**A representative-sandwich model for simultaneously coupled
mechanical-electrical-thermal simulation of a lithium-ion cell under
quasi-static indentation tests**

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Abstract

The safety behavior of lithium-ion batteries under external mechanical crush is a critical concern, especially during large scale deployment. We previously presented a sequentially coupled mechanical-electrical-thermal modeling approach for studying mechanical abuse induced short circuit. In this work, we study different mechanical test conditions and examine the interaction between mechanical failure and electrical-thermal responses, by developing a simultaneous coupled mechanical-electrical-thermal model. The present work utilizes a single representative-sandwich (RS) to model the full pouch cell with explicit representations for each individual component such as the active material, current collector, separator, etc. Anisotropic constitutive material models are presented to describe the mechanical properties of active materials and separator. The model predicts accurately the force-strain response and fracture of battery structure, simulates the local failure of separator layer, and captures the onset of short circuit for lithium-ion battery cell under sphere indentation tests with three different diameters. Electrical-thermal responses to the three different indentation tests are elaborated and discussed. Numerical studies are presented to show the potential impact of test conditions on the electrical-thermal behavior of the cell after the occurrence of short circuit.

Keyword: Lithium-ion battery, Short circuit, Multi-physics simulation, Mechanical crush, Temperature ramp, Indentation

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Introduction

Due to its high energy density, high voltage and low self-discharge rate, Lithium-ion batteries (LIBs) are currently the state-of-the-art power sources for a variety of applications, from consumer electronic devices to electric-drive vehicles (EDVs). The physical phenomena occurring in LIBs are very complicated and take place in different time and length scales (particle, electrode, cell and pack), including electrochemical reactions at the anode and cathode active materials, electron moving in current collectors, heat generation due to charge/discharge, chemical reaction between electrolyte and electrode surfaces, mechanical deformation under external crush, and most importantly, the coupling effect between these multi-physics responses. The understanding of the interaction between different physics at different scales is of great importance; computational models are an efficient way to study multi-physics algorithm and provide insights to the design of safer LIBs. This work intends to study one very practical problem of LIBs: mechanical-abuse-induced short-circuit.

A short circuit in a battery pack can result in deformation and/or venting of the battery [1]. Doughty and Pesaran [2] presented a comprehensive review of mechanical abuse tests of battery cells, modules and packs. There is a significant amount of recent effort focused on the development of abuse test methods. Hatchard et al. [3] developed a

“smart nail” penetration test method for LIB by instrumenting thermocouples on the nail tip, to collect temperature vs. time data at the location of nail penetration. Lamb and Orendorff [4] examined mechanical abuse tests and the results were found to vary significantly with test conditions. However, the research work on simulating the mechanical-abuse-induced short-circuit and subsequent thermal ramp in LIBs are quite limited.

Wierzbicki and Sahraei [5] and Sahraei et al. [6-8] conducted a series of tests to characterize effective mechanical properties of battery components (separator and electrodes), and evaluate the mechanical performance of pouch LIBs and cylindrical LIBs under bending and compression loading conditions, as well as, punch indentation using different shapes of punches. Macro-scale homogenized finite element (FE) models were developed to simulate these tests and presents good correlations. Sheidaei et al. [9] investigated the tensile behavior of a single-layer polypropylene separator in both dry and wet conditions using a dynamical mechanical analyzer (DMA). It was found that the mechanical properties (Young’s modulus and yield stress) are significantly lower when tested in electrolyte solutions, for example, the wet to dry ratio of Young’s modulus in the machine direction is 48.5%. Cannarella et al. [10] presented a straightforward procedure for measuring the compressive (with and without electrolyte) and strain-rate dependent tensile mechanical properties of LIB separators using a universal test machine. Based on Cannarella’s test results [10], Gor et al. [11] developed a material model for predicting elastic response of the studied separators, taking into account the strain-rate effect, viscoelastic and poroelastic. Lai et al. [12-13] and Ali et al. [14] conducted a series of experimental and computational work on representative volume element (RVE)

specimens of prismatic graphite/LiFePO₄ pouch cells. The results indicate that the anode and cathode active material coatings have nearly no load carrying capability under tension and suggest that the compressive response of LIB can be modeled by treating the indicated layers as foam materials. Avdeev and Mehdi [15] characterized experimentally the nonlinear mechanical deformation of cylindrical LIB under lateral impact using a high-speed camera. A homogenized finite element model was developed to estimate the impact time during the drop tests.

In [5-8, 16], it was observed through experimental measurement of the cell voltage that the instant at which the voltage drop occurs correlates with the instant at which the mechanical failure of the battery structure is observed. The short circuit initiation was assumed to be co-located at the same coordinates at which the principal tensile stress first reaches a certain magnitude (for example, 10MPa in [6]). While references [5-8, 16] provide a simple and indirect method for predicting a mechanical-abuse-induced short circuit, a coupled mechanical-electrical-thermal (or multi-physics) model can predict the short circuit in a straight-forward way, and provide more accurate insights into the failure mechanism. And more importantly, the coupled model enables prediction of thermal and electrical responses after the initiation of short-circuit, which are the primary physics governing the failure of the battery.

The mechanical models of LIB cells listed above [5-15] all utilize homogenized macro-scale models, whereas to predict the electrical short it is necessary to explicitly model each individual component of the battery cell. In our recent work [17], a representative sandwich (RS) was developed to predict short-circuit under external crush following a sequential one-way coupling method. By conducting electrical-thermal

analysis on the deformed geometry obtained from the mechanical solver, we successfully captured separator failure induced electrical failure and consequential thermal ramp. It was validated that using a single RS can simulate reasonably well the mechanical response of a full pouch cell. In this work, a simultaneous coupling approach is presented which predicts the simultaneous evolution of electrical-thermal responses associated with mechanical deformation.

