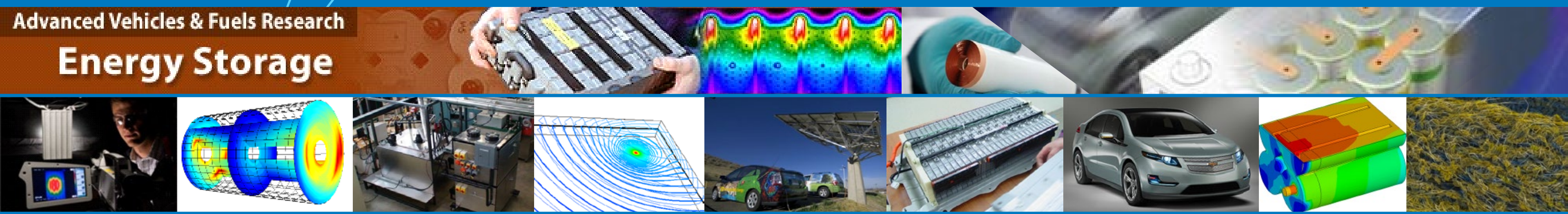
13 th US National Congress on
Computational Mechanics

Representative-Sandwich Model for Mechanical-Crush and Short-Circuit Simulation of Lithium-ion Batteries



Chao Zhang, Shriram Santhanagopalan, Michael A Sprague, Ahmad A Pesaran

National Renewable Energy Laboratory

July 28th, 2015

NREL/PR-2C00-64824

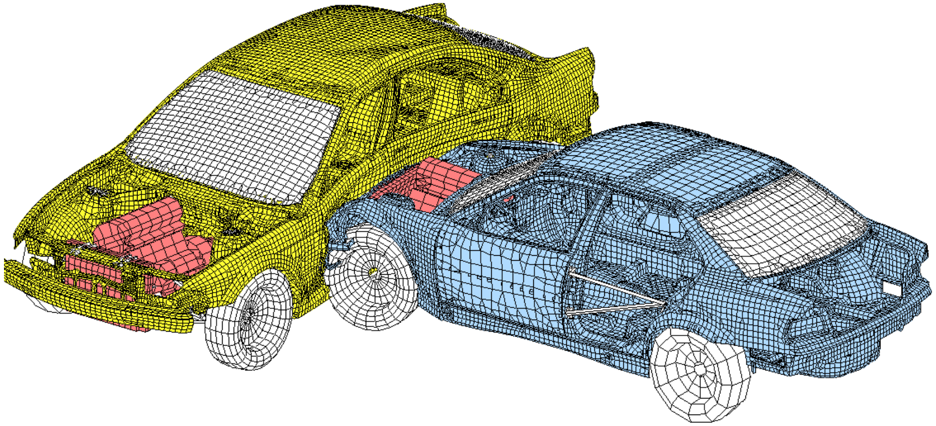
Outline

- Background
  - Mechanical abuse of batteries
  - Motivation
- Mechanical-electrical-thermal model
  - Representative-sandwich model
  - Constitutive models
  - Model validation
  - Coupled electrical-thermal behavior
  - From quasi-static test to impact test
- Summary and Future work

Background

- Battery performance, cost, and **safety** must be further improved for larger market share of HEVs/PEVs and penetration into grid
- 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**
- 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.

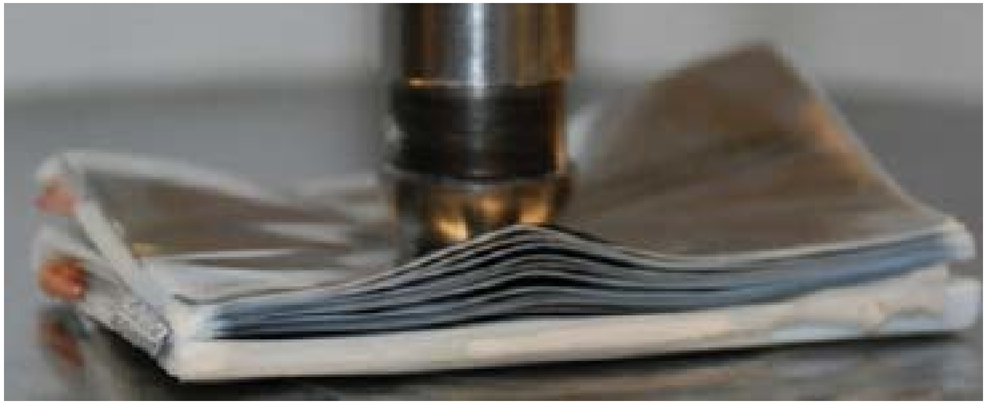
http://www.rushlane.com/wp-content/uploads/2013/05/Crash-test-dummies-at-work-How-they-help-make-your-car-safer.jpg



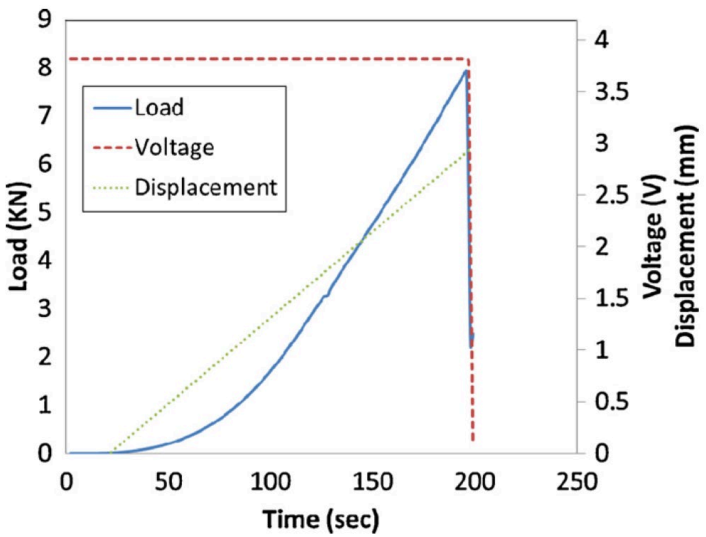
http://i1-news.softpedia-static.com/images/news2/BMW-and-Audi-Are-Using-Linux-2.png

Background: Mechanical Abuse of Batteries

❖ **Pouch cell indentation**

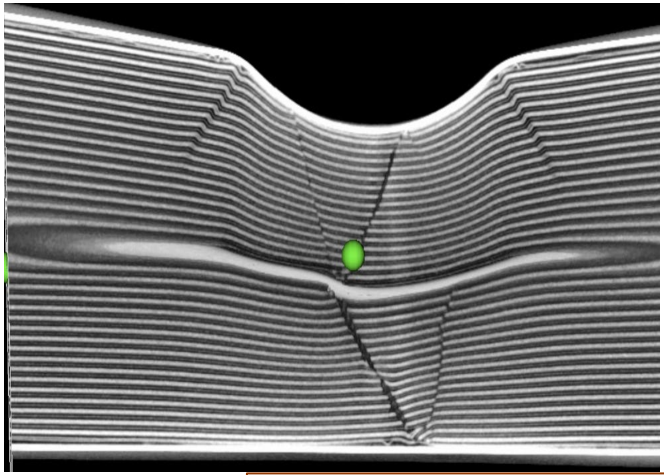


Sahraei et al., J Power Sources 2012



❖ **Cylindrical cell indentation** ❖ **Pouch cell bullet impact**

Origin of mechanical failure is within the active material;
The consequential short-circuit behavior depends on the crack orientation and deformed geometry of the fractured region



