDirect

Journal of Energy Storage

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

Electrochemical-electrical-thermal modeling of a pouch-type lithium ion battery: An application to optimize temperature distribution

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ARTICLE INFO

Article history:
Received 12 October 2016
Received in revised form 15 March 2017
Accepted 17 March 2017
Available online 6 April 2017

Keywords:
Lithium-ion battery
Thermal design
Coupled modeling
Temperature distributions
Tab arrangements

ABSTRACT

This paper presents an electrochemical-electrical-thermal coupled modeling approach for pouch-type lithium ion batteries. In the presented approach, simple and efficient analytical methods are applied to calculate the current density over the current collector and the localized heat generation rate of current collectors. The feasibility of this approach is validated with experimentation. A comprehensive simulation study on the impact of tab arrangements on the temperature distribution of pouch-type lithium ion batteries is conducted. The results demonstrate that symmetrical tab arrangements improve the uniformity of temperature distribution significantly, although they will lead to a very slight increment of the maximum temperature on the surface of pouch cell. Besides, placing the collecting tabs on the opposite sides or long side(s) of battery cell is helpful in lowering its maximum temperature and improving the uniformity of temperature distribution.

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1. Introduction

Lithium-ion batteries (LIB) have been the dominant energy storage technology for portable electronics, and also are the most promising energy storage means for electric vehicles, thanks to their high energy and power densities, low self-discharge rates, and long cycle life [1,2]. However, the excessive temperature rise and non-uniform temperature distribution during charge/discharge still are challenges to LIBs technology, which may reduce battery reliability [3] and even resulted in thermal runaway and safety disasters [4–6]. A plenty of thermal management strategies are proposed to address the thermal issues of LIB [1,7]. For example, cooling systems based on forced air cooling [8,9], liquid cooling [10], or phase change materials (PCM) cooling [11], are attached to LIB packages for avoiding extreme heat accumulation. Furthermore, thermal design of LIB is optimized in order to lower their maximum temperature (T_{Max}) and improve the uniformity of temperature distribution, such as changing the tab configuration [3,12,13].

Modeling and simulation plays an important role in the optimization of LIB thermal design [14,15]. Extensive efforts have been devoted to improve the accuracy and time-efficiency of LIB modeling in the past two decades. The assumption of one dimensional model, which ignores the gradients of the variables in the current collector plane, lowers its accuracy and feasibility [16]. Kim et al. developed a reliable 2D electrical-thermal model [13,14,16,17]. But the accuracy of their model strongly depends on precise measuring and fitting of the relationship between the electrode potential and depth of discharge. Although Multi-scale and Multi dimensional (MSMD) modeling approaches can accurately predict electrochemical, electrical, and thermal characteristics in LIB, the demand on enormous computing resource and time limits its application [18,19]. Recently, Zhao et al. developed a computationally efficient LIB model consisting of 1D electrochemical part and a 3D thermal part [20]. However, Zhao's model doesn't describe the temperature gradient in the two directions parallel to the current collectors. In this context, we report herein an improved electrochemical-electrical-thermal model whereby the temperature distribution across the current collectors are involved using a simple analytical method.

For this study, a pouch-type LIB was modeled. In a pouch-type LIB, which can provide a higher energy density at package level than cylindrical cells, the arrangement of collecting tabs directly affect the current distribution across the current collectors, which in turn affects the heat generation rate (HGR) and temperature gradient [14,16]. There are a total of 6 possible tab arrangements for a pouch-type LIB, which are depicted in Fig. 1 and denoted with Type A1-A3 and B1-B3. Kim et al. studied the case of A1, A3, and B1, and showed that A3 resulted in the lowest T_{Max} [13]. Du et al.

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http://dx.doi.org/10.1016/j.est.2017.03.008
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Nomenclature

$C_{s,0}$	Initial concentration of lithium in solid phase, mol cm^3
$C_{e,0}$	Initial electrolyte salt concentration, mol cm^3
$C_{s,max}$	Maximum concentration of lithium in solid phase, mol cm^3
D_s	Diffusion coefficient of lithium in the electrode particles, cm^2 s^1
D_e	Salt diffusivity in electrolyte, cm^2 s^1
K_i	Heat conductivity of components inside cell
j^{Li}	Reaction current density, A cm^{-3}
L_i	Thickness of components in experimental cell
R_s	Particle radius, μm
r	Radial coordinate along active material particle, cm
ε_s	Solid phase volume fraction
ε_e	Electrolyte phase volume fraction
t_+	Cationic transport number
ρ_i	Density of different components inside cell
σ	Electric conductivity

reported widening the tabs in A3 would lead to a more even temperature gradient, especially at high discharge rate [12]. Samba et al. deem that a symmetrical tab-arrangement trends to improve the uniformity of temperature distribution through comparing the case of A1, A3, B1, and B3 [3]. To our best knowledge, there is still lack of a systematically comparative study of all the 6 possible tab-arrangements.

