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WCCM XII & APCOM VI

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

Chao Zhang, Shriram Santhanagopalan and Ahmad Pesaran

National Renewable Energy Laboratory

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Outline

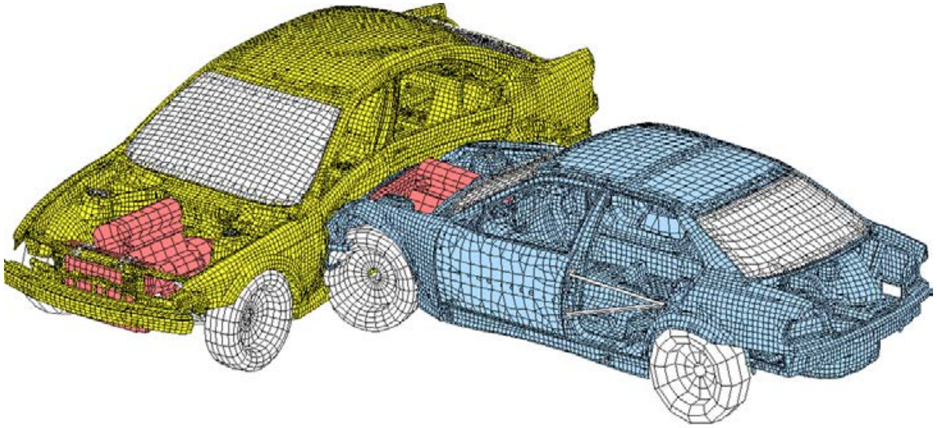
- Introduction
- Coupled Mechanical-Electrical-Thermal Modeling
  - o Constitutive properties of cell components
  - o Progressive failure modeling of single battery cell
  - o Mechanical-electrical failure of a battery module
- Quasi-static and Impact Failure of Lithium-Ion Batteries
- A Novel Multiscale Coupled Mechanical-Electrochemical-Thermal Modeling Framework
- Summary and Future Work

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.

http://www.rushlane.com/wp-content/uploads/2013/05/Crash-test-dummies-at-work-How-they-help-make-your-car-safer.jpg



http://i1-news.softpedia-static.com/images/news2/BMW-and-Audi-Are-Using-Linux-2.png