Pesaran et al., EVS28, 2015

Background: Failure Events

- Vehicle crash → battery crush → cell damaged zone → failure of a separator → electrodes contact →local short → current flow → heat generation → heat rejection not sufficient →*temperature* increase →*reaching above onset* temperature → spontaneous reactions → thermal runaway → smoke and fire

→: may lead to (depending on many factors)

- Simulating all physics and geometry at the same time is challenging and takes a lot of time; simplifications needed
- Our approach:
  - Decouple structure behavior from ECT interactions
  - First, model structural changes after crush,
  - Then, model the characteristics of damaged zone
  - Finally, use it for electrochemical and thermal modeling

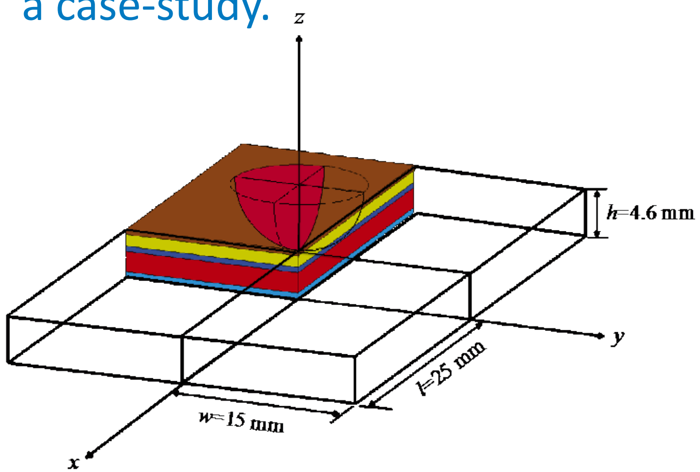
Motivation

Assuming that a short circuit initiates due to failure of separator and electric contact between positive (Cathode) active layer and negative (Anode) active layer:

- Predicting the local failure of separator
- Electrical-thermal analysis on the deformed finite element mesh
- Incorporating Electrical contact to predict crush-induced short circuit
- Predicting post-short thermal ramp behavior of the cell

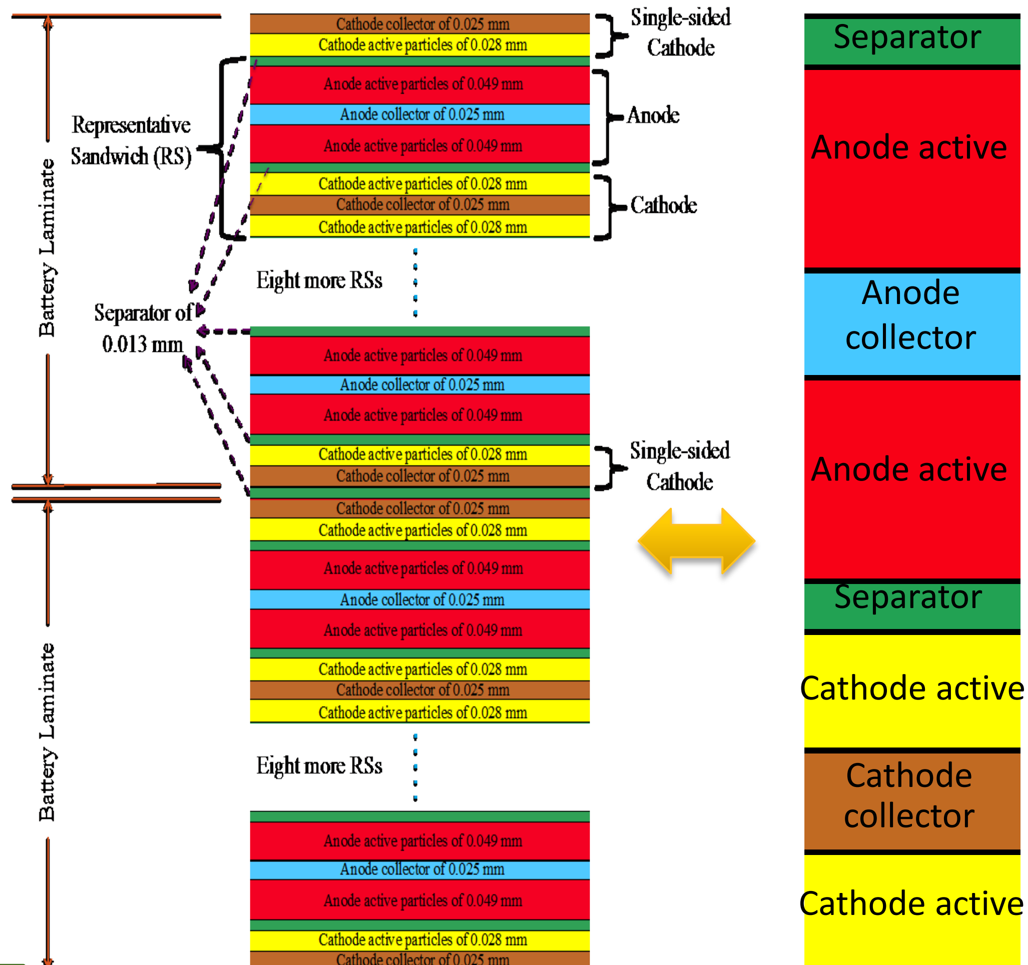
Mechanical-Electrical-Thermal (MET) Model

- A representative-sandwich (RS) finite element model was developed to efficiently simulate the coupled response of a pouch battery cell under mechanical crush.
- Each individual cell component (active material, separator, etc.) is explicitly represented.
- An indentation test is simulated as a case-study.



