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Modeling analysis of the effect of battery design on internal short circuit hazard in $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2/SiO_x$ -graphite lithium ion batteries



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ABSTRACT

The internal short circuit is one of the most severe safety hazards to large format lithium ion batteries. This study aims to reproduce the internal short circuit hazard through experimental and numerical methods to give a better understanding of the effect of laminated battery design on thermal abuse tolerance. A thermal abuse reaction model based on $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2/\text{SiO}_x$ -graphite system is constructed with the assist of differential scanning calorimetry, and accelerating rate calorimetry experiments. The thermal runaway of the sample battery shows a five-stage process, and 11 chemical reactions and other heat sources are sorted out through modeling. Then the model is further simplified and coupled with the electrochemical-thermal model. The whole process of initiation of thermal runaway and heat progression afterward are reproduced. The model is extended to compare batteries with different laminated numbers and electrode sizes on the internal short circuit issue. Results show that different laminate design schemes will result in different hazard patterns. Larger layer number will delay the thermal runaway of the battery, but increase the seriousness of thermal hazard. Thermal tolerance ability can be adjusted without changing battery capacity. This work provides an applicable methodology for tuning layer number and electrode size for battery manufacture for safety concerns.

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1. Introduction

In order to meet the ascending power demand of electric vehicles (EVs), the energy density of next-generation lithium ion battery (LIB) should reach 300-350 Wh kg⁻¹ in the next five years. On the other hand, the continuous growth of cobalt price since 2017 also gives a persistent cost pressure on LIB manufacturers [1]. To cope with the situation, developing nickel-rich cathode material is becoming a trend, which can not only provide high energy density, but also lower the cobalt content in materials effectively. To match with the high capacity cathode, the anode material is also undergoing an evolution. Silicon-based material is considered to be a promising candidate [2,3]. Despite the extraordinary theoretical specific capacity (4200 mAh g^{-1}) of silicon, the considerable volume expansion during cycling severely restrains its practical application [4,5]. To date, to compromise with the technology restriction, the Si and SiO_x doped graphite anodes are the primary choices for high energy density LIBs [6-8]. Therefore, assembling the nickel-rich cathode material and SiO_x doped graphite anode

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https://doi.org/10.1016/j.ijheatmasstransfer.2020.119590 0017-9310/© 2020 Elsevier Ltd. All rights reserved. together to fabricate full cells is a practical approach to enhance the energy density of LIBs.

However, with the increase in energy density, the safety concerns of LIBs should also be considered. It is well known that thermal runaway (TR) of a LIB is directly initiated by high temperature, corresponding to a drastic heat generation process, which can happen under several abuse circumstances like nail penetration, crash, overheat, external/internal short circuit, etc. [9]. As for the application in EVs, the safety of batteries will be challenged under all kinds of situations. In that case, the TR of LIBs should be thoroughly studied.

Among all the abuse circumstances mentioned above, the internal short circuit (ISC) is one of the most unnoticeable and unpredictable. When it comes to application in EVs, the potential danger of ISC should not be underestimated. However, it is challenging to introduce controllable ISC to a battery manually, and the poor reproducibility may be intractable, especially for large-scale power batteries. Hence, numerical simulation has become a powerful tool to reproduce the process and analyze the target system under standard conditions. A lot of simulation works have been carried out on the ISC issue. Zavalis et al. built a 2D single-layered model to simulate current distribution under different types of ISC [10]. Santhanagopalan et al. investigated the ISC induced heat gen-



Fig. 1. Thermal experiments results. (a)-(d) are the DSC tests results of cathode+electrolyte, anode+electrolyte, separator and electrolyte. (e) and (f) are the ARC test results of the sample pouch battery.

eration with a 2D model of a winding-type battery [11]. Chen et al. constructed a 3D multilayer ISC model based on 2D equivalent circuit, and the model is extended to study the ISC location's influence [12]. Spotnitz et al. investigated the thermal abuse reaction progression pattern inside a cylindrical cell initiated by a localized heat spot, which represents ISC in the center [13]. Although ISC and TR have been reproduced in these modeling works, the determining factors on the issue of improving abuse tolerance still need further discussion. The feedback from the model results in battery manufacture is still limited. In order to improve the guidance function of battery modeling on ISC and TR issues, different battery designs should be compared in the abuse tolerance aspect.

The influence factors of battery thermal endurance can involve many aspects, such as material stability, operating condition, battery management system, etc. in addition to that, battery design is also a vital factor to be concerned. Because the ISC induced TR is started with a localized heat spot, the heat transfer process in the battery plays an essential role in the TR initiation stage. During TR afterward, the abuse reactions progression pattern is also dependent on heat transfer and accumulation. Because the heat transfer and accumulation are highly relative to the battery's geometry, thus design optimization is one effective way to adjust battery ISC abuse tolerance.