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

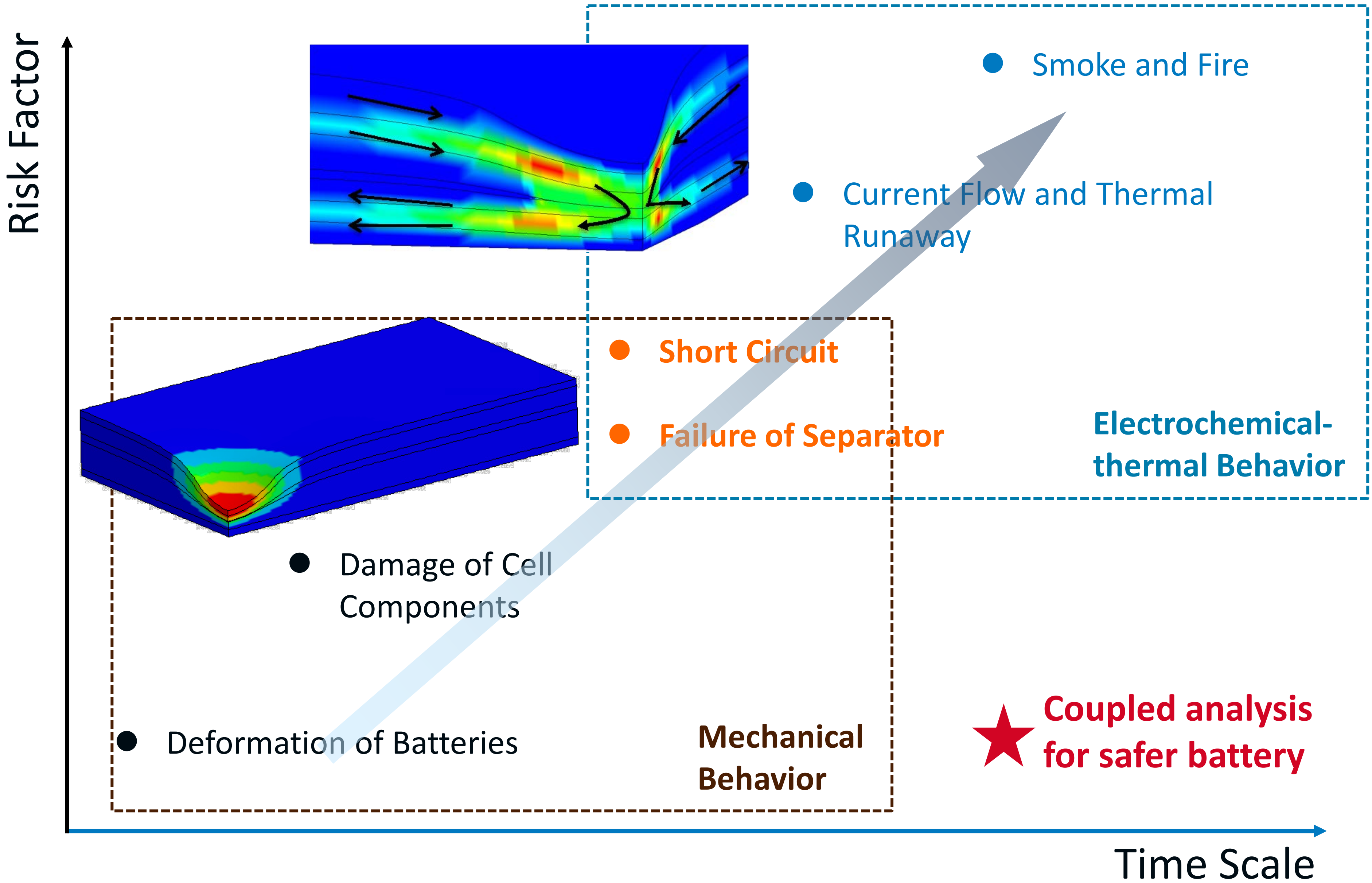
- Design concept

  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

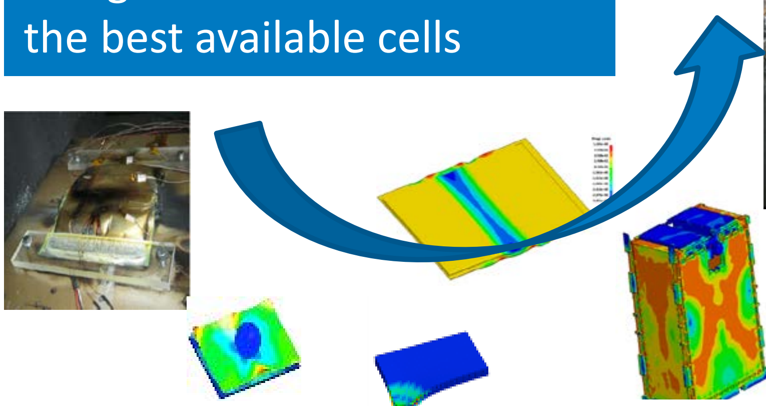


Introduction

❖ 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



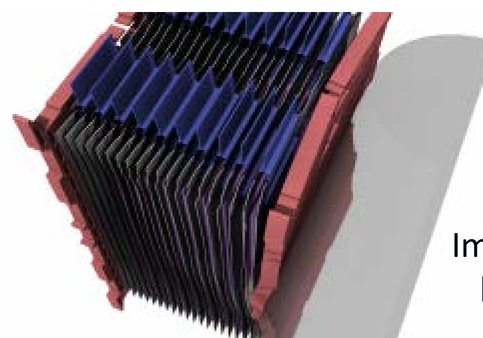
Displacement under Crush

Current density under short-circuit

Pack Response

Finite element models for mechanical crush simulation

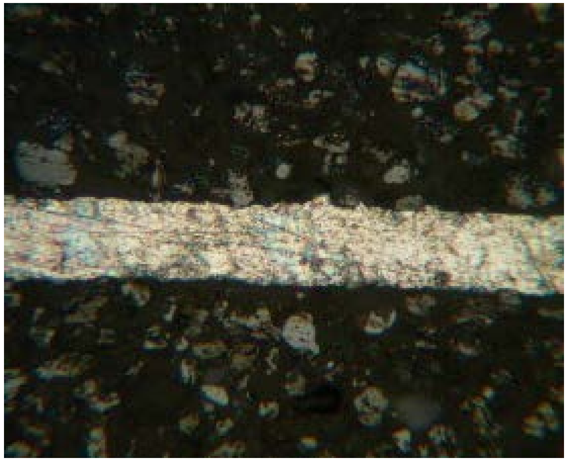
Single cell crush

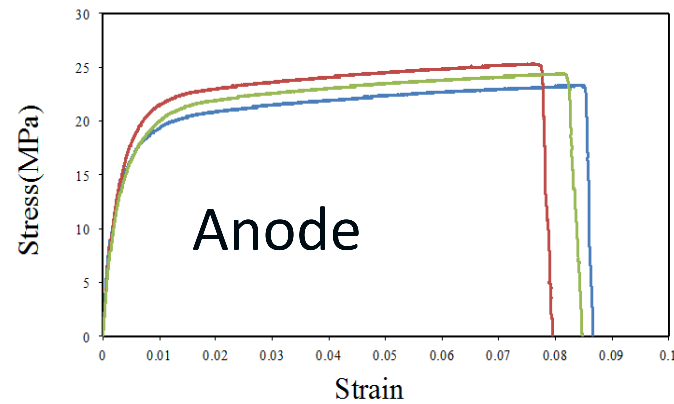


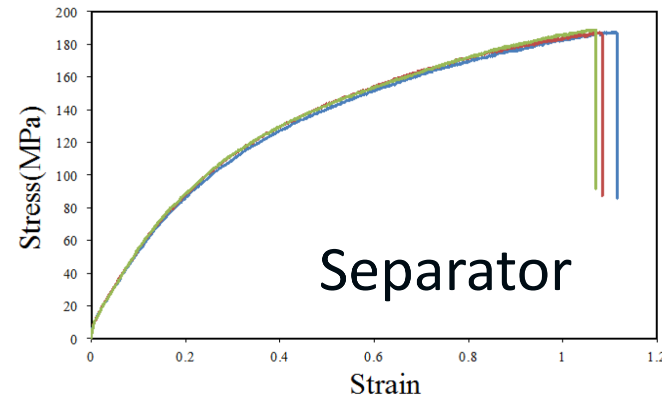
Impact of a 20 cells battery module

Coupled Mechanical-Electrical-Thermal Modeling

❖ Constitutive Properties - Tensile





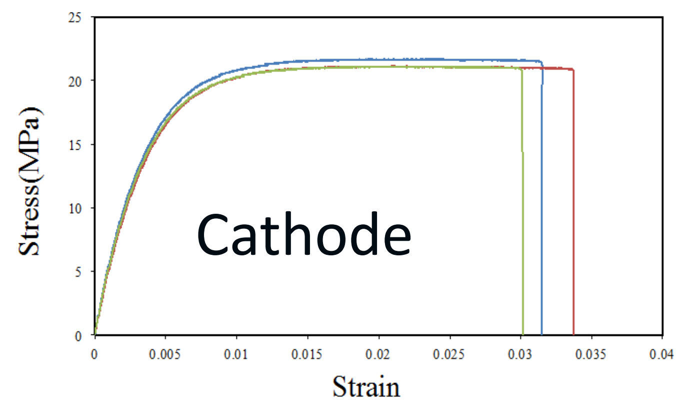


Electrodes:

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

Separator:

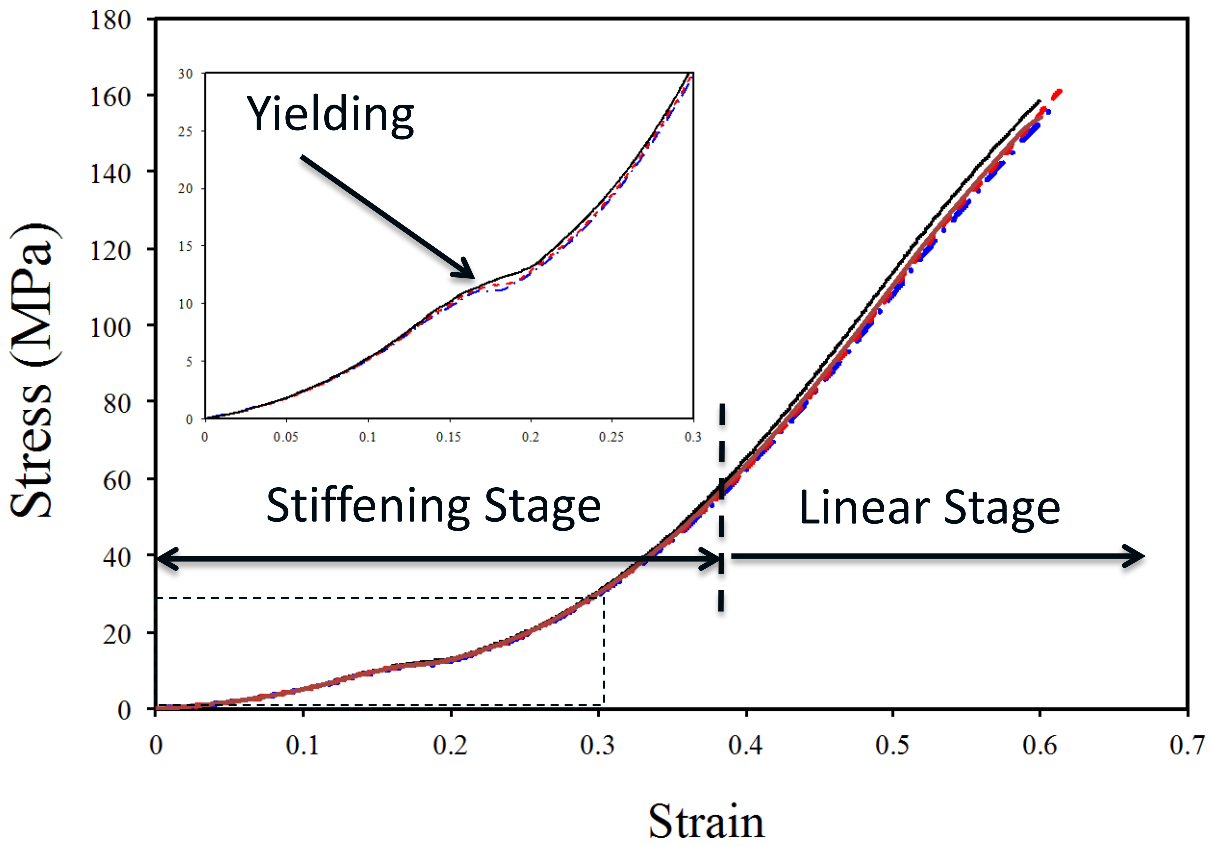
- Multilayer polymer fabrics
- Excellent flexibility



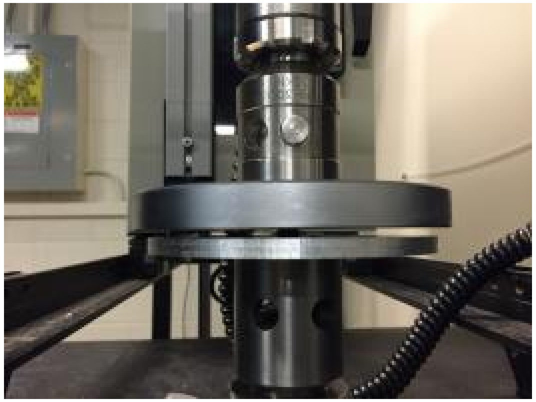
Coupled Mechanical-Electrical-Thermal Modeling