Schematic representation of a indentation test and dimensions of the RS model

Representative-sandwich model

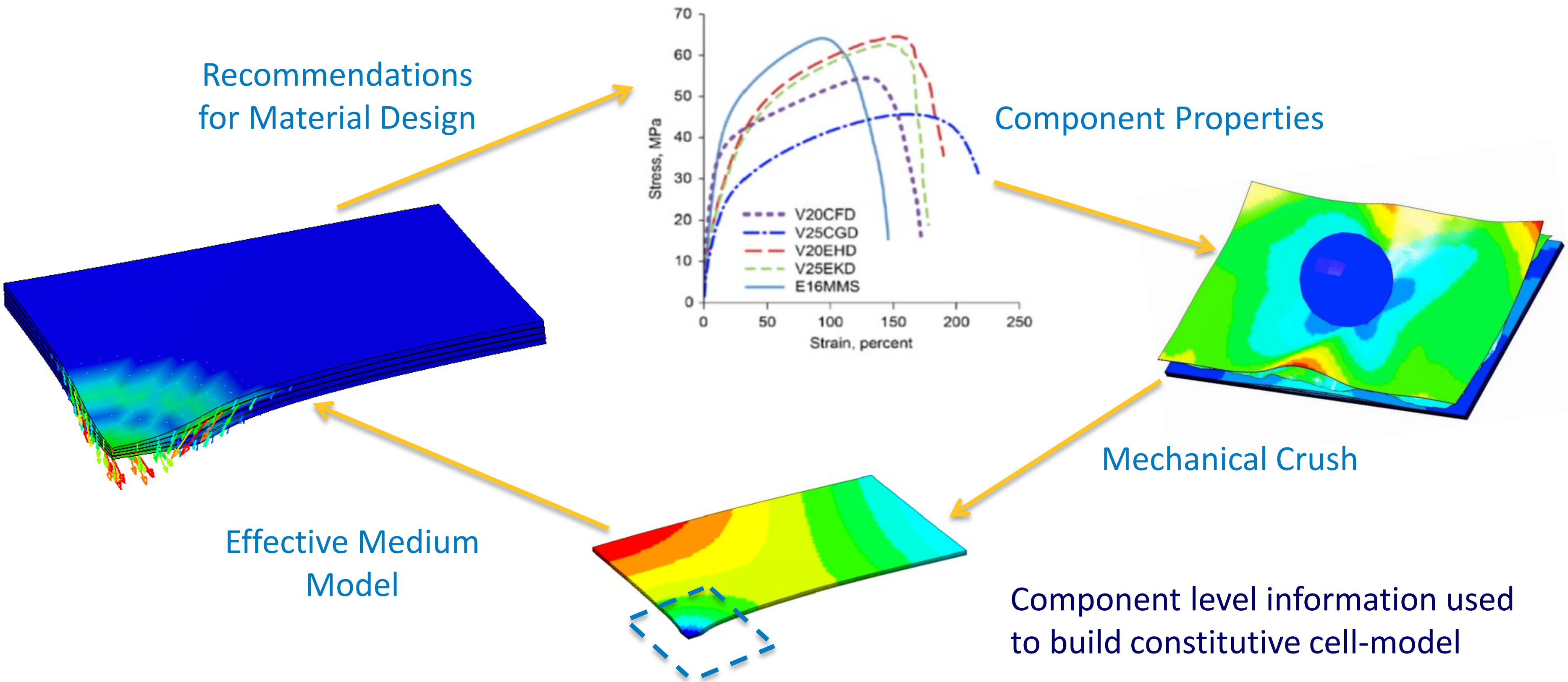


Full pouch cell layout

Single RS

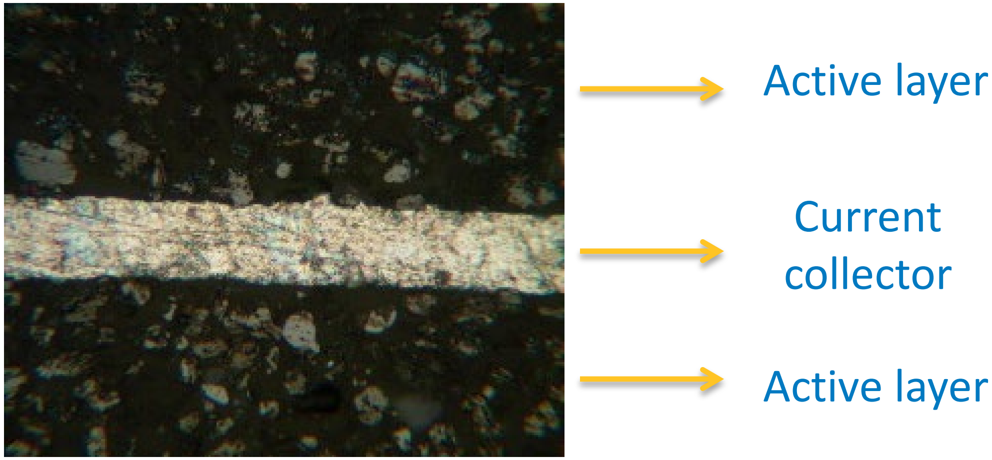
MET Model: Coupling Methodology

- Assuming mechanical crush is a much faster process than electrochemical and thermal response, we developed a **sequential one-way** coupled modeling approach, conducting electrochemical and thermal modeling on top of a mechanically deformed geometry

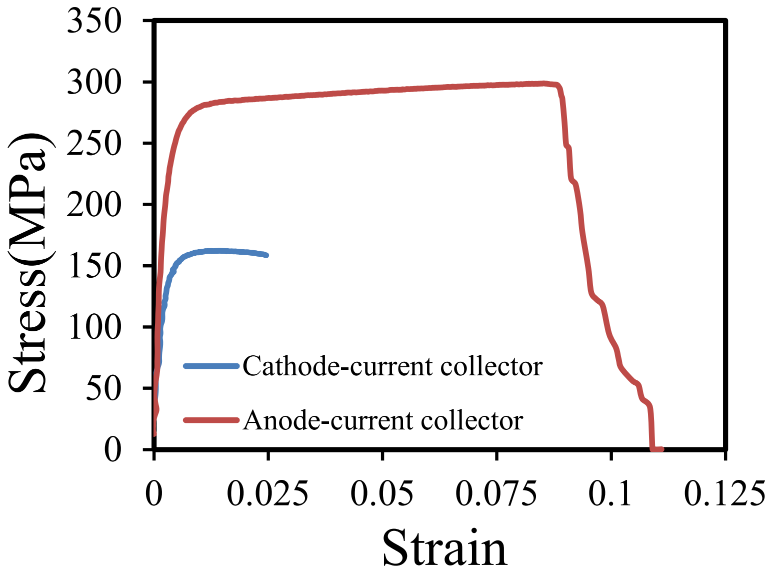


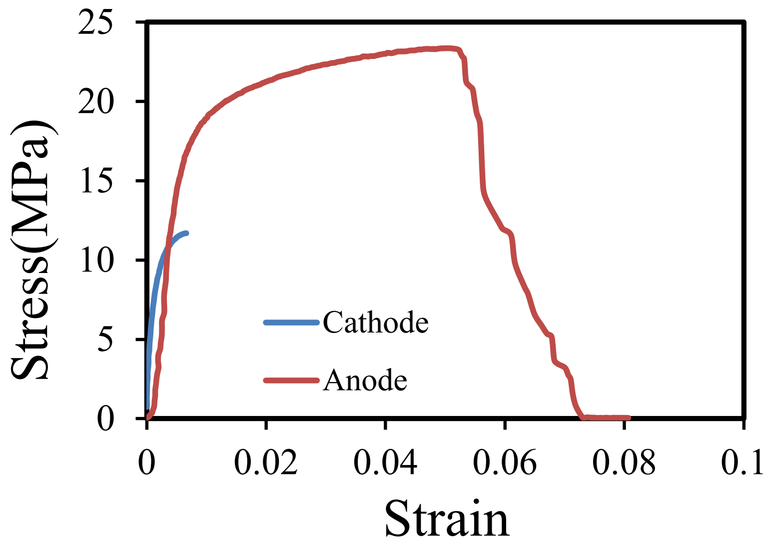
MET Model: Mechanical Properties of Battery Components

❖ **Tensile properties of electrodes**



Cross-section of anode
(Pesaran et al. AMR 2015)