Fig. 2. (a)–(d) are the Arrhenius kinetic model simulation results. (e)–(f) are the fitting results of ARC experiment. (g) shows the primary heat sources contribution to the temperature rise. Negative values including separator endothermic power and Q_{expl} are multiplied by -1 to be able to show in the plot.



Fig. 3. Interpolation function profile of *Q*_{expl}.

As we have discussed, TR reactions model will play an essential role in the modeling work. Many studies have reported on LIBs thermal runaway processes through experiments and modeling methods. Richard and Dahn combined accelerating rate calorimetry (ARC) and differential scanning calorimetry (DSC) to explore the heat generation reactions of graphite anode, and developed reaction model to reproduce the combustion process [14,15]. Huang et al. acquired the thermal analysis kinetics of oxygen release process of NCM111 through fitting DSC results [16]. Feng et al. constructed a thermal runaway model of NCM/Graphite model by fitting ARC experimental data [17]. The model is further applied in a large battery module to analyze the TR propagation. Spotnitz et al. developed a three-dimensional model combined with the one-dimensional model, and predicted the thermal reaction progress during thermal abuse of cylindrical LIBs [13]. However, the kinetics expressions and parameters of these battery TR models are acquired from previous works directly or fitted to experimental data, which ignored the differences in batteries, such as electrolyte composition, electrode composition, manufacturing technique, etc. Thus, acquiring the thermal reaction kinetics from the target battery is essential to improving the reliability of the simulation.

Therefore, in this work, we devoted to analyzing the relation between ISC abuse tolerance and the design of laminated batteries by modeling methods. The thermal abuse reactions model is established based on experimental data and coupled to the electrochemical model to reproduce the process. NCM811/SiO_x-Graphite LIB is selected as the simulation target because its high energy density character not only makes it a promising battery composition system, but also implies serious repercussions when undergoes TR. To the knowledge of the authors, no literature has been found which has established the thermal kinetic model of SiO_x, or NCM811/SiO_x-Graphite system. This work has developed a reliable and applicable methodology to build a 3D finite element method (FEM) model for ISC-TR. The model can provide beneficial insights into laminated battery designing and assessment to assist battery manufacture.

2. Model development

In order to describe the whole process of ISC hazard, a multidimensional multi-physics model has to be built. The model construction process includes two major parts: thermal abuse model derivation and coupling with an electrochemical-thermal model. The thermal abuse model accounts for the TR of battery, which consists of expressions of thermal abuse reactions and other heat sources. Afterward, by coupling with the electrochemical-thermal model, the initiation of ISC and TR and heat propagation can be interpreted.

To ensure the kinetics model can reflect the battery chemistry correctly, we present an approach to acquire theoretical expressions base on experimental analysis of DSC and ARC tests. DSC can reveal the reaction composition, onset temperature, enthalpy change and etc., while the ARC test, can reflect the combustion characteristics of the overall battery system. Although the real abuse situation may differ from DSC and ARC tests in temperature rising rate, the reactions and other heat sources are the same. Thus the kinetics acquired can be applied in ISC abuse situation.

The electrochemical-thermal model is built based on our previous work [18], and extended in this work to analyze ISC circumstance with incorporated thermal abuse model. Several laminate designs are cross-compared to extract feature information about ISC hazard.

The commercial laminated pouch battery is provided by Tianjin JEVE Power Industry Co., Ltd. The battery capacity is 12 Ah, with NCM811 as the cathode (mass ratio of NCM811: 97.75%) and SiO_x/graphite composite as the anode (mass ratio of SiO_x: 10.5% and graphite: 84.92%). All thermal tests were conducted after the battery was charged to 4.2 V.

2.1. Thermal abuse model

2.1.1. DSC experiments and data analysis

DSC experiments were conducted on the main battery materials to acquire thermal parameters for the kinetics expressions. The samples were obtained by dissembling the battery. Four kinds of samples were prepared, including cathode+electrolyte, anode+electrolyte, separator, and electrolyte. The four tests basically covered all thermal generation reactions in the battery [13,19,20]. Before analyses, both cathode and anode materials were rinsed and soaked in dimethyl carbonate (DMC) for 1 h, and then dried under vacuum condition. Then, 4 mg of cathode material, 2 mg of anode material and 1.8 μ L electrolyte (based on the battery composition) were sealed in a steel crucible. The DSC measurements were conducted from 35 °C to 400 °C under Ar atmosphere with the heating rate of 5 °C min⁻¹.

DSC data are shown in Fig. 1(a)–(d). The reaction between cathode and electrolyte exhibits two peaks. Within the temperature region of 100–300 °C, NCM811 undergoes a series of phase transitions from layered structure to M_3O_4 -type spinel, then to rock salt [16,21–23]. Both processes involve intensive release of oxygen, which reacts with electrolyte and cause heat dissipation. Therefore the first peak located around 200 °C is designated as a superposition of the reactions between two-stage-release oxygen and electrolyte [24]. The peak located at 380 °C is considered to be the reaction of binder [25].