❖ Constitutive Properties - Compression

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

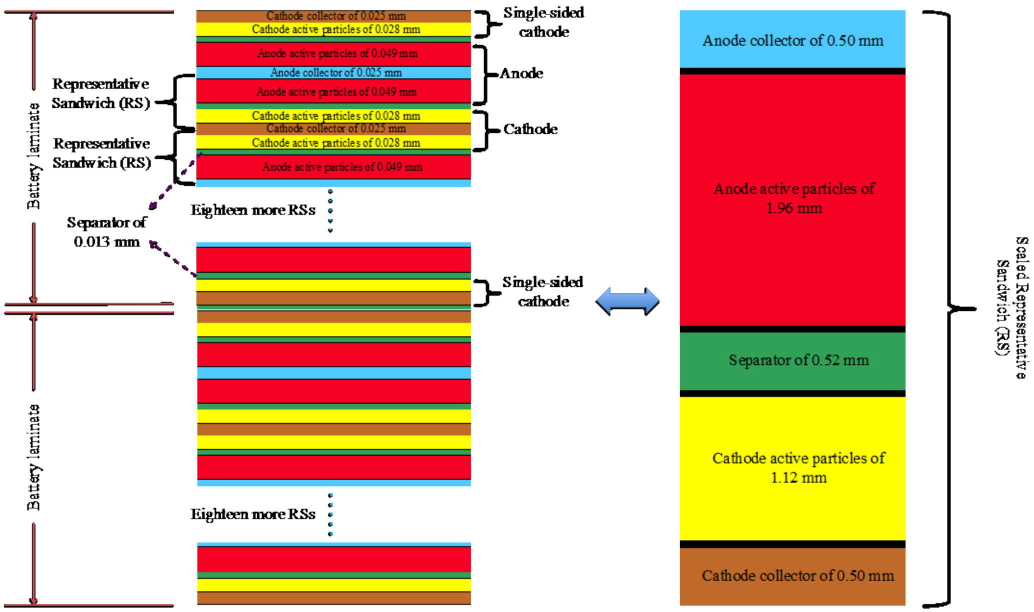


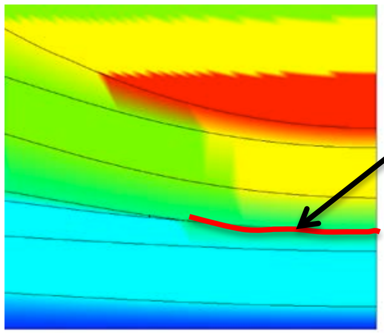
Compression curves of cathode



Coupled Mechanical-Electrical-Thermal Modeling

- Representative sandwich model





Separator fracture results in electrical contact between electrodes

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

- Coupled modeling

Electrical Solver

$$\vec{j} = -\kappa_s \vec{\nabla} \phi$$

$$\vec{E} = -\vec{\nabla} \phi$$

→

Joule Heating

$$E_{Joule} = \frac{\vec{j} \cdot \vec{j}}{\kappa_s}$$

$$Q = \frac{\dot{E}_{Joule}}{V}$$ →

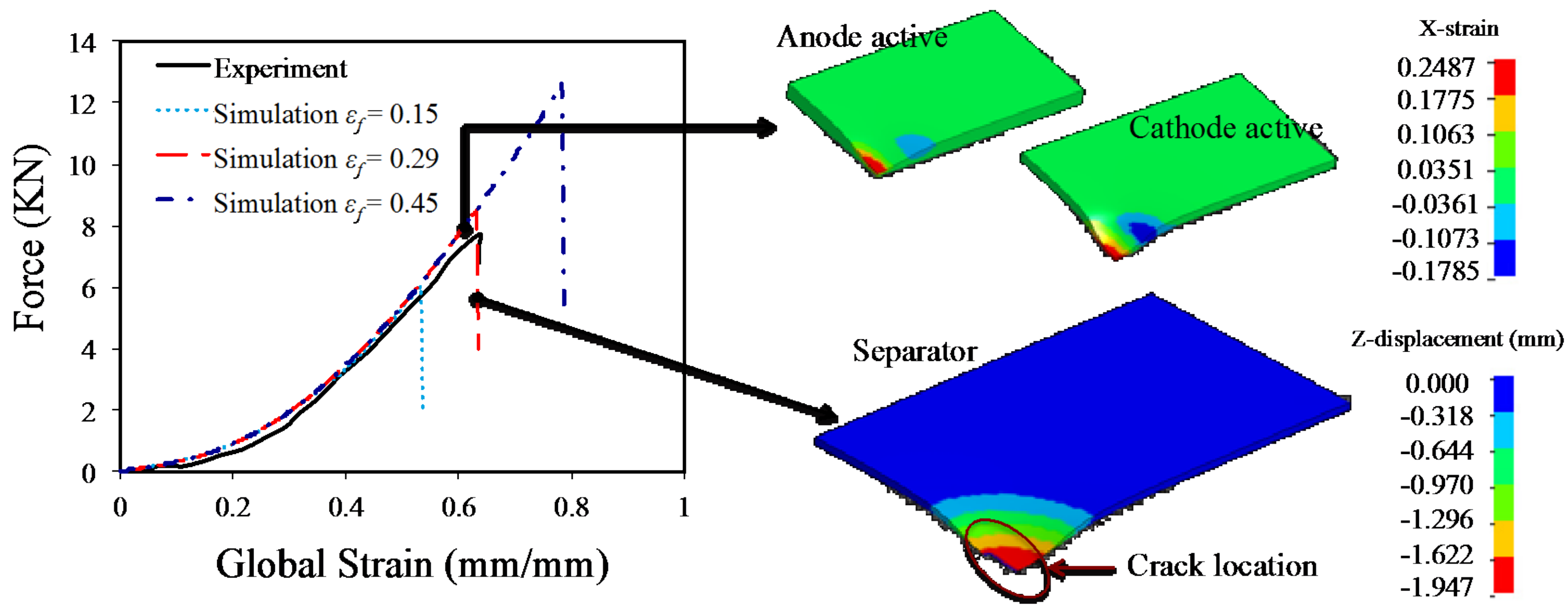
Thermal Solver

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}[K_{ij} \frac{\partial T}{\partial x_j}] + Q$$