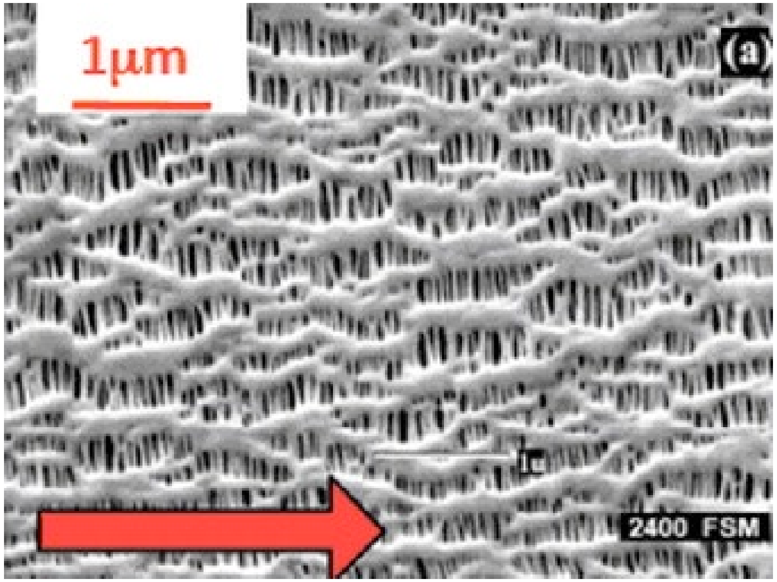




- Porous active layers
- Perfect bonding between active layers and current collector
- Brittle fracture behavior of active layers leading to earlier failure of current collector

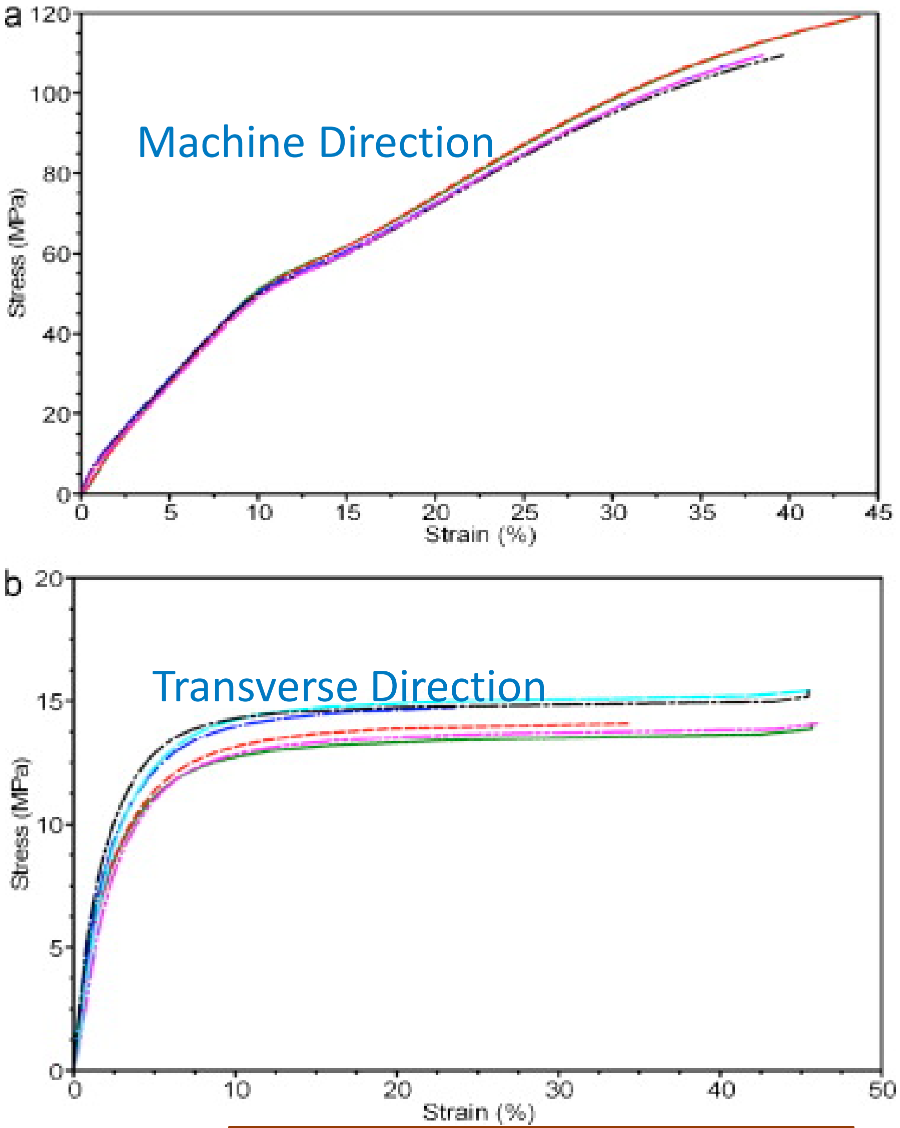
MET Model: Mechanical Properties of Battery Components

❖ Tensile properties of separators



SEM image of separator
(Sheidaei et al., J Power Sources 2014)

- Porosity about 40%
- Anisotropic tensile behavior
- Significant higher tensile failure strain than the electrodes



Sheidaei et al., J Power Sources 2014

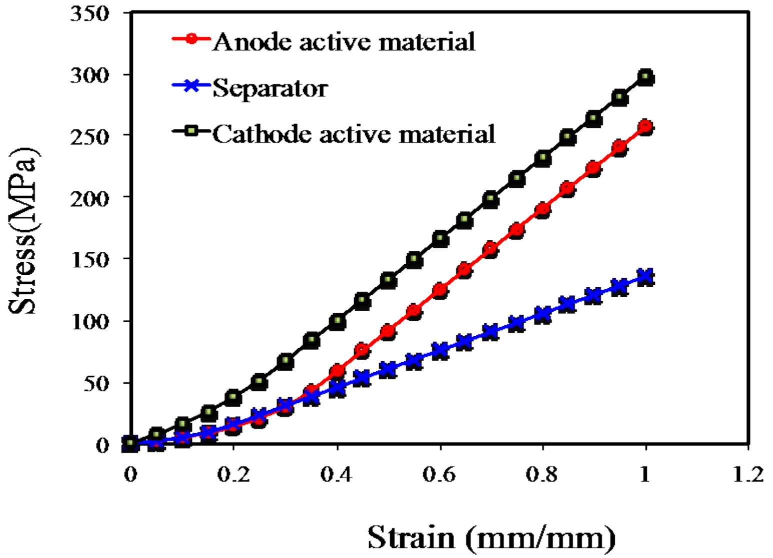
MET Model: Mechanical Properties of Battery Components

Compressive properties of electrodes

- Compressive properties of the thin porous layers can hardly be measured directly.
- An analytical procedure was developed to derive through-thickness stress-strain responses for active materials and separator from compressive experimental data of a full pouch cell.