The remainder of the paper is organized as follows. Section 2 presents theory and governing equations of the coupled mechanical-electrical-thermal model. The description of finite element model set-up, including mesh, constitutive models and boundary conditions is presented in Section 3. The results presented in Section 4 consist of correlation of mechanical model with experiments, prediction of mechanical failure induced short-circuit, numerical studies of different indentation conditions and the interaction between mechanical failure and post-short electrical-thermal responses.

2. Coupled mechanical-electrical-thermal model

The coupled mechanical-electrical-thermal model is built in a commercial finite element software LS-DYNA [18] using modules available by default: solid mechanics solver, thermal solver and electromagnetic (EM) solver. The basic equations for these three solvers are introduced below.

The mechanical solver is used to solve for deformation and predict failure of a structure suffering external or internal loading conditions. The explicit mechanical solver seeks a solution to the momentum conservation equation

$$\sigma_{ij,j} + \rho f_i = \rho u_{i,tt} \quad (1)$$

where σ_{ij} denotes components of stress, u_i denotes components of displacement, ρ is the density, f_i is the body force density and t is time. The comma on $\sigma_{ij,j}$ denotes covariant differentiation, similarly, $u_{i,tt}$ denotes acceleration. For a solid, the constituent (stress-strain) relationship can be written as follows:

$$\sigma_{ij} = C_{ijkl} \gamma_{kl} \quad (2)$$

where C_{ijkl} is the stiffness matrix, and the components of strain γ_{kl} are related to displacement by the following relationship

$$\gamma_{kl} = \frac{1}{2} \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad (3)$$

where x is the coordinate. And the indexes i, j, k and l equal 1, 2, and 3 corresponding to x, y and z directions. A detailed description of the constitutive material models used here is provided in [18].

The LS-DYNA EM solver employs the eddy current approximation [19], which assumes a divergence free current density and no charge accumulation. Two equations constituting the system response will be solved:

$$\nabla(\kappa \vec{\nabla} \phi) = 0 \quad (4)$$

$$\kappa \frac{\partial \vec{A}}{\partial t} + \vec{\nabla} \times \left(\frac{1}{\mu} \vec{\nabla} \times \vec{A} \right) + \kappa \vec{\nabla} \phi = \vec{j}_s \quad (5)$$

where magnetic vector potential $\vec{A}$ and electric scalar potential ϕ are two unknowns to be solved; κ is the electrical conductivity, μ is the magnetic permeability and $\vec{j}_s$ is the source current density. After solving the above two equations, the Lorentz force $\vec{F}_{Lorentz}$ and Joule heating energy E_{Joule} can be computed as:

$$\vec{F}_{Lorentz} = \vec{j} \times \vec{B} \quad (6)$$

$$E_{Joule} = \frac{\vec{j} \cdot \vec{j}}{\kappa_s} \quad (7)$$

where $\vec{j}$ is the current density.

For the thermal solver, the governing equations of conduction of heat in a three-dimensional solid is given by:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} [k_{ij} \frac{\partial T}{\partial x_j}] + Q \quad (8)$$

where T is temperature, c is specific heat, k_{ij} is thermal conductivity and Q indicates heat generation rate per unit volume Ω .

In LS-DYNA, the mechanical, EM and thermal solvers, are fully coupled with each other. Figure 1 shows the interactions between the LS-DYNA mechanical, thermal and EM solvers. The three solvers have distinct time steps, and generally the mechanical time step is a lot smaller than the EM and thermal time steps. At each mechanical time step, the EM and thermal field values are calculated by linear interpolation. At each EM time step, the EM solver and the mechanical solver interact, during which the EM solver communicates the Joule heating term E_{Joule} to the thermal solver while the thermal solver communicates the temperature to the EM solver.

At each EM time step, the EM solver communicates the Lorentz force described in Eq. (6) to the mechanical solver resulting in an extra force in the mechanical governing equation (Eq. (1)):

$$\sigma_{ij,j} + \rho f_i + F_{Lorentz} = \rho u_{i,tt} \quad (9)$$

The mechanical solver returns the displacements and deformation of the structure to the EM solver. Similarly, at each thermal time step, the thermal solver communicates temperature to the mechanical solver while the mechanical solver communicates the value of the plastic work $W_{plastic}$ to the thermal solver. The plastic work and Joule heating are the predominant sources of heat generation in our case; so Eq. (8) can be rewritten as follows:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} [k_{ij} \frac{\partial T}{\partial x_j}] + \frac{\dot{W}_{plastic} + \dot{E}_{Joule}}{V} \quad (10)$$

where the dot indicates the time derivative and V is the volume of the element. We should note that there is no explicit representation of temperature in the governing equation for the mechanical and EM solvers. The material properties, like conductivity κ and stiffness C_{ijkl} , evolve as a function of the temperature. However, due to the limited availability of experimental data, in this work, all the material properties are considered to be temperature independent throughout the whole analysis.

In typical electrochemical battery models [20-21], the magnetic field is not considered assuming $\vec{A} = 0$ all over. Then the electrical potential can be obtained by solving the following two equations:

$$\vec{j} = -\kappa_s \vec{\nabla} \varphi \quad (11)$$

$$\vec{E} = -\vec{\nabla} \varphi \quad (12)$$

where $\vec{E}$ is electrical field. These are simplified versions of Eqs. (4) and (5). Contributions from the electrolyte to the short-circuit are assumed to be negligible (κ_s is

the solid phase conductivity) – given that the difference between the electronic and ionic conductivities is four orders in magnitude or larger.