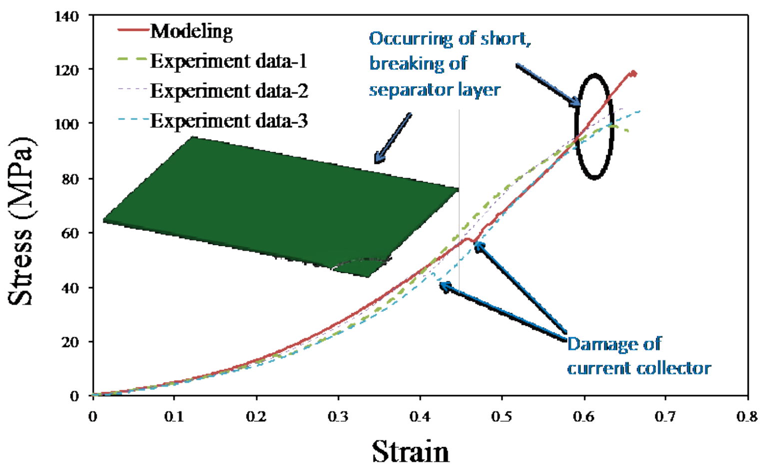
K_s could be a function of temperature

Coupled Mechanical-Electrical-Thermal Modeling

- Hemisphere indentation



- Cylindrical indentation

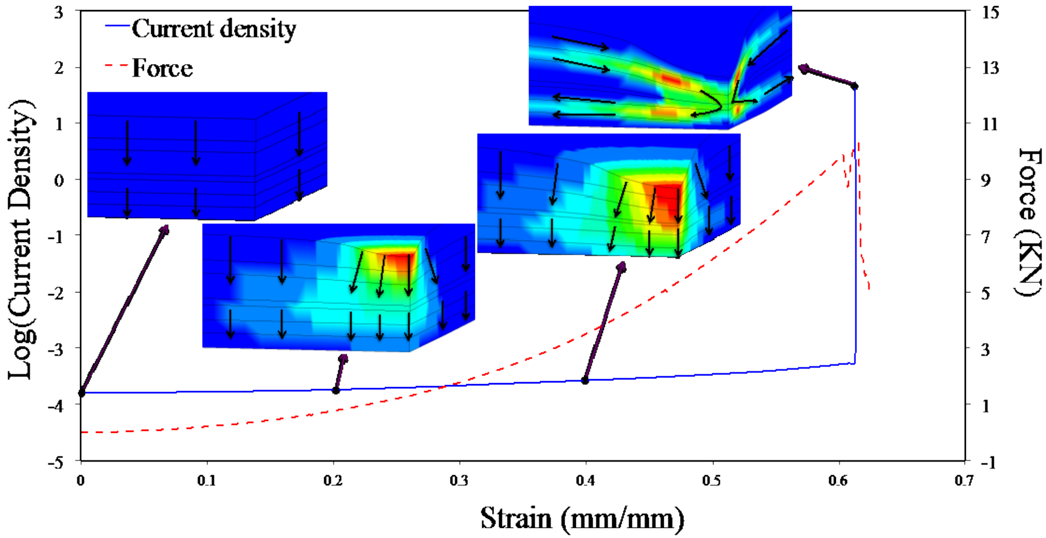


- Different separator cracking pattern under different loading conditions;
- The main failure behavior includes: electrode tensile cracking, electrode compressive failure, interface shear failure and separator tensile failure et al.

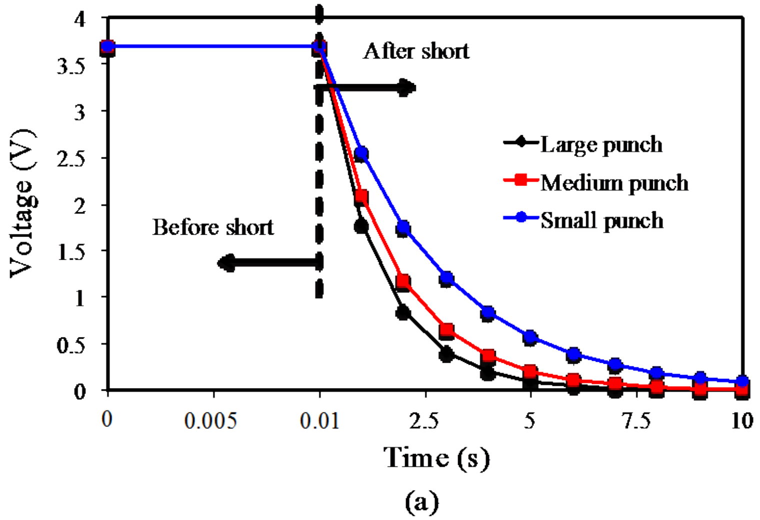
Zhang et al. J. Power Source, 2015

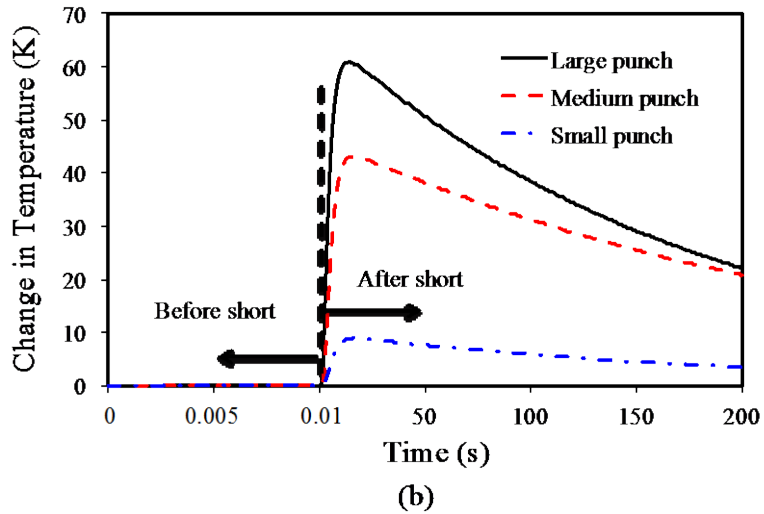
Coupled Mechanical-Electrical-Thermal Modeling

❖ Electrical-thermal Responses



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





Voltage drop and temperature increase following by a mechanical abuse induced short circuit