Constitutive Equation

$$\sigma = \begin{cases} \dfrac{E_{\max}(e^{\beta\varepsilon}-1)}{\beta e^{\beta\varepsilon_p}} & \varepsilon < \varepsilon_p \\ \dfrac{E_{\max}(1-e^{-\beta\varepsilon_p})}{\beta} + E_{\max}(\varepsilon-\varepsilon_p) & \varepsilon \geq \varepsilon_p \end{cases}$$



- E_{max} condensed modulus;
- ε_p porosity;
- β gradation factor – determined through fitting experimental data

Zhang et al., J Power Sources 2015

MET Model: Mechanical Properties of Battery Components

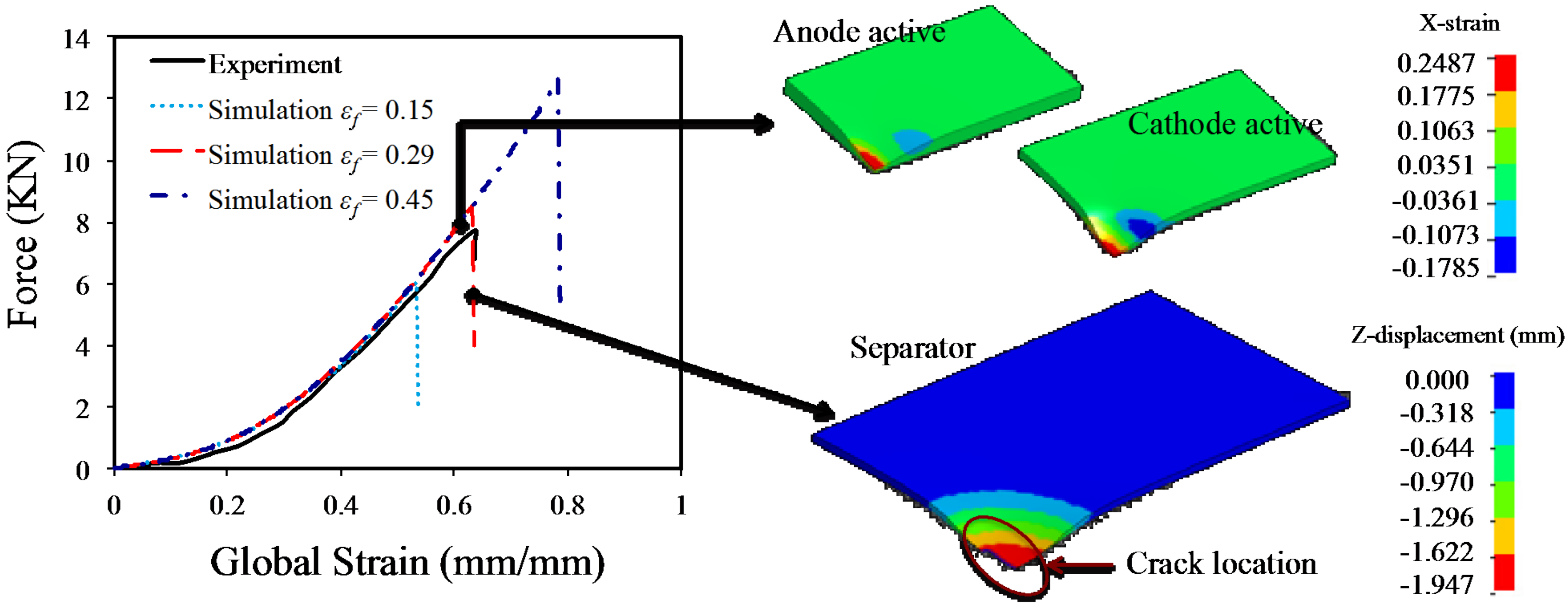
❖ Material models

- The porous active materials and separators are treated as homogeneous solid materials and modeled using LS-DYNA MAT126 MODIFIED-HONEYCOMB
- The current collectors are modeled using MAT24 LS-DYNA MAT PIECEWISE-PLASTICITY

Consider the separator failure is corresponding to the fracture of the structure:

1. We treat the electrodes perfect plasticity beyond tensile failure strain;
2. Tensile failure strain is assigned for the separator;
3. Parametric study is conducted to correlate experimental data.

MET Model: Model Correlation

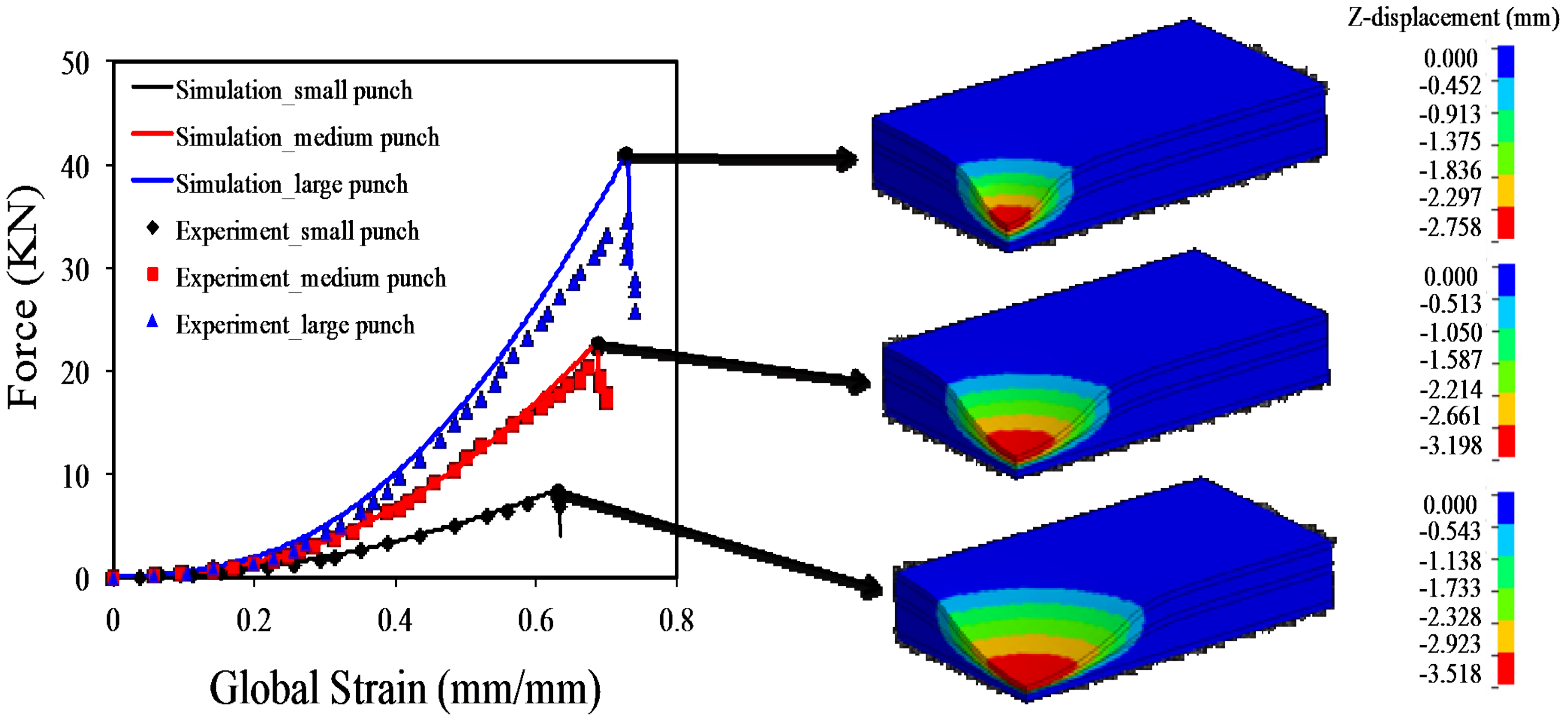


❖ The crack of the separator initiated exactly the center of the structure

❖ The active layers are more likely cracked before the failure of separator

MET Model: Simulation of Different Indentation Tests

- The failure shape of lithium-ion battery under indentation tests with three different punch diameters are studied.



MET Model: Electrical-Thermal Modeling

- An electrical simulation is run on the deformed geometry by imposing an arbitrary voltage across the terminals and monitoring the current distribution across the different layers, to obtain the magnitude of the short.