The goal of this study is to predict the initiation of short circuit and its consequential evolution of electrical properties (current and voltage) and temperature, and more importantly, the effect of external deformation on the electrical and thermal response of the cell. The information obtained from these simulations is extremely helpful for the studying the electrochemical responses.

3. Numerical model

The Lithium-ion battery studied in this work is a small LiCoO_2 pouch cell. The nominal capacity of the cell is 740 mAh with a nominal voltage 3.7 V. To simulate the local damage and predict the short circuit, it is necessary to model each individual component (separators, collectors and active materials) of the battery structure. In this work, a finite element model was built to explicitly model each individual component without loss of computational efficiency or accuracy. We use the electrical contact between active materials following the failure of the separator as a criterion for short circuit.

3.1 Representative sandwich model

The detailed stacking and dimensions of the studied pouch cell were reported by Sahraei et al. [7]. It was found that the pouch cell was composed of two separate laminates; each can be considered a multi-layered plate, made from cathodes, anodes and separators. A cross-sectional view is shown in Figure 2(a). A cathode and anode are each composed of collector and active layers. A representative sandwich (RS) is introduced to define the repeating layout as shown in Figure 2(a). Each RS contains a cathode active

material layer, a cathode current collector layer, an anode active material layer, an anode current collector layer and one separator layer. The casing material is not considered in this study, since its contribution to the mechanical response or the initiation of short circuit can be isolated from the response of the cell components as reported by Sahraei et al. [7].

The whole pouch cell contains about 165 layers, and can be estimated to be comprised of 40 representative sandwiches. The modeling of all the 165 layers (the full pouch cell model) is computationally very costly. One simplifying approximation is to represent the 40 representative sandwiches as one single equivalent but thicker RS (shown on right side of Figure 2(a)), where each layer has a proportionately larger thickness.

The schematic representation of an indentation model is shown in Figure 2(b). Due to symmetry, we only consider one quarter of the actual in-plane domain in our finite element model to save computational time. The geometry in our FE representation has a length l of 29.75 mm, a width w of 17 mm, and thickness h of 4.6 mm. The bottom surface (i.e. $z = 0$) of the battery models is constrained in the thickness direction (z -direction). The indentation tests were conducted with rigid spheres with diameters 12.7 mm, 28.575 mm and 44.45 mm in three different test cases, respectively, moving downward in the z -direction at a constant speed to accomplish the loading process in 0.01 second. Although the loading speed is much higher than that in a typical quasi-static experiment, the simulations are still considered quasi-static since we were able to verify that the kinetic energy was less than 1% of the total energy.

The battery model was meshed using solid elements, with 18 elements through the thickness (z-direction), 100 elements along the length (x-direction) and 60 elements through the width (y-direction) resulting a total of 108000 elements for the RS model. The indenter is modeled as a rigid sphere.

3.2 Mechanical constitutive models of battery components

The development of an accurate constitutive model is essential for building a predictive model. The preliminary test results by Lai et al. [12-13] and Sahraei et al. [7-8] suggest that the electrodes and separator have significantly different tensile and compressive responses due to the presence of porous active materials. Separator is also known to be anisotropic under in-plane tensile loading conditions. Sheidaei et al. [9] identified that the separator shows different tensile response in the machine direction and transverse direction. In this work, anisotropic constitutive models are developed for the active materials and separator based on reported experimental results. The current collectors are simulated as isotropic elasto-plastic materials.

3.2.1 Separator and active materials

In the present study, the porous active materials and separator are treated as homogeneous solid materials and LS_DYNA material model MAT126 (MAT_MODIFIED_HONEYCOMB) is utilized in combination with the co-rotational solid element type. The material model has an orthotropic nonlinear elasto-plastic constitutive behavior based on experimentally determined stress-strain curves, which are defined separately for all normal and shear stresses. The components of stress tensors are considered to be fully uncoupled, which means that the Poisson's ratio is zero, consistent with the mechanical test observations for LIBs [12]. The elastic modulus increases from

initial uncompacted modulus to the compacted modulus depending on the relative volume.

Based on the previous experimental observations [7], we assume that the active materials are isotropic with the same mechanical properties in all three directions but different responses under tension and compression. The separator is assumed to be isotropic under compression but orthotropic under tension, where the tensile response in the through-thickness direction is assumed to be the same as that in the machine direction (y-direction of Fig. 2(b)). Based on the tensile experimental data of similar materials by Lai et al. [12-13], piece-wise linear stress-strain curves are developed to describe the tensile behavior of anode and cathode active materials as shown in Figure 3(a). Figure 3(b) shows the piece-wise linear stress-strain curves of separator under tension in machine and transverse directions, developed based on the tensile experimental data of similar material by Sheidaei et al. [9].

The mechanical response of the active material layers and the separator are more complicated due to the presence of porosity. Currently, there is no experimental work reported in literature measuring the compression properties of active materials. In our previous work [17], an alternate analytical procedure was developed to estimate the effective compressive stress-strain response of these porous layers from existing compression data experimentally measured using the full pouch cell. Figure 3(c) shows the compressive stress-strain curves of active materials and the separator.

The stress-strain curves (one curve each for the active materials and two curves for separator) are then implemented into the corresponding material models as the normal loading curves. The shear loading curves use the same curve as normal loading

conditions but with a scale factor 0.45 according to [22]. Other material parameters (for example, initial modulus, compacted modulus and volume fraction et al.) in the Honeycomb model are derived from the implemented stress-strain curves (see Fig. 3).