In this article, we present our newly developed electrochemical-electrical-thermal coupled modeling approach for LIB. A 1D electrochemical sub-model is used to calculate HGR of the cell unit. The position-varying HGR of the current collectors, which are derived from current density difference, are calculated by an analytical method. HGR of collecting tab is also calculated by analytical method. The temperature distribution is obtained by importing the calculated HGRs into a 2D thermal sub-model. The presented modeling approach is first validated with experimental data. Afterwards, a comprehensive study on the influence of tab locations on the thermal behaviors of pouch-type LIB is conducted, with the hope to help the optimization of battery thermal design.

2. Modeling

2.1. Model description

Fig. 2a displays the 700 mAh pouch-type LIB manufactured by Chengdu Interstellar Li-ion Battery Tech Co. Ltd, that is modeled in this study. The parameters of this battery are listed in Table 1. In the modeling, a single electrode plate pairs, as shown in Fig. 2b, are used as an equivalent substitute for the repeating units of positive and negative electrode plates in the molded LIB. The feasibility of this simplification had been validated by comparing simulation to the experimentation [3,19,21–23].

The presented model consists of a 1D electrochemical sub-model, a 2D electrical sub-model, and a 2D thermal sub-model. The modeling and simulation are conducted using COMSOL4.3b software and the modeling process is depicted in Fig. 3. The HGR of the cell unit consisting of cathode, anode, and electrolyte are calculated by the 1D electrochemical sub-model reported elsewhere (see details in SI) [20]. The Joule heat at different

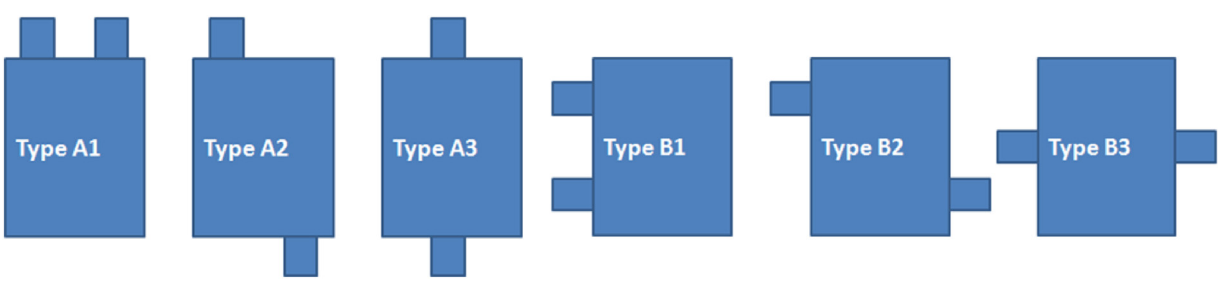

Fig. 1. Schematic illustration of 6 possible collecting tab arrangements.

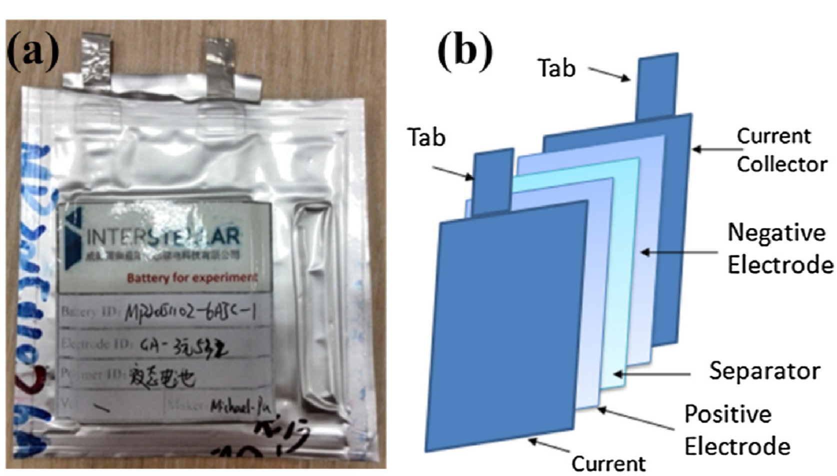

Fig. 2. (a) Photograph of the modeled LIB; (b) Single electrode plate pair configuration.

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