Electrical Solver

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

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

Joule Heating

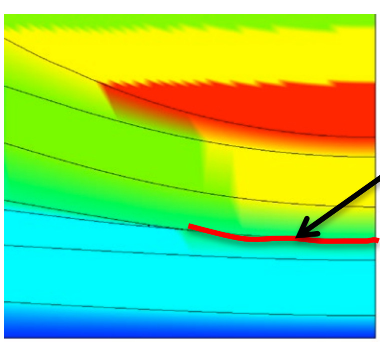
$$E_{Joule} = \frac{\vec{j}\cdot\vec{j}}{\kappa_s}$$

$$Q = \frac{\dot{E}_{Joule}}{V}$$

Thermal Solver

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

K_s could be a function of temperature

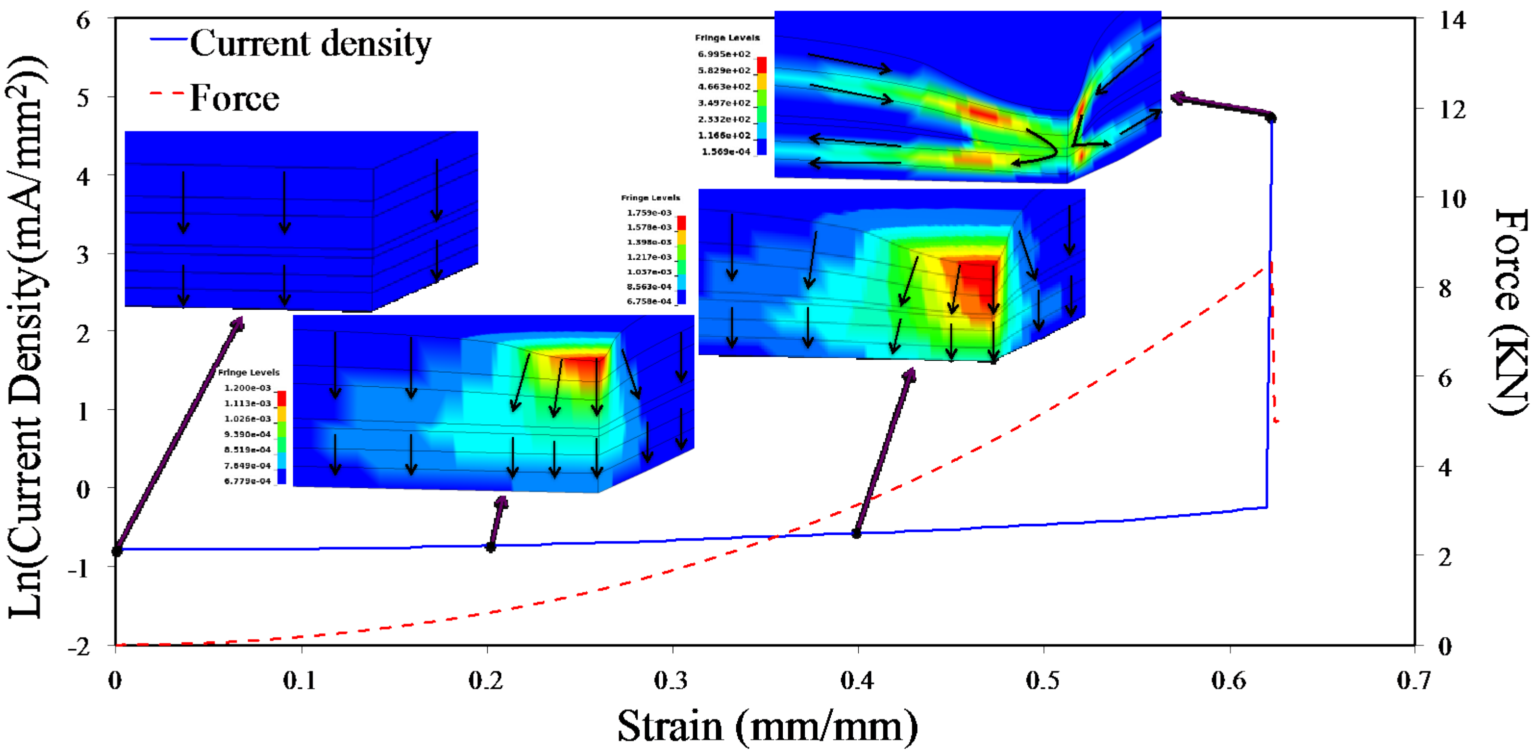


Separator fracture (element erosion) results in electrical contact between electrodes

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

MET Model: Electrical-Thermal Modeling

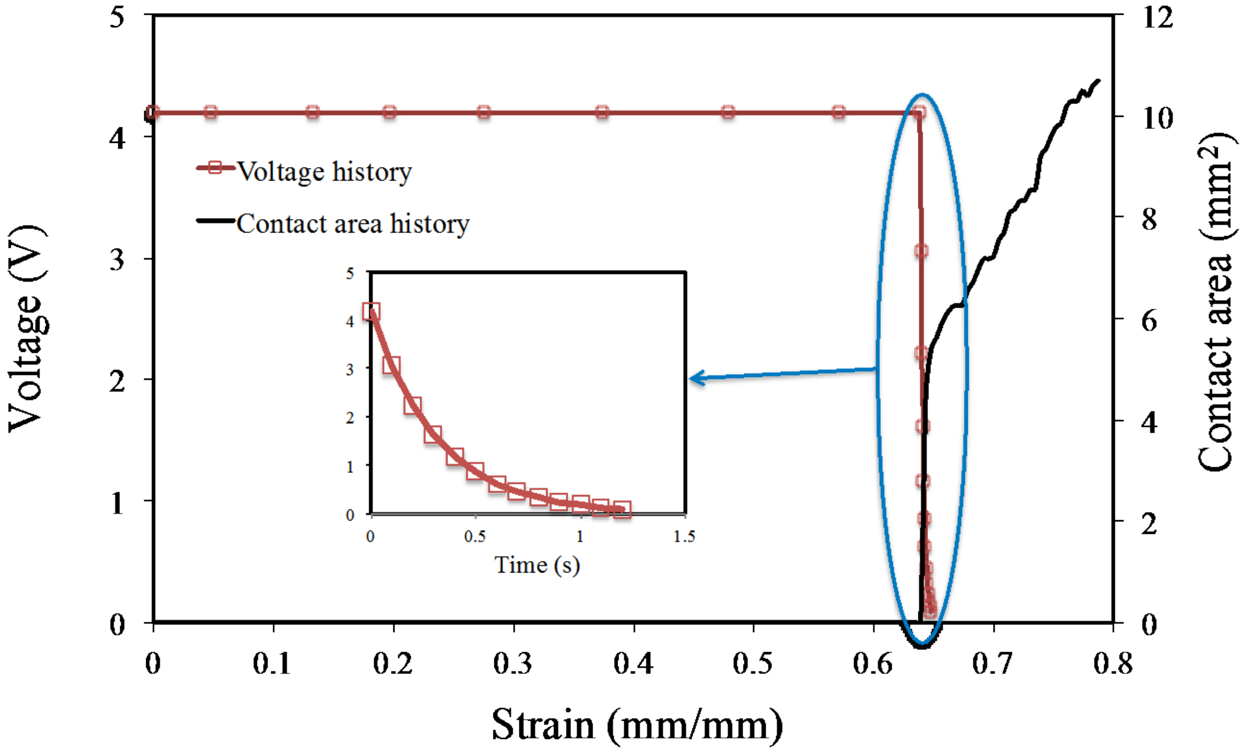
- In the results shown below, short circuit initiates due to failure of separator and electric contact between positive (Cathode) and negative (Anode) active layers
- The onset of short circuit is predicted, which occurs simultaneously with the mechanical fracture of the battery structure.