3.2.2 Collectors

In previous work by Sahraei et al. [7] and Lai et al. [12], a series of experiments were conducted to characterize the tensile and compressive properties of the battery components. It was suggested that the current collectors can be modeled using the piece-wise plasticity representation in LS-DYNA. In this work, the MAT_PLASTIC KINEMATIC representation [18], a computationally effective model for isotropic-hardening plasticity, is used to describe the mechanical behavior of the current collectors. The associated properties to be specified as input parameters with this representation in LS-DYNA are shown in Table 1. These material properties for the current collectors were obtained by Hill [23] using similar materials.

3.3 Electrical-thermal model

There is no experimental data available for the electrical or thermal properties for the materials used in the cells studied here. The electrical and thermal properties of a $\text{LiMn}_2\text{O}_4/\text{LiC}_6$ battery [24] are used in our model. Table 2 shows the electrical conductivity and thermal properties for each component of the LIB. Although the actual properties of the battery studied may be different from these values, the results obtained using the data referenced in Table 2 still provide a reasonable electrical-thermal response for predicting the short-circuit initiation and post-short phenomena.

For the simultaneously coupled simulation, a constant voltage of 3.7V is applied between the top and bottom surfaces of the RS. The evolution of voltage after initiation

of a short circuit is studied by calculating the internal voltage drop caused by the sudden decrease in resistance due to the short-circuit. For thermal simulations, a default adiabatic boundary condition is used for the symmetrical surfaces ($x = 0$, $y = 0$). For the other four external surfaces ($x = -w$, $y = -l$, $z = 0$ and $z = h$), a convection boundary condition is defined to model heat exchange between the surroundings and the battery cell:

$$q = k_{ij} \frac{\partial T}{\partial x_j} = h(T - T_{\infty}) \quad (13)$$

where q is the heat transferred per unit time and per unit area, h is heat transfer coefficient which is defined as $15 \text{ W}/(\text{m}^2 \cdot \text{K})$ in this work based on experimental measurements reported by Maleki et al. [25], T_{∞} is the temperature of the surroundings which is considered as constant at 298 K. An initial temperature 298 K is applied to all the elements.

3.4 Mechanical and electrical-thermal failure criterion

The objective of this work is to predict the structure fracture induced electrical short-circuit of LIB under quasi-static indentation. Proper failure criteria and failure parameters should be implemented and defined to enable this capability.

Simulation of mechanical failure of cell components has rarely been reported in the literature. This work intends to study the separator failure induced cathode-anode short-circuit behavior, and we anticipate that the failure of the separator material will occur well in advance before other forms of short-circuit (e.g., anode/aluminum etc.) can take place. In previous work [17], a maximum volume-strain failure criterion was applied to simulate mechanical failure of separator. We carried out a parametric study on the maximum through-thickness volume-strain value of the separators using the single-RS model, and found that when failure strain equals 0.93 (which means that the thickness of

the element is compressed to 7% of initial thickness), the numerically predicted and the experimentally measured global failure strains match.

In this work, the maximum tensile failure criterion implemented with the Honeycomb Model was utilized to simulate separator failure. The tensile failure strain of separator varies a lot depending on the polymer component, manufacturing process and specimen preparation. Avdeev et al. [26] tested the static and dynamic tensile behavior of Celgard C480 tri-layered separator and reported failure strains of 35% and 400% in machine direction and transverse direction at a strain rate of 0.1 /s, respectively. Lai et al. [13] reported a failure strain range of 50% to 80% for separator of a LiFePO₄ battery cell. The tensile test results of polypropylene separator reported by Venugopal et al. [27] shown that the failure strain in transverse direction is about twice of that in machine direction. In the current work, parametric study was conducted to estimate the tensile failure strain of the separator layer assuming that the onset of separator failure coincides with battery cell fracture.

One limitation of the simultaneous modeling approach is that element erosion is not compatible with the EM solver. To overcome this issue, we first conducted a mechanical only simulation to correlate the mechanical indentation test results and recorded the critical global displacement u_f of indenter at the moment of cell fracture. Then we conducted the simultaneous simulation by applying exactly the amount of critical displacement u_f to the indenter and disabling mechanical failure criterion. Through this method we can obtain exactly the same deformed geometry at the instant of cell fracture. The electrical contact is defined by a distance-based criterion, which means electrical contact initiates when the distance between two parts is below a certain

threshold value d_c . Once the mechanical failure criterion is satisfied, no more loading will be added which means that the indenter will be held in place without further movement. There will be no further deformation or relaxing happened inside the pouch cell beyond the instant of mechanical failure.

Whereas existing models assume initiation of electrical contact following mechanical failure of separator layer, our approach calculates the current flow across the component layers that border the element subjected to mechanical failure and utilizes the resultant voltage drop to determine the short resistance. This process allows us to introduce additional failure criteria based on the electrical and thermal properties of the different layers coming into contact across the instance of mechanical failure. For instance, in this work, the criterion for electrical failure is the instantaneous local current density exceeding a preset value, for example, 0.01 C, which corresponds to a current density of 13.12 mA/mm² for a 740 mAh cell when the area of elements subject to mechanical failure is 0.785 mm². Thermal failure is set to initiate when the temperature across the element in question exceeds the melting point of the corresponding material (e.g., 144 °C or 417 K for the separator). However, mechanical failure sets in instantaneously compared to the thermal response, which is usually distributed over a span of several seconds. Accordingly, in this work, we present our methodology for linking the mechanical-failure criterion with the follow-on electrical activity and discuss some preliminary thermal responses.