The reaction between anode and electrolyte shows three exothermic peaks. The anode is composed of graphite, SiOx, and binders. In addition, an extra solid electrolyte interface (SEI) layer will be formed after lithiation. It can be deduced that these four peaks may be originated from reactions related to these four species. The first broad peak starts at about 90 °C is assigned to SEI decomposition [14,15]. The second peak within the region from 225 °C to 275 °C is a superposition of two peaks, implied by the abrupt change of slope at 265 °C. The first one is located around 245 °C, attributed to the reaction of LiC₆ and electrolyte [25–29]. The second sharp peak located at 270 °C is designated as the Li_xSi reaction with electrolyte [30,31]. And the last small peak at 300 °C is corresponding to the reaction of binders [25].

The decomposition of the electrolyte itself is located above 210 °C. Firstly started with the decomposition of LiPF_6 shown as a small endothermic peak. The subsequent two distinguishing

Table 1

Thermal dynamic parameters of exo/endothermic reactions. Part of parameters' fitting is referred to Ref. [13,17].

sample	х	$H_{x}/J\ g^{-1}$	$m_{\rm x}/g$	c _x	$A_{\rm x}/s^{-1}$	$E_{\rm x}/J mol^{-1}$	$n1_x$	$n2_{x}$
cathode+	cat1	25.08209	73.76	0.999	6.22e8	9.50e4	2	1
electrolyte	cat2	34.39599	73.76	0.999	1.442e9	1.07e5	2	0
	binder	16.38511	73.76	0.999	1.077e19	2.688e5	1	0
anode+	SEI	200.00	39.375	0.15	1.667e15	1.145e5	5.5	0
electrolyte	graphite	30.08209	39.375	0.999	3.151e15	1.80e5	2	0
	silicon	11.39599	39.375	0.999	6.151e16	1.82e5	1	1
	binder	10.38511	39.375	0.999	4.9679e15	1.99e5	1	0
separator	sep	-6.2928	7.90	0.999	3.40e37	3.11e5	2	0
electrolyte	LiPF ₆	-1.57440	12.5	0.999	1.50e10	1.14e5	1	1
	ele1	16.70	12.5	0.999	2.95e7	9.20e4	2	1
	ele2	2.26	12.5	0.999	3.10e7	1.02e5	1	1

Table 2

Parameters of the lumped model.

A_{lump}/s^{-1}	$E_{lump}/J \text{ mol}^{-1}$	n _{lump}	C _{lump}	H _{chem} /J
2.011e11	1.108e5	2	1	7.320e3
1.013e10	1.172e5	2.7	1	1.006e5

exothermic peaks represent the reactions between PF_5 and solvent or additive [32–34]. The separator melts from 125 °C to 150 °C, and shows an endothermic peak. It can be seen that the exothermic power of cathode and anode are much higher than that of electrolyte and separator. Therefore, the dominant heat contribution during TR should be related to the former two reactions.

2.1.2. ARC tests and TR data analysis

ARC test was operated under heat-wait-seek mode. The temperature step of the initial external heating program was 5 °C. Once the sample battery's self-heating rate exceeds the detection limit of 0.03 °C min⁻¹, ARC will maintain an adiabatic environment. Then the battery was self-heated by its exothermic reactions under adiabatic condition until thermal runaway. The temperature of battery was determined by the average value of two thermal couples on the opposite sides of the battery. The heat capacity of battery was also calculated by a constant power heating program.

Fig. 1(e) shows the evolution of sample temperature in ARC tests. Before 660 min, the battery is heated by the instrument in a stair-like mode with a 5 °C step. When the sample temperature reaches 91 °C, the temperature rise rate reaches 0.03 °C min⁻¹, and the test program enters into track mode (i.e. it maintains adiabatic condition and stops the external heater, as well as starts the self-heating of battery) until thermal runaway.

In order to get a better understanding of the TR process in the aim of guiding model construction, we can divide the curve into five regions (Fig. 1(f)):

- I The self-heating rate is lower than the detection limit, and the sample is heated by external heater.
- II The track mode starts, and the self-heating rate is relatively low, corresponding to the long flat plateau in Fig. 1(e).
- III The heating rate starts to increase until the TR critical temperature.
- IV Sever heat release causing a sample temperature burst. Because the temperature rises too fast, the sampling points are very sparse.
- V The battery undergoes a massive explosion at about 500 °C, and the explosion causes an intensive heat release and mass eruption, leading to a much lower heating rate until it reaches the highest temperature.