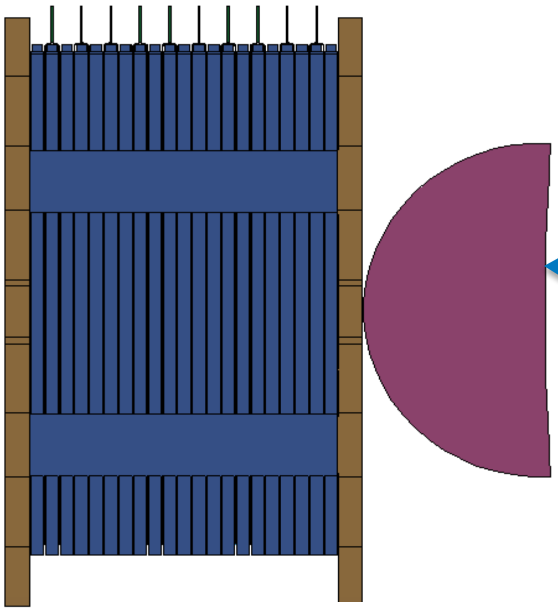
- The established approach captures the evolution of current density and temperature ramp.
- It was utilized to study the interaction between mechanical failure and short circuit behavior to identify the origin of experimental variation.

Zhang et al. J. Power Source, 2015

Mechanical-electrical failure of a battery module

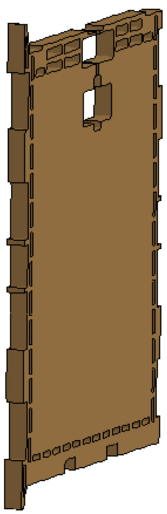
❖ Impact simulation

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.

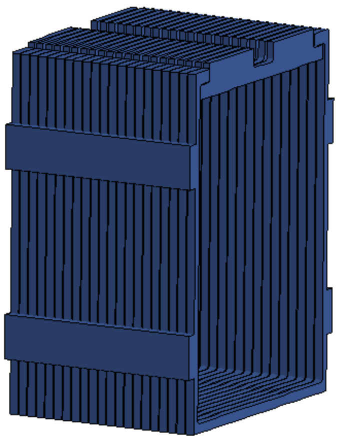


Mass of impactor 32 Kg;

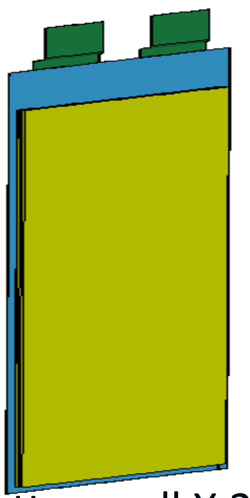
impact speed 6.26 m/s to represent the experimental condition



Front and back panel



Middle frame



battery cell X 20

Total number of elements: 0.5 million

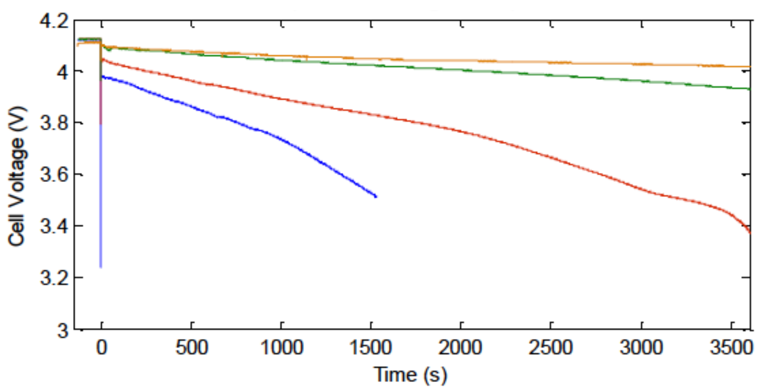
Computational time: 30 hours using 60 large memory CPUs

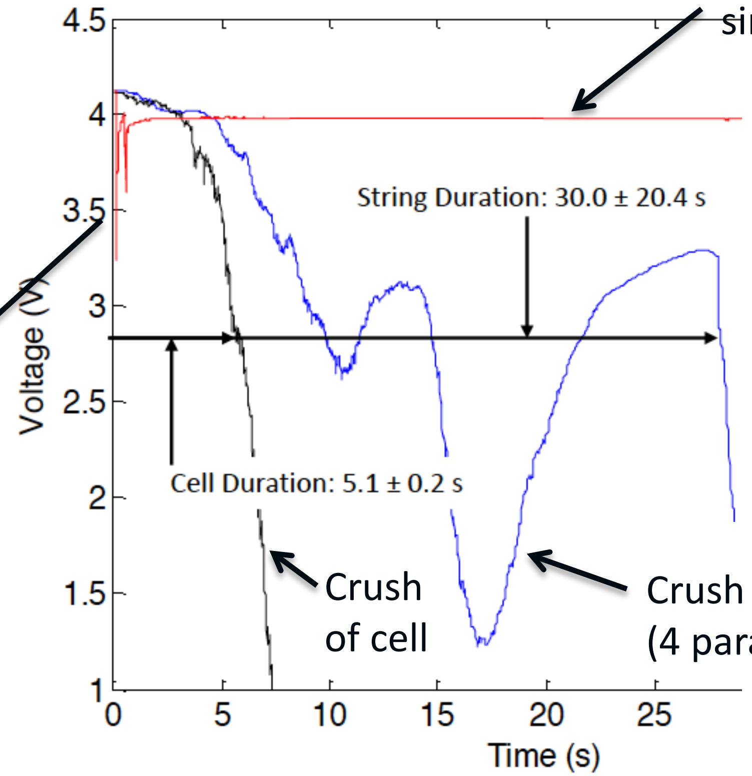
Quasi-static and Impact Failure of Lithium-Ion Batteries

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)