The numerical models are solved on a High Performance Computer system equipped with a total of 31,104 Intel Xeon processors providing a total of about 608 TeraFLOPS or Trillion floating point calculations per second. The computational time for

the mechanical only simulation is 8 hours using 60 CPUs, while the computational time for the simultaneous coupled model is 16 hours also using 60 CPUs.

4. Results and Discussion

4.1 Calibration of the mechanical model

Previous experiment results [8] have identified that a simultaneous voltage drop and temperature increase was detected at the moment of force drop (fracture of structure). Thus, before conducting the coupled simulation, it is necessary to correlate the mechanical model with experimental results. An efficient mechanical modeling strategy is established with the capability of predicting the onsite of mechanical fracture and enabling coupled modeling of electrical and thermal behaviors.

The mechanical model is validated through comparison of the numerically predicted and experimentally measured force vs. global-strain curves (See Fig. 4). Utilizing the constitutive and failure models described in the previous sections (3.2 and 3.4), the mechanical responses of the cell subjected to indentation using spherical indenters of three different diameters (12.7 mm, 28.575 mm and 44.45 mm named as small punch, medium punch and large punch, respectively) were simulated. Experimental indentation tests corresponding to these results, on the pouch cell described in Section 3 were conducted by Sahraei et al. [8] using the hemispherical punches at a loading rate of 1 mm/minute and monitoring the voltage simultaneously. A significant finding of the experimental results was the fact that the electrical short circuit detected from the drop in cell voltage coincided well with the drop in the load due to mechanical failure.

In our work, the global strain is defined as the applied displacement of rigid sphere over the initial thickness of the RS model. The force is recorded as the reaction

force of the rigid sphere in the through-thickness direction (z -direction). The maximum tensile failure strain of separator is obtained through a parametric study comparing the numerical predicted force-strain curves with experimental curves. Figure 4(a) shows the parametric study of the mechanical responses for the small punch indentation test obtained by varying the tensile failure strain of separator. It is found that the numerically predicted global failure strain of the battery cell increases with the increase of tensile failure strain for the separator layer. And when the tensile failure strain of separator equals 0.29, the numerical predicted and the experimentally measured global failure strain match.

We note that the failure strain value used for the indentation model is much lower than the experimental measured value in a uniaxial tensile test. This is because under a structure-level test some other local premature damage events, for example, cracking of electrodes, may cause earlier failure of the separator. The strain contour of active materials at the instant before the fracture of battery cell is shown in Fig. 4(a), from which we can see that the maximum tensile strain value of the active materials is about 0.2487 exceeded the experimental detected tensile failure strain 0.03 (reported by Lai et al. [13]). This suggests that during the indentation tests before the failure of separator, the active material layers are very likely subjected to cracking. Although this cracking of electrodes may not affect much the resistance of the battery cell across the terminals, it would very likely induce localized concentration of the stress/strain response, and result in an earlier failure of the adjacent layers (i.e., the separator and the current collector). However, in this work the tensile response of active materials after cracking is described using material models for perfect plasticity. Since we do not implement failure/damage

material models for the electrodes, the numerically correlated tensile failure strain value for separator layer serves as an effective failure strain that compensates for the effects of failure events (e.g. electrode cracking) that precede the tensile failure of the separator.

The failure shape of the separator layer is also shown in Fig. 4(a). The crack initiated exactly the center of the structure ($x=y=0$, Fig.2 (b)) and propagated along the y -direction (machine direction). The cracking behavior is consistent with the characterized fracture image using X-ray CT scanning, which is likely due to the anisotropic feature of separator and the in-plane aspect ratio (length/width). The successful prediction of the cracking behavior further elaborates the significance of the presented single-RS model.

Figure 4(b) presents a comparison of the numerical and experimental results for indentation tests using punches of three different diameters. The single-RS model predicts well the force-strain responses under all three indentation conditions, showing the suitability of the materials models presented here in capturing the mechanical response of the pouch cell components, and the viability of using the single-RS model to predict the global mechanical response of the full pouch-cell. The latter observation is important when scaling these models to simulate the response of multi-cell modules or battery packs. The single-RS model is capable of predicting the onset of failure within the pouch cell under indentation and enables a lumped representation of the cell, with the ability to incorporate the mechanical properties of the individual cell components.

We note that the onset of the cell fracture under different indentation conditions are predicted through parametric studies of tensile failure strain for the separator layer, shown in Fig. 4(a). The parametric study results in different tensile failure strain values for the three indentation conditions, which are 0.29 for the small punch, 0.17 for the

medium punch and 0.15 for the large punch. This is because the tensile strain of the separator is related to the indenter diameter. A smaller indenter produces a sharp deformation and results in a relatively higher maximum tensile strain for the same indentation depth.

4.2 Simultaneously coupled mechanical-electrical-thermal simulation

In the previous section, the single-RS model presented was correlated with experimental results to predict the mechanical response and onset of structure fracture. The correlated models are then applied to simulate simultaneously the mechanical-electrical-thermal responses of the battery cell during indentation tests, through incorporating the electrical-thermal model described in Section 2, Section 3.3 and 3.4.

4.2.1 Prediction of electrical short-circuit

One main focus of this work is to predict the onset of electrical short-circuit during a mechanical crush. For the simultaneous coupled mechanical-electrical-thermal model, the distance-based criterion is utilized for the electrical contact initiation. Figure 4(b) shows the overall displacement contour of the battery cell at the moment of fracture, from which we identified that the maximum through-thickness displacement of the battery cell (loading distance of indenter) is 2.758 mm, 3.198 mm and 3.517 mm for the three indentation conditions. To predict the electrical short-circuit, we assume the indenter stops moving once the structure fails, which means there will be no further deformation after the mechanical failure of battery cell. The critical distance d_c of electrical short-circuit of LS-DYNA model is taken as the minimum thickness of the separator at the instant of cell fracture (contour plots of Fig. 4(b)).