Accordingly, the heat sources during the TR process can be classified into five categories: (1) external heater, (2) self-heating be-

cause of exothermic reactions. (3) the heat transfer between battery and environment after the cooling program starts to function, (4) heat release and mass eruption during explosion, and (5) massive ISC. The former four sources have been noted earlier in the article, and the fifth needs a further explanation. During TR, direct contact between cathode and anode may happen due to separator collapse [35], which may be the fuse detonating the TR of batteries. According to Feng's work, the existence of extra heat dissipation can be verified by the comparison of total heat generation [17]. In this work, the heat capacity C_p is measured to be 1.280 J g⁻¹ K⁻¹. By multiplying the battery mass (M = 194.56 g) and total temperature change during track procedure (91.00 °C to 587.83 °C), we can get the theoretical total heat dissipation of 1.2341×10^5 J. According to the DSC results, the total chemical reaction heat dissipation $(1.0732 \times 10^5 \text{ J})$ lower than the theoretical total heat dissipation $(1.2341 \times 10^5 \text{ J})$ as expected. Considering the explosion, the actual total heat generated during TR should be even larger. Thus, extra heat dissipation due to the contact between cathode and anode is confirmed to be existing.

2.1.3. Thermal reactions kinetics and battery TR model

This part of modeling work is done in MATLAB. The exo/endothermic reactions can be expressed in the Arrhenius relationship as follows [17]:

$$\frac{dc}{dt} = A \exp\left(-\frac{E}{RT}\right) f(c) \tag{1}$$

$$f(c) = c^{n1} (1 - c)^{n2}$$
⁽²⁾

where A is the pre-exponential factor, E is activation energy, f(c) is mechanism function, c is normalized concentration describing the degree of reaction.

For DSC simulation, the heat flow is calculated as follow:

$$P = \sum_{x} \left(H_x \frac{dc_x}{dt} \right) \tag{3}$$

where *H* is the enthalpy of reaction.

The fitting results are shown in Fig. 2(a)-(d), and the parameters are listed in Table 1.

The TR model is a zero dimension model. The temperature of the battery, T, is calculated by:

$$\frac{dT}{dt} = \frac{Q_{total}}{C_0 M} \tag{4}$$

We constructed the TR model base on the five heat sources described in Section 2.1.3. The total heat generation power is calculated as:

$$Q_{total} = Q_{heat} + Q_{chem} + Q_{conv} + Q_{expl} + Q_{ISC}$$
(5)

The external heat power Q_{heat} is set as a constant of 0.7 W for simplification. All the reactions involved in the DSC fitting are



Fig. 4. Fitting result of the lumped model. (a) Heat generation fitting of thermal reactions. (b) (c) Comparison of the original model and lumped model fitting results of ARC experiment data.

Table 5				
Summary of governing	equations in the	electrochemical-therma	1 model	[40 - 43]

Conservation of charge	$ \nabla \cdot (-\sigma_{s} \nabla \phi_{s}) = -A_{\nu} i_{loc} \nabla \cdot (-\sigma_{leff} \nabla \phi_{l} + (\frac{2\sigma_{leff}RT}{F})(1 + \frac{\partial lnf}{\partial lnc})(1 - t_{+}^{0}) \nabla lnc_{l}) = A_{\nu} i_{loc} $
Effective liquid phase conductivity	$\sigma_{l,eff} = \sigma_l \varepsilon_l^{1.5}$
Specific surface area	$A_{\nu} = \frac{3\varepsilon_l}{r_p}$
Local current density	$i_{loc} = i_0 \left(\exp\left(\frac{\alpha F \eta}{RT}\right) - \exp\left(\frac{-(1-\alpha)F \eta}{RT}\right) \right)$
Exchange current density	$i_0 = Fk_x c_{s,max}^{0.5} (c_{s,max} - c_s)^{0.5} c_l^{0.5}$
Overpotential	$\eta = \phi_s - \phi_l - E_{eq}$
Heat source	$Q_{h} = -(i_{s}\nabla\phi_{s} + \sigma_{l,eff}\nabla\phi_{l}) + (\eta + T\frac{\partial E_{eq}}{\partial T})A_{\nu}i_{loc}$
Heat conservation	$\rho_{eff}C_p \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + Q_h$

included, and the same kinetic parameters are used to calculate Q_{chem} :

$$Q_{chem} = \sum_{x} \left(H_x m_x \frac{dc_x}{dt} \right) \tag{6}$$

The power of convective heat transfer, *Q_{conv}*, between battery and environment during cooling procedure is calculated by:

$$Q_{conv} = hS(T_{amb} - T) \tag{7}$$

The convective heat transfer coefficient, *h*, is set to 10 W m⁻² K⁻¹ [17]. The surface area of the battery, *S*, is 0.05 m². Ambient temperature, T_{amb} , is 250 °C as the cooling program starts.