Evolution of current density during a mechanical indentation test

MET Model: Electrical-Thermal Modeling

- The voltage evolution before and after short can be predicted using the coupled modeling approach.
- The present approach can capture the gradual drop of voltage (inset of figure below), which is important in designing safety features to prevent propagation of failure.

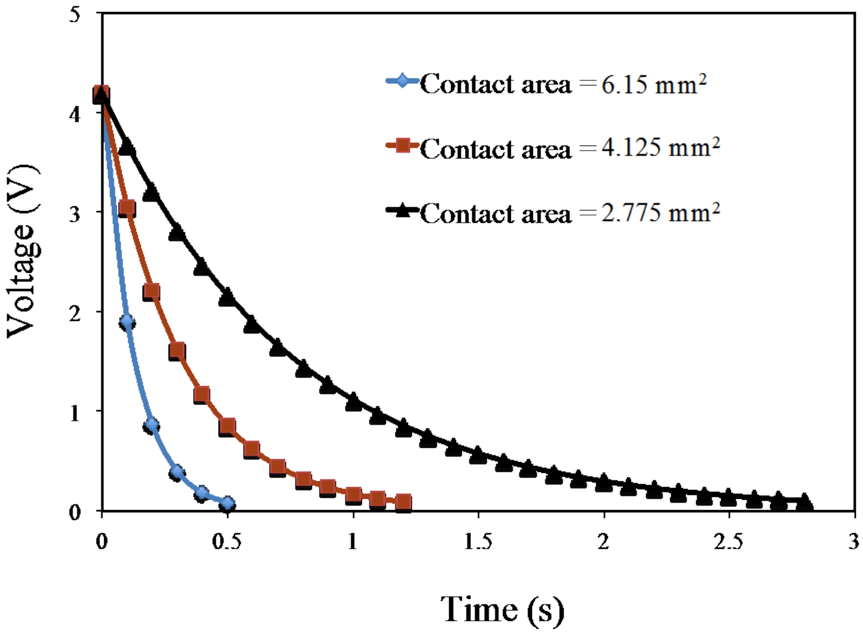


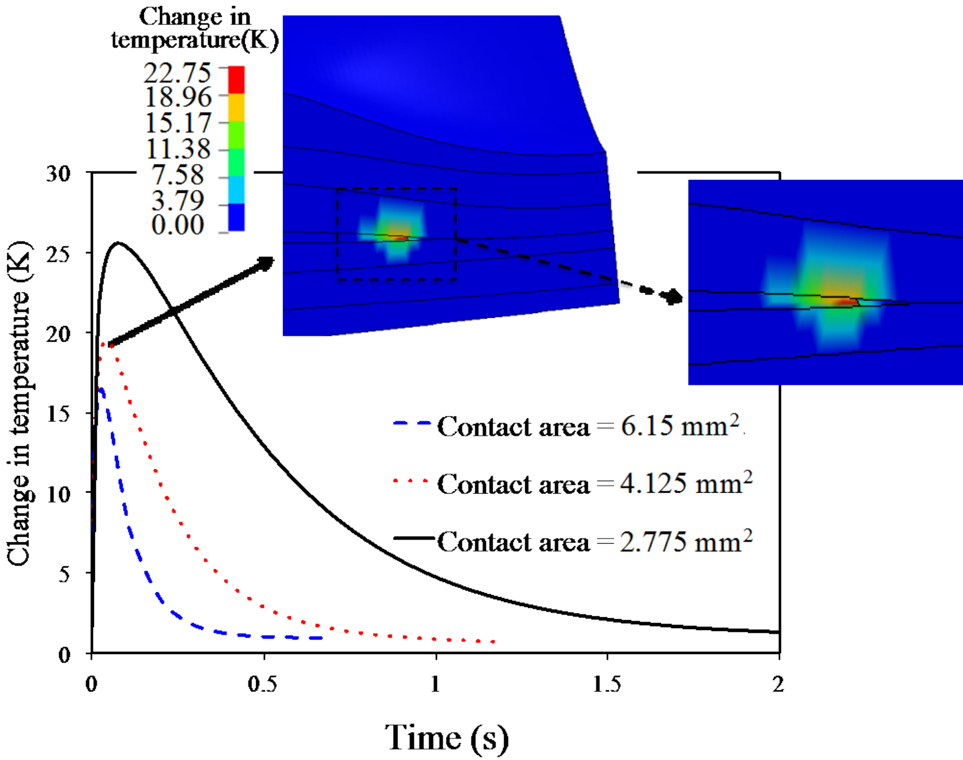
Evolution of voltage and short-circuit area before and after short circuit

MET Model: Electrical-Thermal Modeling

- The thermal ramp after short circuit can also be predicted using the coupled modeling approach.
- The coupled model shows the potential to study different short-circuit conditions, for example, evolution of electrical contact area as the short proceeds.