Complete Voltage Response for Cells after Impact





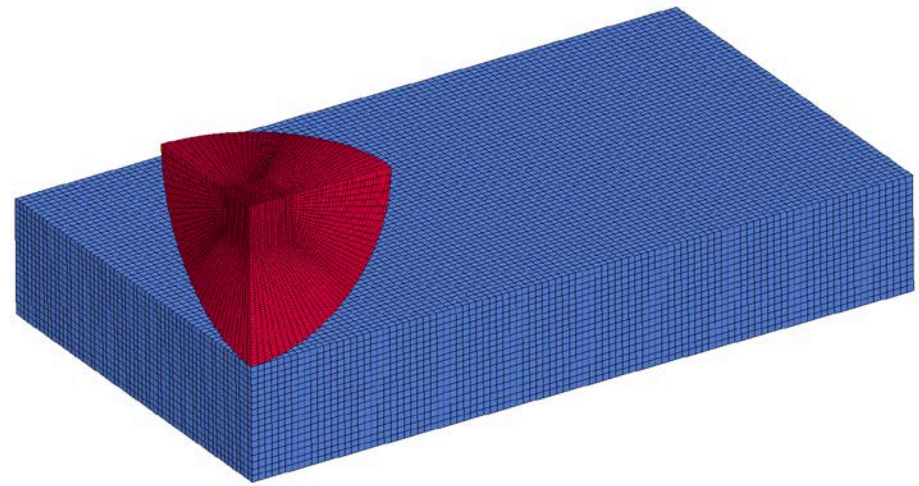
	Peak Load (kN)	Peak Temperature (°C)	Cell Duration
Static Crush	77.3±3.4	300~350	5.1 ±0.2s
Impact	79.3±1.1	25~70	hours