 Q_{expl} is heat-releasing power of the explosion. The critical temperature is 490.7 °C. Due to the unpredictable chaotic process, Q_{expl} is fitted to experiment data, and illustrated in Fig. 3. t = 0 s represents the instant that the battery exploded. Aside from the heat release, by weighing the mass of battery before and after TR test, the mass loss is also considered in the model. After the test, the mass of the whole battery drops from 194.56 g to 88.52 g. By taking the weight of packaging materials into account, the active material loss is 61.1%. Considering the model simplicity, the mass loss is treated as an instant event at the moment of the explosion.

Massive ISC has been simulated in several research articles. The equation we chose to model Q_{ISC} , shown in Eq. (8), follows the works of previous researchers [17]. ΔH_{ISC} is total electric energy the battery contains, calculated by integrating the charging profile

as 1.5625×10^5 J. Δt is the equivalent ISC duration set as 10 s. Due to material combustion, the electric energy that can be released will reduce. We use a lumped reaction ratio factor ξ to describe the electric energy loss. Since the separator has no contribution to electric energy release, it is excluded in the calculation of ξ . In addition, because of the active material loss at explosion, Q_{ISC} instantly drops 61.1%.

$$Q_{ISC} = \frac{1}{\Delta t} (\Delta H_{ISC} \xi - \int Q_{ISC} dt)$$
(8)

$$\xi = \frac{\sum_{x} \int H_{x} m_{x} c_{x} dt - \int H_{sep} m_{sep} c_{sep} dt}{\sum_{x} (H_{xi} m_{xi} c_{xi}) - H_{sepi} m_{sepi} c_{sepi}}$$
(9)

2.1.4. Kinetic modeling results and model reduction

Thermal behavior of battery during TR has been reproduced successfully, which further verifies the kinetic parameters in Table 1. Through numerical simulation, the internal processes can be separated and classified. Fig. 2(g) shows the heat contribution of anode, cathode, separator, electrolyte reactions, and other primary heat sources. Because separator melting is endothermic, the heat power shown in the plot is actually opposite to the real data. In the beginning, the self-heating power of the battery is quite low. As entering temperature tracking mode, the reactions of anode (mainly the decomposition of SEI) are the primary heat sources at the beginning, which corresponds to stage II in Fig. 1(f). After that, the reactions on cathode become dominant, which is stage III. Then the sample temperature reaches the critical point, TR is

Table 4

Summary of parameters used in the electrochemical-thermal model. The parameters are measured or provided by manufacturer if not explicitly indicated otherwise.

Geometric parameters					
L _{length}	Length of battery	197 mm			
Lwidth	Width of battery	104.5 mm			
L _{CC, pos}	Thickness of positive current collector	13 µm			
L _{CC, neg}	Thickness of negative current collector	6 µm			
Lpos	Thickness of positive electrode	68 µm			
Lneg	Thickness of negative electrode	88 μ m			
Lsep	Thickness of separator	16 µm			
r _{p, pos}	Particle radius of positive active material	4.82 μ m			
r _{p, neg}	Particle radius of negative active material	6.33 μm			
ε _{l, pos}	Porosity of positive electrode	0.249			
€ _{l, neg}	Porosity of negative electrode	0.261			
ε _{l, sep}	Porosity of separator	0.450			
Electrochemical	l				
parameters					
Cmax, pos	Maximum lithium ion concentration of	46,123 mol m ⁻³			
	positive active material				
Cmax, neg	Maximum lithium ion concentration of	$52,225 \text{ mol } \text{m}^{-3}$			
	negative active material				
soc _{pos} e	State of charge of positive electrode	0.335			
soc _{neg} e	State of charge of negative electrode	0.675			
k _{pos} [39]	Reaction rate coefficient of cathode	1e-11 m s ⁻¹			
k _{neg} [39]	Reaction rate coefficient of anode	3e-11 m s ⁻¹			
c _l	Electrolyte concentration	1000 mol m ⁻³			
$\sigma_{s, pos}$	Solid phase conductivity of cathode	11.99 S m ⁻¹			
$\sigma_{s, neg}$	Solid phase conductivity of anode	598.8 S m ⁻¹			
$\sigma_{CC, pos}$	Conductivity of positive current collector	5.998e7 S m^{-1}			
$\sigma_{CC, neg}$	Conductivity of negative current collector	$3.774e7 \text{ S m}^{-1}$			
σ_l [45]	Electrolyte conductivity	$1.5091^{-9}c_l(-1.05e7 + 668.0c_l + 0.494c_l^2 + 7.4e4T - 17.8c_lT - 8.8610^{-4}$			
		$c_l^2 T - 61.1846T^2 + 5.7078c_l^2 T^2)S m^{-1}$			
D ₁ [39]	Electrolyte diffusivity	$10^{-4} \times 10^{-4.43 - \frac{54}{7-229-5c_l} - 0.22c_l} m^2 s^{-1}$			
$t^{0}_{+}[39]$	Transfer coefficient	0.38			
$\frac{\partial lnf}{\partial lnc}$ [39]	Activity	$(0.601 - 0.24c_l^{0.5} + 0.893(1 - 0.0052(T - 294))c_l^{1.5})(1 - t_+^0)^{-1} - 1$			

e = estimated.