Effect of electrical contact area on voltage drop and thermal responses

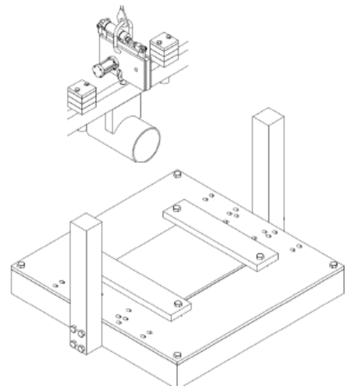


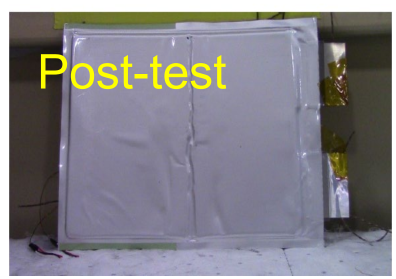


Highlights on the location and value of maximum temperature

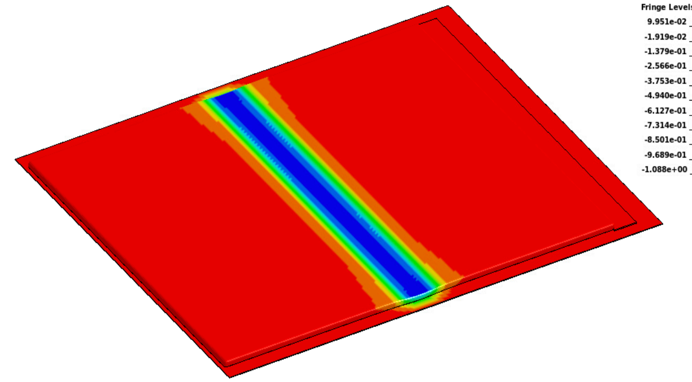
Impact of Lithium-ion Battery Cell

Test Facility and Set Up

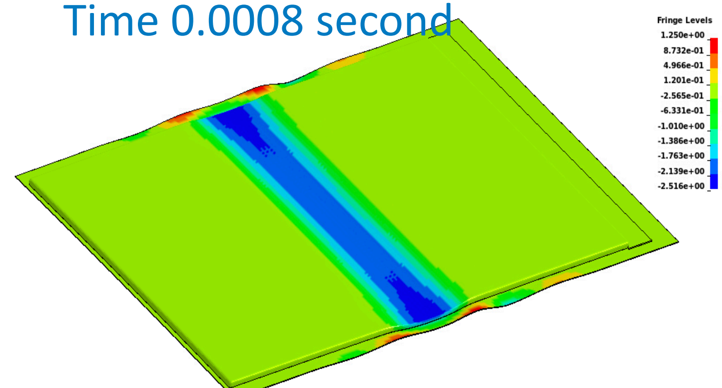




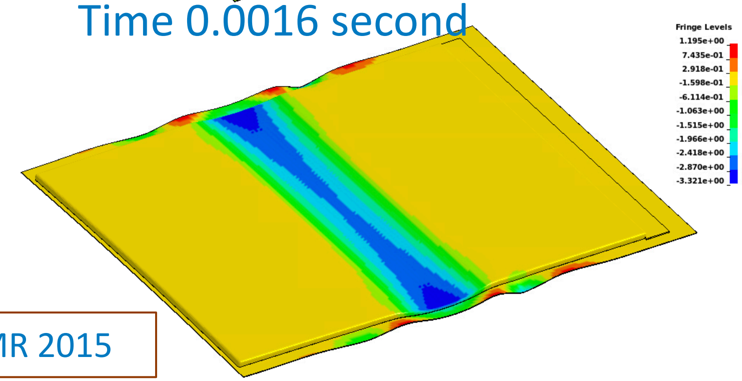
Time 0.0004 second



Time 0.0008 second



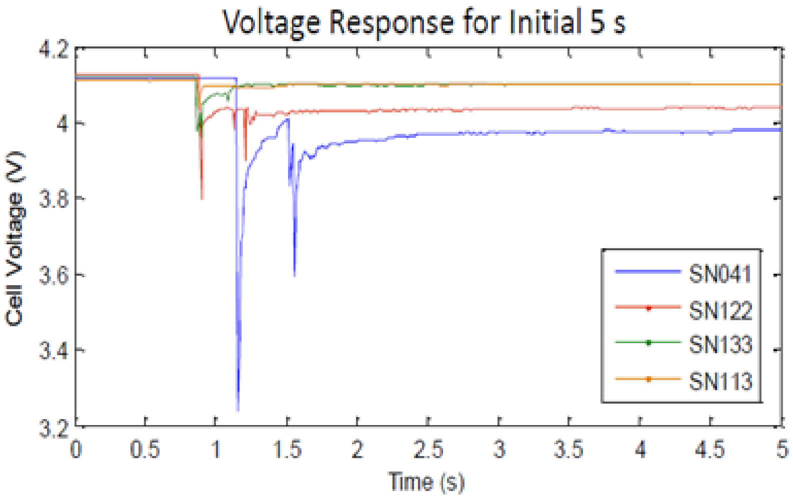
Time 0.0016 second

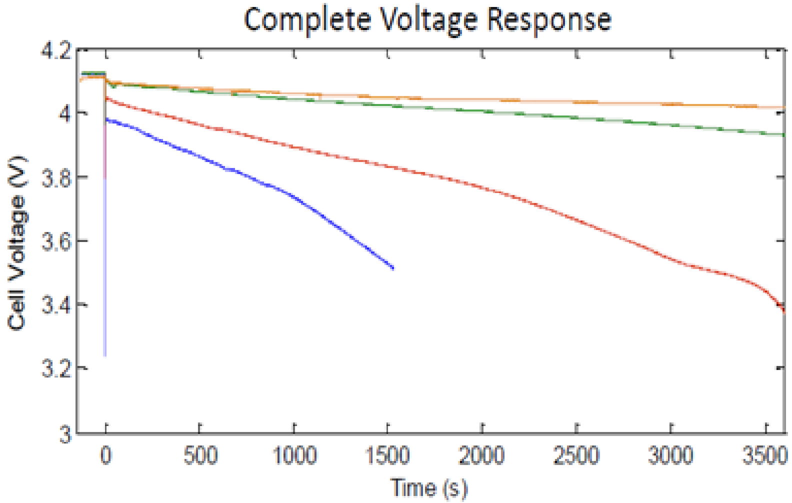


- The variables controlled to vary the impact of the load include the initial height (1m, 2m) and the weight of the load (32 kg, 14 kg).

Santhanagopalan et al. AMR 2015

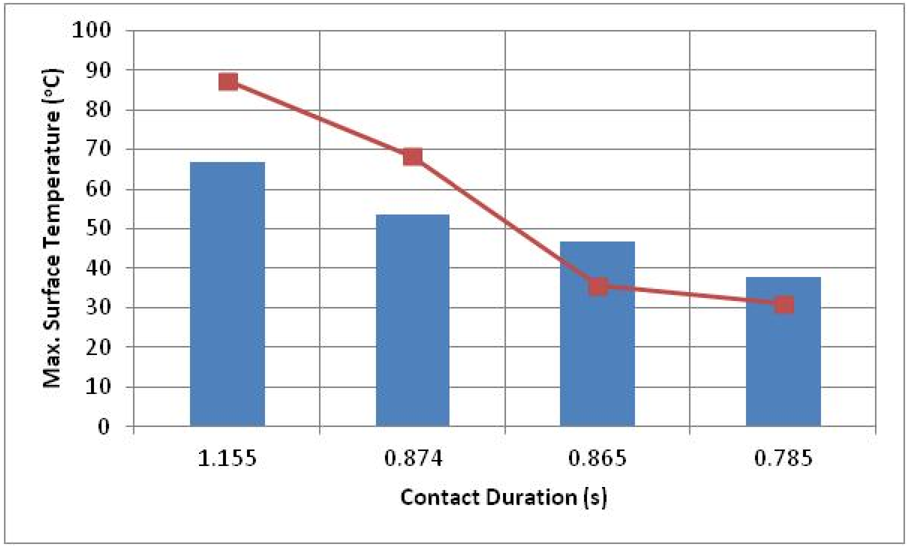
Impact of Lithium-ion Battery Cell





Cell voltage history during the impact test

Santhanagopalan et al. AMR 2015



Maximum surface temperature: model (line) versus experiments (bars). The contact duration corresponds to experimentally measured length of contact between the cell and the impactor during the impact test during the four test cases.

- Effect of impact is localized—several layers of the cell remain intact;
- Pouch material does not rupture under the load conditions used for the test;
- The rebounding of voltage is most likely associated with the recovering of elastic strain after unloading.

Summary

- We developed a unique sequential approach for coupled mechanical-electrical-thermal simulation of lithium-ion battery
- A single representative sandwich (RS) model was developed, correlated well with experimental results and predicted fracture of the structure
- Sequential mechanical-electric-thermal coupled simulation was conducted using the single RS model. It predicts the initiation of short-circuit and consequential voltage evolution and thermal history

Future Work

- Simultaneous two-way coupled modeling approach
- Generic material models for battery cells and cell components
- High strain rate impact loading conditions
- Modeling of progressive damage process

Acknowledgements

The NREL Team

Chuanbo Yang
Gi-Heon Kim
Lei Cao

Funding

Brian Cunningham
Dave Howell

Collaborations

NATIONAL RENEWABLE ENERGY LABORATORY

Thanks !

The End