Coupled Mechanical-Electrochemical-Thermal Analysis of Failure Propagation in Lithium-ion Batteries

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Outline

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  o Progressive failure modeling of single battery cell
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• Quasi-static and Impact Failure of Lithium-Ion Batteries
• A Novel Multiscale Coupled Mechanical-Electrochemical-Thermal Modeling Framework
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Introduction

❖ Safety of Lithium-Ion Batteries under Mechanical Abuse

• One emerging concern for electrical vehicle industry is the safety performance of batteries, especially under mechanical failure; significant investment is being made to develop new materials, fine tune existing ones, and improve cell and pack designs to increase performance, reduce cost, and make batteries safer.


Introduction

**Challenges**

- Critical component or property that controls the structural strength or failure of separator.
  - complicated constitutive properties of cell components
  - varies under different loading conditions
  - internal damage status or residual stress
- Design concept
  - robust external protection or tolerate cell deformation
  - effect of cell deformation on battery performance

**Modeling, simulation, and design tools** can play an important role
- Provide insight on how to address issues,
- Reduce the number of build-test-break prototypes, and
- Accelerate the development cycle for new products.
Introduction

- Short Circuit
- Failure of Separator
- Damage of Cell Components
- Smoke and Fire
- Current Flow and Thermal Runaway

Risk Factor

Mechanical Behavior

Electrochemical-thermal Behavior

Coupled analysis for safer battery

Deformation of Batteries

Time Scale
Introduction

**Approach**
- Damage initiation and failure propagation in the cell component level;
- A single representative sandwich (RS, 7 layers) model to represent the periodically stacked multilayer (100+ layers) structure;
- Simultaneously coupled multiscale mechanical-electrochemical-thermal modeling;
- Investigated the interaction of mechanical damage on short-circuit behavior.

Design better Batteries from the best available cells

Finite element models for mechanical crush simulation

Displacement under Crush

Current density under short-circuit

Pack Response

Single cell crush

Impact of a 20 cells battery module
Coupled Mechanical-Electrical-Thermal Modeling

- Constitutive Properties - Tensile

Electrodes:
- Porous active material layer
- Perfect bonding between active layers and current collector
- Low failure strain (less than 10%)
- Failure initiates in current collector

Separator:
- Multilayer polymer fabrics
- Excellent flexibility
Coupled Mechanical-Electrical-Thermal Modeling

- Constitutive Properties - Compression
  - Compression of the thin porous layers show multi-stage deformation process.

![Compression curves of cathode](image)

- Linear Stage
- Stiffening Stage
- Yielding

Strain

Stress (MPa)
Coupled Mechanical-Electrical-Thermal Modeling

- **Representative sandwich model**

- **Coupled modeling**

**Electrical Solver**

\[ j = -\kappa_s \nabla \phi \]

\[ E = -\nabla \phi \]

**Joule Heating**

\[ E_{\text{joule}} = \frac{j \cdot j}{\kappa_s} \]

\[ Q = \frac{E_{\text{joule}}}{V} \]

**Thermal Solver**

\[ \rho c \frac{\partial T'}{\partial t} = \frac{\partial}{\partial x_i} \left[ K_{ij} \frac{\partial T'}{\partial x_j} \right] + Q \]

*\(K_s\) could be a function of temperature*

The contact area (eroded volume of separator layer) has a strong impact on the consequential electrical-thermal responses.
Coupled Mechanical-Electrical-Thermal Modeling

- **Hemisphere indentation**

  - Different separator cracking pattern under different loading conditions;
  - The main failure behavior includes: electrode tensile cracking, electrode compressive failure, interface shear failure and separator tensile failure et al.

- **Cylindrical indentation**

  - Different separator cracking pattern under different loading conditions;
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Zhang et al. J. Power Source, 2015
Coupled Mechanical-Electrical-Thermal Modeling

**Electrical-thermal Responses**

Current density across the active material before and after a short-circuit at different levels of total strain

- The established approach captures the evolution of current density and temperature ramp.
- It was utilized to study the interaction between mechanical failure and short circuit behavior to identify the origin of experimental variation.

Zhang et al. J. Power Source, 2015
Mechanical-electrical failure of a battery module

**Impact simulation**

1. Simulate the impact response of a battery package using simultaneous electrical-mechanical-thermal model;
2. Predict the failure of battery cell and temperature distribution;
3. Evaluate the safety of battery package.

- Mass of impactor 32 Kg;
- Impact speed 6.26 m/s to represent the experimental condition

Front and back panel

Middle frame

Battery cell X 20

Total number of elements: 0.5 million

Computational time: 30 hours using 60 large memory CPUs
Similar peak loads applied to cell over different time scales produced different voltage responses:

- For static crush, instantaneously drop of voltage, significant reactions and thermal runaway were observed; (hard short)
- For impact, the pouch remained intact, moderate temperature rise. (soft short)

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**Peak Load (kN) | Peak Temperature (°C) | Cell Duration**
---|---|---
Static Crush | 77.3±3.4 | 300~350 | 5.1 ±0.2s
Impact | 79.3±1.1 | 25~70 | hours

Santhanagopalan et al. AMR, 2015
Limitations of Existing Approach

- Progressive failure process across the layered structure;
- Prediction of short circuit propagation across the cell;
- Simultaneously coupled modeling of mechanical abuse induced short circuit.

Macro-scale 3D homogenized mechanical-thermal model

Meso-scale quasi-3D mechanical-thermal model

Pseudo 2D electrochemical-thermal model

\[ \frac{d\bar{\epsilon}}{dt}, T \]

\[ \sigma, \sigma_i, \bar{\epsilon}, \varepsilon_i, T' \]

\[ R_{\text{short}}, K_s, dt', t', T \]

\[ T' \]
Mechanical-Electrochemical-Thermal Modeling

- **Single Element Benchmark Study**

- **Short Resistance** ($\Omega \cdot \text{m}^3$)
  
  Different types of shorts can be distinguished by the short area for the different failure modes of the separator layer, e.g., tensile failure or shear failure.

  \[
  R_{\text{short}} = A_{\text{short}} \sum \frac{1}{K_{s(i)}^2}
  \]

- **Temperature**

  Temperature is assumed to be uniform across each LSDYNA macro element. And the temperature rise is calculated based on the generation of joule heating energy and electrochemical reaction heats.
The effect of short resistance on the abuse responses

- With the decrease of short circuit resistance, the instantaneous increase of current and voltage drop increases, the discharging completes in a much quicker manner.
- The temperature profile is consistent with the voltage/current evolution profiles, a lower short-circuit resistance does not always produce a higher temperature: there are trade-offs between the cell’s energy content, how fast it can be dissipated as heat in the electrochemical models versus heat transfer rates away from the point of generation.
Summary

• We present experimental and modeling approach on the crashworthiness of battery structures from single cell to battery module;
• We investigated the variation of failure behavior of batteries under different loading conditions;
• We developed unique modeling approach and proposed new approach on the safety performance of battery under external mechanical abuse;
• Further efforts are necessary on modeling the progressive failure process in the component level and solid methodologies on coupling the mechanical failure with electrochemical-thermal behaviors
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