initiated by massive ISC. One detail worth to be noticed is that the normalized concentration of separator reaches 0.0012 at the massive ISC triggering temperature, which implies that the separator has been totally burnt down at this point. This simulation result agrees with prior researchers' work that massive ISC may happen after separator collapse. The phenomenon further supports the existence of massive ISC indirectly. The intensive release of QISC boosts other reactions, increasing the heat generation power. After the explosion, the temperature ascending rate quickly drops to about 6 °C min⁻¹. By comparing Fig. 2(e) and (f), we can conclude that SEI decomposition is the primary heat source at the beginning stage of self-heating. The reactions of cathode start the transition region between low self-heating to TR. The reactivity of cathode is the determining factor of the plateau in Fig. 1(e). Once the temperature goes over the threshold, the combustion is out of control. In conclusion, through numerical modeling, the chemical part is separated from the chaos, and can be applied in the electrochemicalthermal model later.

Nevertheless, the reaction composition is too complicated, which consists of 11 dependent variables. If applied directly in the FEM model, it will bring too many freedom degrees in the model, making it difficult to converge during calculation. Therefore, the model needs to be further simplified. Empirical equations like Arrhenius equations and Gaussian pulses can be used [36–38]. The shortcoming of the previous works is that the empirical equations are acquired by fitting the thermal test results of a whole battery. The reference data are not enough to calibrate the model, and the true processes may be hidden. In order to make the empirical model as authentic as possible, and increase the reliability of simulation results, we deduced the empirical equations from the thermal dynamic model stated foregoing.

The empirical equations should be able to reflect the lump heat behavior of 11 reactions, and also applicable in a vast temperature rate range which would be expected in the real thermal abuse situation. Base on the experiment and simulation results, the self-heating process is generally composed of two primary heat sources: small heat generation before TR, and large heat generation during TR. In light of the connection between separator collapse and ISC, the reaction of separator is separated, and treated as an independent process. Thus in the following parts, the ISC triggering condition will be changed to separator collapse. The critical normalized concentration is set as 0.0012. In total, we decided to use three Arrhenius equations to fit the total heat generation curve to simulation results, which are calculated by putting reactions in external forcing heat condition of different constant temperature rising rate. Eqs. (10) and (11) are derived, where H_{chem} is the total heat of chemical reactions, and Q_{chem} is the heat dissipation power. Table 2 lists the fitted parameters. Fig. 4 shows the fitting results. Although the lumped equation loses some accuracy in detail, the general picture of energy dissipation is captured without losing kinetic characteristics. The lumped model shows good agreement with experimental data and the original model. The equations can be used in the following FEM model.

$$\frac{\mathrm{d}c_{lump}}{\mathrm{d}t} = A_{lump} \exp\left(-\frac{E_{lump}}{RT}\right) c_{lump}^{n_{lump}} \tag{10}$$

$$Q_{chem} = H_{chem} \frac{\mathrm{d}c_{lump}}{\mathrm{d}t} \tag{11}$$

2.2. Electrochemical-thermal model

The electrochemical-thermal model is established based on the test data of 57 Ah LIBs in COMSOL Multiphysics using lithium-



Fig. 5. Comparison between simulation results and measured values. (a)-(c) are battery charge voltage curves, and (d)-(f) are battery average surface temperatures. The applied currents are 30 A, 42 A, and 57 A, respectively, from left to right.

ion battery module and heat transfer module. The parameters are adopted from Ref. [39] and experiment data. The geometry structure of the model is identical to the sample battery with 31 positive electrodes and 32 negative electrodes. The electrodes are welded to the tabs on the opposite side along the length direction. It is set up based on the P2D (pseudo-2-dimensional) method, which has been widely used in the LIB modeling [40-43]. The kernel of the P2D method is porous electrode method advanced by Newman and Doyle [44], in which the porous structure of the electrodes is homogenized by introducing porosity into relevant equations and parameters. In the model, four independent variables are solved: ϕ_s, ϕ_l, c_l and T, accounting for solid phase potential, liquid phase potential, liquid phase concentration and temperature, respectively. In order to include the solid phase diffusion's effect into the model, an extra dimension is embedded in the porous electrode domain to calculate the solid phase concentration of intercalated lithium. A series of equations are applied to describe the complex physics in the battery. A Nernst-Planck-Possion equation modified by concentrated solution theory is used to describe the liquid phase. Possion equation is used to describe the solid phase. The interface Faradaic reactions are governed by Butler-Volmer equation. We use Fick's Law to calculate the diffusion processes in liquid and solid phase. The equilibrium potentials and the temperature derivatives of equilibrium potentials of both electrodes are adopted from our previous work as interpolated functions [18]. The main governing equations are listed in Table 3, and the parameters are listed in Table 4. Simulation results are compared with the test results as shown in Fig. 5. Details of the model construction and verification have been thoroughly discussed in our previous work [18].