Table 3 summarizes the model parameters and results for the simultaneous simulation of three different indentation cases. Based on the electrical failure criteria, a current larger than 0.0074 A (0.01 C) will be sufficient to create a short-circuit in the cell. The battery cell is considered electrically failed based on the detected current value at the moment of cell fracture. In Table 3, the short-circuit resistance R_s is calculated using the Holm's formula [28]:

$$R_s = \frac{1}{2\kappa_s a} \quad (14)$$

where a is the radius of electrical contact surface assuming that the contact surface is close to that of a circle: contact area equals πa^2 . And the contact area is calculated as integral of surface areas for separator elements with thickness lower than d_c . The data of electrical contact resistance is useful when correlating the experimental abuse test with theoretical solutions. We note that this quantity is not a necessary component for the presented coupled model. In Table 3, we find that the short-circuit area is much smaller than our previous work using sequential method [17], where the deformed geometry for short-circuit calculation has electrical contact area more than 2.775 mm^2 . This result highlights the advantage of this simultaneous coupled modeling approach in capturing the onset of electrical short-circuit and providing more detailed insights on the abuse tolerance of the battery cell.

Figure 5 shows the evolution of current across the electrical contact area for the three different indentation tests. All three cases show the same electrical behavior during the test: there is a small increase in the current before the onset of short-circuit, due to the thickness decreasing induced decrease of electrical resistance; a sharp increase in current is detected at the moment of failure due to the initiation of short-circuit, which

corresponds to the current density contour plot for the peak point (cell fracture and electrical failure). It is noticed that the maximum concentration of the current density occurs in the anode active layer due to its relatively higher conductivity than the cathode active material.

Comparing the three different indentation tests, we found that there is an increase of short-circuit area with the increase of indenter size which is consistent with the mechanical deformation distribution (Fig. 4(b)) and illustrated in the current density contour plots (Fig. 5) where the current density concentration area is larger for the indentation test with larger indenter. As discussed in the previous work [17], the electrical contact area has a significant impact on the short-circuit behavior. The current at the moment of short will be larger, due to the relatively lower short resistance when there is a larger electrical contact area. This will then result in a faster voltage drop and a lower local maximum temperature. We note that the short-circuit behavior depends also on the electrical conductivities of the materials in contact.

4.2.2 Prediction of thermal ramp after short-circuit

Understanding the voltage evolution behavior after the short circuit is of great significance, both for designing a safer battery, as well as for design of post-event containment measures. As demonstrated in previous experimental work [4], there is little change to the cell voltage before short-circuit. With the initiation of electrical contact, the voltage and resistance of the cell structure drops to very small values. Using the same methodology described in [17], we obtained the evolution of voltage after the short-circuit as shown in Fig. 6 (a). In Figs 6-7, the time $t=0.01$ second corresponds to the instant the short-circuit occurs or mechanical fracture. While in experiments [8], an

immediate drop in the cell voltage was observed for the three indentation tests, the numerical simulations predict a gradual decrease of voltage. This result provides some additional insights on the interaction between the electrical and thermal behavior following short-circuit and is especially useful in explaining the temperature ramp after short-circuit. For the same cathode-anode short, as expected, the simulated voltage drop for the large punch indentation test (largest electrical contact area) is faster than the other two tests. This result, when extrapolated, is useful in explaining why short-circuits involving very small contact areas do not result in thermal runaway. The voltage drop is so slow that any heat generated from such shorts is dissipated before sufficient temperature rise can result in a runaway. On the other hand, when the contact area is exceedingly large, the energy content of the small format cell is released within milliseconds before the current density can rise to sufficiently large values to generate any heat; whereas, a large-format cell will continue to have sufficient energy available across the same time-scale, and will generate sufficient heat to result in the follow-on reactions.

The voltage drop is incorporated into the simultaneous model, which is then used to predict the temperature response during the whole period before and after short-circuit. The temperature at the cell surface was calculated at: the farthest point ($x = -29.75$ mm, $y = -17$ mm of the top surface) from the short location, and the results are shown in Fig. 6(b). As observed from Fig. 6(b), the temperature increase before the short is negligible (less than 0.1 K). Temperature spikes are observed upon incidence of short-circuit. The surface temperature of the cell increases gradually by about 9 K, 42K and 60 K for the small punch test, medium punch test and large punch test, respectively, and then starts

dropping at a much lower rate due to the convection between the surrounding air and the cell. A larger punch produces a relatively higher temperature due its higher current which produces more Joule heating energy. Figure 7(b) shows the histories of Joule heat per volume for the three indentation tests after the occurrence of short-circuit. As from Fig. 7(b), Joule heating for the large-punch indentation test is about six times of that for the small-punch indentation test. Also due to the larger contact area, the Joule heating energy increases faster and flattens out earlier.

The predicted temperature ramp is similar to the experimentally observed results reported by Sahraei et al. [8]. The change in the maximum surface temperature also matches the experimental results [8] (10 K for the small punch test, 50 K for the medium punch and 40 K for the large punch) in a reasonable manner. In the experiments, the medium punch test produces a higher temperature rise than the large punch, which is likely due to the variation of contact area at the moment of short. At the moment of structural failure, the local deformation or damage event (e.g. cracking, fracture) is very rapid process, which will result in significantly different contact areas at the instant of short-circuit. For the instant of short-circuit, a large contact area will produce a higher short-circuit current, a faster voltage drop and a higher local temperature rise. Further discussion on this topic is presented in the next section.