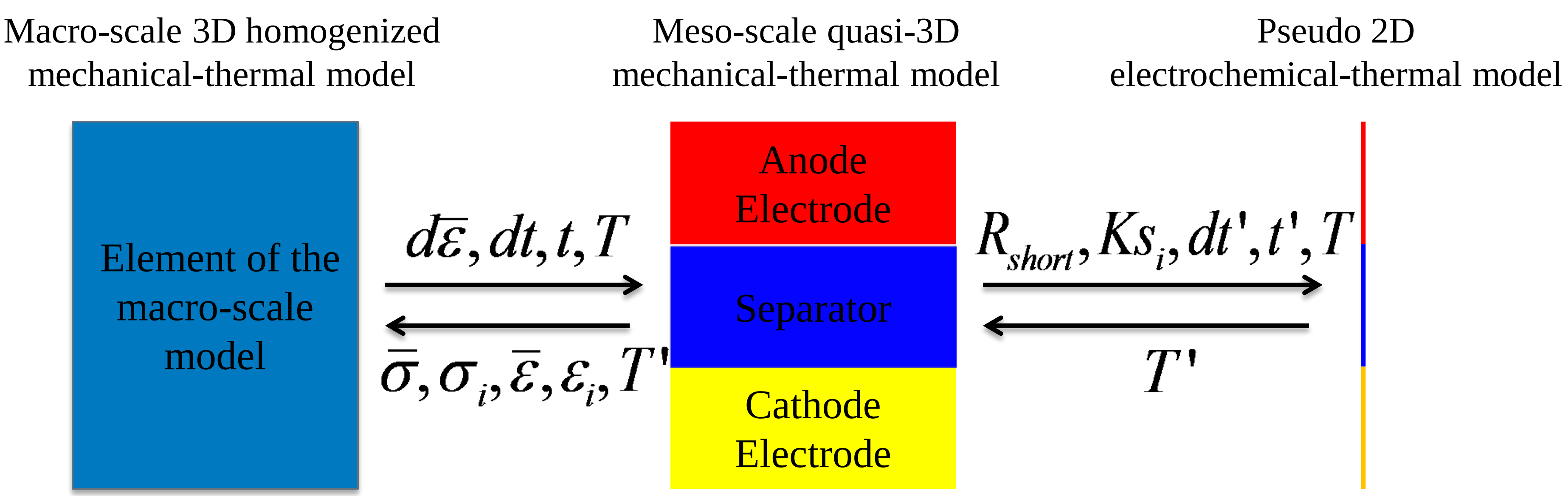
Santhanagopalan et al. AMR, 2015

Mechanical-Electrochemical-Thermal Modeling

❖ Limitations of Existing Approach

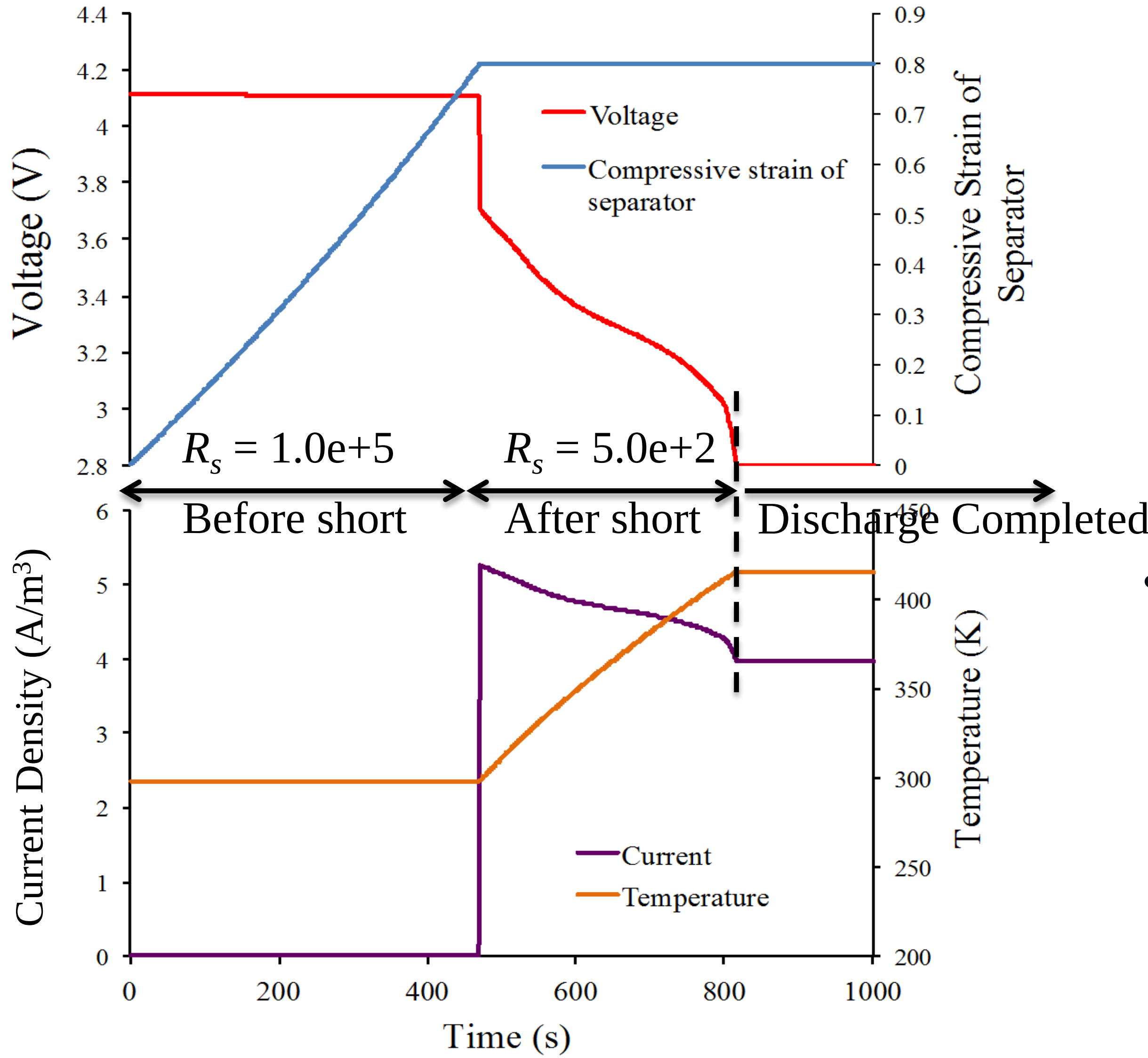
- Progressive failure process across the layered structure;
- Prediction of short circuit propagation across the cell;
- Simultaneously coupled modeling of mechanical abuse induced short circuit.





Mechanical-Electrochemical-Thermal Modeling

❖ Single Element Benchmark Study



- Short Resistance (Ω•m³)

Different type of shorts can be distinguished by the short area for the different failure modes of separator layer, e.g. tensile failure or shear failure.

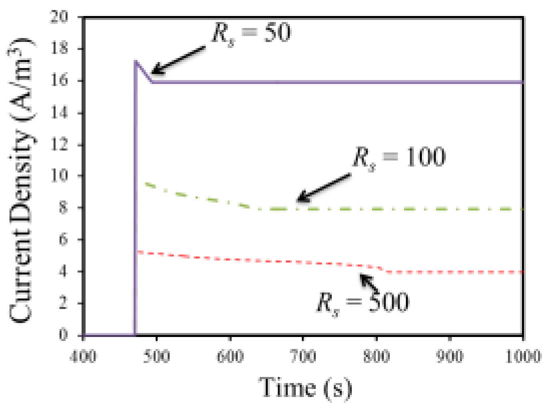
$$R_{short} = A_{short} \sum \frac{1}{\kappa_s^{(i)}}$$

- Temperature

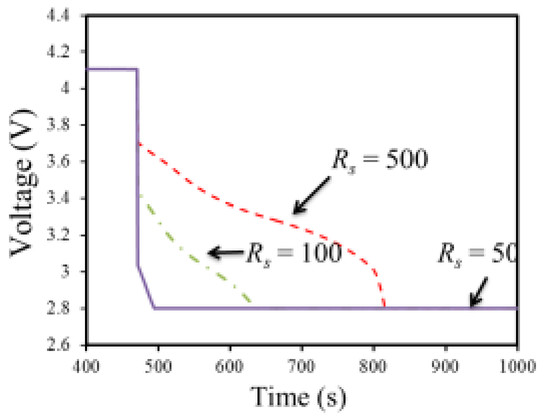
Temperature is assumed to be uniform across each LSDYNA macro element. And the temperature rise is calculated based on the generation of joule heating energy and electrochemical reaction heats.

Mechanical-Electrochemical-Thermal Modeling

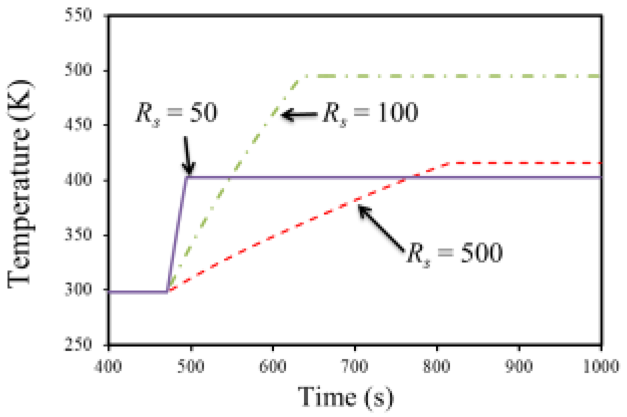
❖ The effect of short resistance on the abuse responses



Current Profile



Voltage Profile



Temperature Profile

- 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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