The calibrated electrochemical model is further extended to simulate the internal short circuit situation. An ISC point is introduced directly into the electrochemical-thermal model. Except for the short circuit induced by the lithium dendrite or other metal deposition, the direct contact between positive and negative electrodes caused by the separator damage, shrinkage or displacement is the most probable situation. This makes the edge of the battery to be the most probable place for ISCs to exist. Therefore, we choose an area in the corner of the middle layer to be the ISC lo-



Fig. 6. Model geometry of C31/A32 battery and T-C13/A14 battery. The ISC area shown is magnified.

Table 5 Thermal parameters of TR model.					
$\rho_{\it eff}/\rm kg~m^{-3}$	$C_p/\mathrm{J}~\mathrm{kg}^{-1}~\mathrm{K}^{-1}$	λ_{eff}/W	$\lambda_{\textit{eff}}/W~m^{-1}~K^{-1}$		
		λ_{ν}^*	λ_p^*		
2886.2	1280.0	1.03	16.23		

 ${}^*\lambda_{\nu}$ is heat conductivity along the normal direction of electrode surface, λ_p is the component along the parallel direction of electrode surface. Both are calculated according to Ref. [39].

cation, as shown in Fig. 6. The contact resistance between cathode and anode is 120 Ω mm². The ISC induced heat generation Q_h is also modified by lumped reaction ratio factor ξ , as shown in Eq. (12). ξ_{ave} is the average value in the ISC point vicinity.

$$Q_h = \begin{cases} Q_h, \ \xi_{ave} > 0.001\\ 0, \ \xi_{ave} < 0.001 \end{cases}$$
(12)

TR lumped model is coupled with the electrochemical-thermal model. TR model treats the battery as a homogenous media



Fig. 7. Electrochemical model results (without thermal reactions coupling) of (a) discharge current generation in different layers at 0 s, (b) current contribution ration of core three layers at 0 s, (c) total short circuit current at 0 s and (d) battery voltage change within 170 s. Thermal runaway of batteries with different layer numbers is shown in (e). C31/A32 battery does not undergo TR within 300 s. Durations of heat spread to the whole battery after the TR are denoted in the plot.

[38,46–48]. The governing equation is

$$\rho_{eff}C_p\frac{\partial T}{\partial t} + \nabla \cdot \left(-\lambda_{eff}\nabla T\right) = Q \tag{13}$$

where ρ_{eff} is the density of battery, C_p is the specific heat capacity, and λ_{eff} is the heat conductivity, which is also an anisotropic

parameter. Q is heat source term as follows:

$$Q = Q_h + Q_{chem} + Q_{ISC} + Q_{con\nu}$$
(14)

 Q_{chem} and Q_{ISC} are expressed in Eqs. (6) and Eq. (8), (9). Q_{conv} is expressed in Eq. (7), but the ambient temperature T_{amb} is set to 298.15 K. Parameters are listed in Table 5.



Fig. 8. Comparison between C7/A8, C13/A14 and T-C13/A14. (a) Current source distribution in different layers. (b) Voltage change within 170 s without exothermic reactions. (c) Heat progression during TR.

3. Results and discussion

3.1. Batteries with different layer numbers

For laminated batteries, the number of electrode layers is an important design parameter. In our model, various batteries with the same electrode geometry but different laminated layers are investigated. Batteries with different layer numbers are denoted as cathode number/anode number (e.g. C31/A32 represents a battery consists of 31 layers of cathodes and 32 layers of anodes, respectively). Fig. 7(a) shows the distribution of current generated in each cell layer. All layer current shows an ascending trend as layer number decreases. The highest column corresponds to the ISC layer, and along with its two neighbor layers, the three core layers give the highest layer current. Due to the difference in electronic conductivity between positive and negative electrodes, the influence on two neighbor layers is different. Typically, the neighbor layer on the positive side generates more current than the neighbor layer on the negative side. The percentage of current arising from the core three layers are displayed in Fig. 7(b). It can be seen that the ratio is decreasing as layer number goes up, and other healthy layers are the major current sources. However, despite the ratio change, the total ISC current remains unchanged, because of the same initial voltage status (4.2 V). Fig. 7(c) shows that all current values are located between 3.09 A and 3.10 A. The discrepancy of 0.01 A has no difference to the batteries with such a large capacity. However, because of different battery capacities, the discharge rate will be larger for lower capacity batteries, which causes lager polarization in the electrochemical system. This can be observed in Fig. 7(d). Battery voltage goes down as capacity decreases. Because the positive/negative electrode tabs are welded together, the solid potential at tabs are identical. Thus, as shown in Fig. 7(a), larger polarization in thin battery causes a larger current generation in each layer. It also implies that the ISC detection through battery voltage drop is more difficult for large scale batteries, but more effective for small scale batteries.