The energy history can provide additional insights on the overall mechanism of failure during the whole test. Figure 7(a) compares the kinetic energy, mechanical strain energy and Joule heating energy histories for the small-punch indentation test. Once the mechanical fracture takes place, the indenter stops loading, so the mechanical strain energy and kinetic energy are constant beyond time zero. Before the occurrence of short-

circuit, we notice that the kinetic energy is much smaller than the strain energy indicating that this is a quasi-static test. On the other hand, the Joule heating energy is the lowest which explains why there is negligible temperature change before the onset of short-circuit. At the instant of short-circuit, a sharp increase of Joule heating energy is observed due to a sudden increase in the current. The total Joule heating energy exceeds the mechanical strain energy within several seconds and dominates the later stage.

We note that in this work, we do not take into account the effect of chemical or electrochemical reactions that follow the initiation of short-circuit event. Since the initial State of Charge (SOC) of the cells reported in this study was 10%, no extreme rise in temperature was observed in our calculation results, nor during the experiments reported in [8]. Under these circumstances, the rate of heat dissipation is faster than the heat generation due to Joule heating. So the temperature spike is not likely to cause any other failure events (e.g., melting of cell components). With the presence of follow-on reactions (e.g., in a fully charged cell), the heat generation will be much more significant and result likely in thermal runaway. The modeling results reported here predict the conditions leading to the onset of failure; these results serve as input feeding into the electrochemical models for the predicting the runaway response including the abuse reactions.

4.3 Numerical studies of interaction between mechanical failure and short-circuit behavior

As discussed in the previous section, the short-circuit behavior varies significantly under different test conditions. To further investigate the interaction of mechanical failure and short-circuit behavior, numerical studies are conducted assuming three different

loading conditions for the small punch indentation test. Case-1: Stop loading after structure fracture; Case-2: Continue loading after the structure fracture; Case-3: Unload the indenter after fracture of the structure.

Figure 8 (a) plots the displacement profile of the indenter for the three different loading cases. Assuming a constant voltage applied between the top and bottom surface, one can then capture the evolution of current under different loading conditions. Figure 8(b) compares the logarithm of the current history for these three loading conditions. As expected, the current is a constant under loading condition corresponding to Case-1 and keeps increasing under Case-2 due to increasing electrical-contact area. It is noticed that within a very short period of 0.0002 second, corresponding to 0.06 mm in displacement, the current increases from 0.053 A to 1.055 A, which is about 20 times larger than that of Case-1. This small displacement may not affect much the mechanical test results, but causes a significantly different post-short electrical behavior. So it is expected that during a realistic test, the electrical-thermal behavior varies a lot even for the same pre-defined test conditions.

During Case-3, the current decreases back after the initiation of short-circuit. As we know the mechanical deformation of a deformed solid includes two parts: elastic strain and plastic strain, of which the elastic strain will be reset to zero when external loading condition is removed. So for the indentation test we are studying, once the indenter is removed, there will be a rebounding of the cell thickness, especially for the porous layers (active materials and separator) where large elastic strain presents. Figure 8(c) plots the minimum thickness history of the separator layer, as we can see at the moment of short-circuit, the thickness is slightly lower than the electrical failure criteria

and then the thickness increase immediately to about 0.09 mm with the removal of indenter. The numerical results of these three different loading conditions suggest that the short-circuit behavior suffers significant variation changes in the experimental conditions. It highlights the necessity to develop more controllable abuse test methods to further understand the failure mechanisms. For example, to study the short-circuit behavior under a constant electrical contact area, the indenter should be held in place, without moving once mechanical failure is achieved.

The understanding of the effect of rebounding behavior is important; as it explains the possibility that sometimes no short-circuit is observed even though mechanical failure is observed. Our most recent experiment work reveals that during an impact test, the voltage of the LIB cell shows an immediate drop and then returns back to a value slightly lower than initial voltage. After the impact test, the voltage remains constant for an hour indicating that no more short-circuit is present. The present numerical results successfully explain the possible mechanism associated with the mechanical-electrical interaction of LIB cell during different test conditions, and proves the capability of our models explaining high-speed impact test results.

Conclusions

In this work, we presented a simultaneous coupled mechanical-electrical-thermal modeling approach for predicting mechanical-abuse-induced short circuit behavior of lithium ion cells under different indentation test conditions. The representative sandwich model was modified and improved to enhance its accuracy in predicting short-circuit location and thermal spike behavior, as well as, be compatible with the mechanical-electrical-thermal solvers.

The mechanical model successfully predicts the onset of structure fracture and captures the local cracking behavior of LIB under three different indentation conditions. The simultaneous coupled model predicts accurately the initiation of short circuit due to structural fracture and post-short thermal and electric responses through using a distance based electrical contact criteria. It is identified that the maximum current density located in the anode active material and a larger indenter size creates a larger electrical contact area.

Numerical studies of three different test conditions after onset of short circuit reveal that the electrical current changes significantly due to the movement profile of indenter. It is observed that the short-circuit may be eliminated if the indenter is removed after the occurring of short circuit, due to the rebounding of separator thickness which breaks the electrical contact between anode active and cathode active layers.