Since the ISC current is identical, which means the same heat generation will be expected, the battery temperature shall be controlled by the heat transfer process, which is closely related to battery geometry. By coupling the TR kinetic model, the heat progression is obtained. Fig. 7(e) compares the thermal progressions of the 5 battery models. The battery with 31 cathodes and 32 anodes does not undergo TR within 300 s, but the other batteries show the heat progression starting from the short circuit point, and spreading to the whole battery.

Two parameters stand out when describing ISC-TR process: the TR triggering time and the duration of heat progression, which reflects the safety time and the average heat dissipation power respectively. It shows that the two parameters are synergistically affected by battery capacity and geometry. Because a smaller thickness will limit the heat transfer, the generated heat is forced to be accumulated in the local region, leading to faster temperature accumulation in the corresponding region. In the case of the thick batteries, the limited heat generated at one point should spread out easier. Thus, the local heating rate is lower. As illustrated in Fig. 7(e), the TR triggering time increases from 20 s to over 300 s as layer number goes up. It can be concluded that the initiation of TR will be delayed for batteries with larger thickness. However, the duration of heat progression decreases from about 50 s to 30 s. Considering the difference in capacity, thick batteries will be much more destructive during

TR due to higher heat amount generated and higher dissipation power.

3.2. Different design for specific capacity

To further investigate how battery design affects ISC and TR, we constructed a battery model of C13/A14 battery of the same capacity with more pieces of electrodes but smaller size. The electrode length is 7/13 times of C13/A14 battery, and denoted as T-C13/A14. The current distribution and voltage change of T-C13/A14 are compared with C7/A8 and C13/A14 in Fig. 8(a) and (b). The total short current is 3.10 A, which is almost the same as the previous simulation results. As previously concluded in Section 4.1, voltage curves of C7/A8 and T-C13/A14, which have the same capacity, are closely located. But the potential of T-C13/A14 is slightly positively deviated from C7/A8, due to the electrode size difference. This result indicates that ISC induced voltage drop is mainly affected by battery capacity, and slightly deviates due to structure difference. Current generated in ISC layer of T-C13/A14 battery is 0.2546 A, which is 61.66% of C13/A14 (0.4129A), and 50.71% of C7/A8 (0.5021A). Moreover, the current contribution of the core three layers also drops down to 19.87%. Despite smaller electrode capacity, the other healthy layers currents are even larger than that in C13/A14, due to a much lower battery voltage. Heat progressions during TR are illustrated in Fig. 8(c). Through the comparison, we can find that the battery thickness actually dominants the critical ignition time, no matter the difference in capacity. The starting point of T-C13/A14 is approximately the same as C13/A14. It should also be noticed that the TR duration of T-C13/A14 is shorter than that of C7/A8, implying a more severe hazard. Therefore, under the same designed capacity, a thicker structure will delay the ignition of battery, but increase the heat releasing power. Generally, the duration of safety time and heat dissipation power are contradictive. The longer the duration of safety time is, the higher the heat dissipation power will be.

4. Conclusion

A kinetics model has been established based on DSC and ARC experiments analysis which reveals the TR mechanism of NCM811/SiO_x-Graphite LIB. 11 individual reactions and other heat sources have been characterized during TR. A novel approach of model reduction is proposed, reducing the complex chemical heat sources to two lumped expressions, which not only ensured good agreement with experimental and original model results, but also significantly reduced computation load in coupled FEM model.

By coupling thermal abuse kinetics into electrochemicalthermal model, we conducted a detailed study of the internal short circuit phenomenon. The electrode size and stack layer number are analyzed for laminated batteries under the same ISC circumstance. The effect of laminate number on total ISC current is limited, which is mostly determined by battery capacity. As the laminate number increases, the TR onset will be delayed, but the TR heat dissipation will be more serious, which implies much more severe explosion damage. For the specific ISC condition and design schemes, the onset time varies from 20 s to over 140 s, and the TR progression duration varies from 50 s to less than 30 s. The modeling work results demonstrate that the effect of laminate structure design should be taken into consideration critically when assessing the ISC abuse endurance of the battery. The trade-off between the duration of safety time and heat dissipation power needs to be made in the battery module application. This work presents a reliable methodology of ISC and TR model construction, and also provides important references for designing and manufacturing of large format LIBs.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Chaoyue Liu: Conceptualization, Methodology, Software, Investigation, Formal analysis, Writing - original draft, Writing - review & editing. **Hang Li:** Methodology, Software, Validation, Investigation. **Xiangbang Kong:** Validation, Investigation, Writing - review & editing. **Jinbao Zhao:** Conceptualization, Supervision, Project administration, Funding acquisition, Writing - review & editing.

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