The simultaneously coupled modeling technique is useful in studying the safety behavior of lithium-ion cells under mechanical abuse, especially in studying the interaction of mechanical failure and short-circuit behavior. It is a helpful tool for evaluating the safety performance of a battery cell and designing more efficient and safer battery structures. Future work should focus on investigating more complicated crush conditions (multi-axial crush, impact and battery module crush etc.).

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Figure Captions:

Figure 1: Interactions between mechanical, electromagnetic and thermal solvers for the simultaneously coupled modeling approach: in this study, a two-way coupling methodology is established that resolves the deformed geometry, electrical and thermal responses simultaneously. The Joule heating generated from the electrical simulations and mechanical plastic work both serve as source terms for the thermal simulations. The electrical and mechanical simulations in turn utilize temperature as an input parameter from the thermal simulations. And the mechanical solver communicates displacement information to the electrical simulation producing continuously changing electrical resistances while the electrical solver communicates the Lorentz force to the mechanical simulations as an extra force.

Figure 2: (a) Cross-sectional view of a pouch cell and schematic of a representative sandwich (RS): the pouch cell is represented by a single RS which explicitly represents the thickness proportions of each individual component; (b) schematic and dimensions of the single RS indentation model: a quarter of the actual domain is utilized in the finite element model based on symmetry; (c) schematic of electrical connections for the single RS model and full pouch cell model: in this work, scaled electrical conductivity properties are utilized for each individual component of the single RS model to theoretically match the overall Joule heat.

Figure 3: Constitutive properties for the active materials and separator: (a) tensile responses for the anode and cathode active materials: elastic-perfectly-plastic stress-strain curves are calculated based on experimental measurements from [13]; (b) tensile stress-strain curves for the separator in machine direction and transverse direction [9]: the

separator has a considerably higher elastic modulus, yield stress and tangent modulus in machine direction than those in the transverse direction; (c) compressive stress-strain curves for the active material and separators, obtained using an analytical method described in [17].

Figure 4: (a) Correlation of numerically predicted and experimentally measured force-strain curves for the small punch indentation test, and numerically predicted deformation of separator and active materials at the instant of cell fracture. A failure strain of 0.29 was found to best match the experimental data from [8]. The crack in the separator layer propagates along the y-direction (see Fig. 2(b)) consistent with experimental observation; (b) comparison of numerically predicted and experimentally measured force-strain responses for three different indentation tests, and numerically predicted deformation of battery cell at the instant of cell fracture. With an increase of indenter diameter, the maximum indentation depth at the moment of fracture increases indicating that the larger punch test results in a later fail of the cell.

Figure 5: Evolution of average current (A) across the active material before and after short circuit at the electrical contact area, and isotropic-view of the current density (A/m^2) distribution in the battery cell for the three different indentation tests: (a) small punch, (b) medium punch and (c) large punch. The maximum current density is identified to be located in the anode active layer. The short circuit current increases with the increase of indenter diameter due to the increase in the electrical contact area.

Figure 6: Electrical-thermal responses before and after short circuit for three different indentation tests: (a) voltage evolution; (b) change in temperature history. For the same battery cell, with the increase of electrical contact area, the voltage drop has increasingly

larger time constants, and consequentially results in a sharper temperature ramp. The maximum changes in surface temperature for these three indentation tests match the experimental results in a reasonable manner.

Figure 7: (a) Comparison of energy histories before and after short-circuit for the small punch indentation test: the mechanical strain energy dominates the stage before short while the Joule heating energy takes over after occurrence of the short-circuit. The relatively smaller magnitude of kinetic energy compared with strain energy indicates that we are studying a quasi-static test; (b) comparison of history of Joule heat per volume for the three different indentation tests: the Joule heating for the large-punch indentation test increases faster and flattens out earlier due to its larger electrical contact area.

Figure 8: (a) Indenter displacement profile for three different loading conditions; (b) histories of the average current across the active material at the short-circuit location for the three different loading conditions of (a): the current history after the occurring of short varies significantly under these three different loading conditions. Further loading (Case-2) produces a continuously sharp increase in the current over a very short period, while removing the indenter results in rebounding of the separator thickness and decreasing of the current; (c) evolution of minimum separator thickness during the indentation test under loading condition Case-3: the separator thickness history demonstrates the presence of thickness rebounding and explains the presence of voltage rebounding behavior during the impact tests.

Table 1: Mechanical parameters for current collectors of a Lithium-ion cell [23]

	Young's Modulus (GPa)	Poisson's Ratio	Yield Stress (MPa)	Tangent Modulus (MPa)
Cathode Collector	70	0.36	180	700
Anode Collector	110	0.35	210	1100

Table 2: Electrical-thermal parameters for each component of the Lithium-ion battery [24].

	Separator	Cathode Active	Cathode Collector	Anode Active	Anode Collector
Electrical conductivity (S/m)	1.0E-5	38	3.8E+7	100	6.0E+7
Thermal conductivity (W/m•K)	1	5	200	5	380
Heat capacity (J/Kg•K)	700	700	870	700	381

Table 3: Numerical parameters and modeling results of LIB cell under different indentation tests

Test cases	Critical displacement of cell (mm)	Critical distance for electrical short-circuit (mm)	Short-circuit area (mm ²)	Short-circuit current (A)	Short-circuit resistance (Ω)
Small punch	2.758	0.0390	0.352	0.053	21.64
Medium punch	3.198	0.0368	0.824	0.142	14.16
Large punch	3.517	0.0350	1.300	0.258	10.50

Figure 1

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Figure 2

Figure 3

Figure 4

(a)

(b)

(c)

Figure 5

(a)

(b)

Figure 6

(a)

(b)

Figure 7

(a)

(b)

(c)

Figure 8