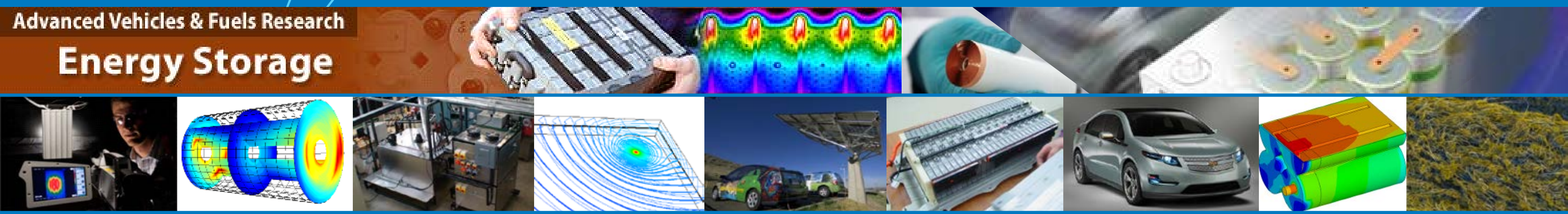
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Coupling of Mechanical Behavior of Lithium Ion Cells to Electrochemical-Thermal Models for Battery Crush



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Outline

- **Introduction**
- **Background**
- **Mechanical-electrochemical-thermal model**
  - Characterization of cell components
  - Battery cell level abuse tests and homogenized models
  - Representative-sandwich model
  - Coupled electrical-thermal model
  - Link mechanical to ECT model
- **Summary and Future work**

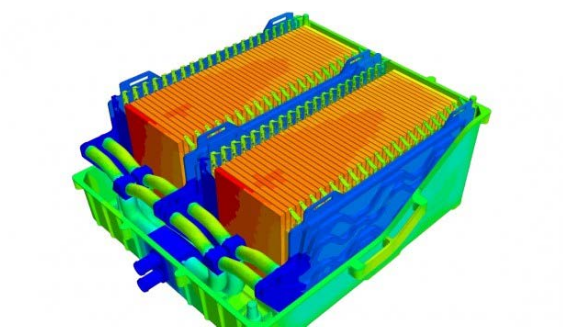
Introduction

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


Public domain photos courtesy of NHTSA

State-of-the-art Vehicle Battery Modeling

- US Department of Energy launched CAEBAT (Computer Aided Engineering for Electric Drive Batteries) activity supporting development of lithium ion battery CAE and simulation tools
- DOE funded NREL to develop high-fidelity and/or fast research models for electrochemical-thermal, life, and safety simulations
- First phase of CAEBAT activity resulted in commercial software for electrochemical-thermal design of EDV batteries



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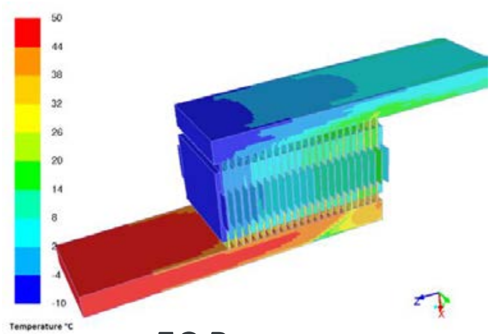
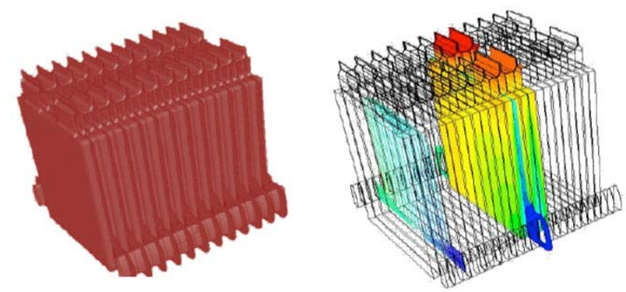


EC Power



ANSYS

- In the second phase of CAEBAT, DOE funded NREL to couple mechanical models with electrochemical-thermal models to simulate crash-induced crush
- NREL's approach for MECT is discussed this presentation

Modeling Battery MECT After Crush

- Vehicle crash → battery crush → cell damaged zone → separator failure → electrode contact → local short → current flow → heat generation → insufficient heat rejection → *temperature* increase → *reaching above onset* temperature → spontaneous reactions → thermal runaway → smoke and fire

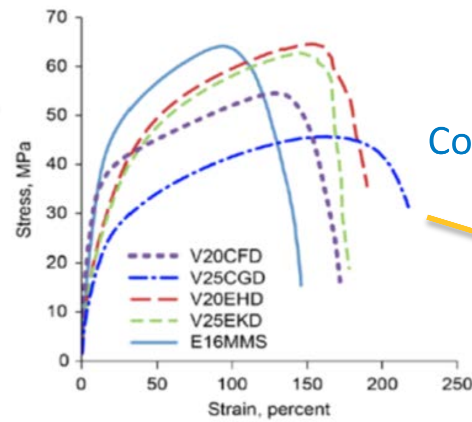
→: may lead to (depending on many factors)

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

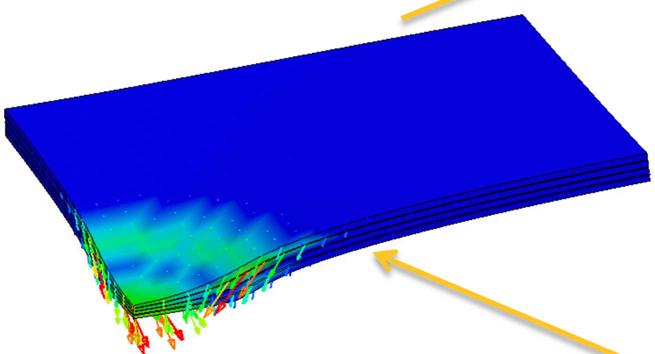
MECT Model: Coupling Methodology

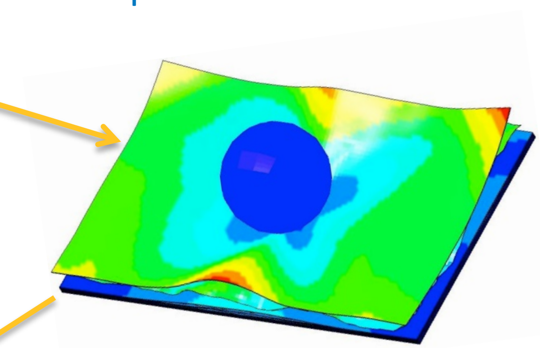
- Assuming mechanical crush is a much faster process than electrochemical and thermal response, we developed a **sequential one-way** coupled modeling approach, conducting electrochemical and thermal modeling on top of a mechanically-deformed geometry

Recommendations for Material Design



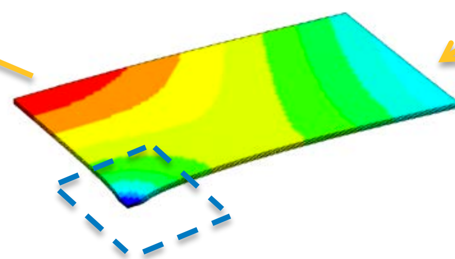
Component Properties





Object indentation

Effective Medium Model

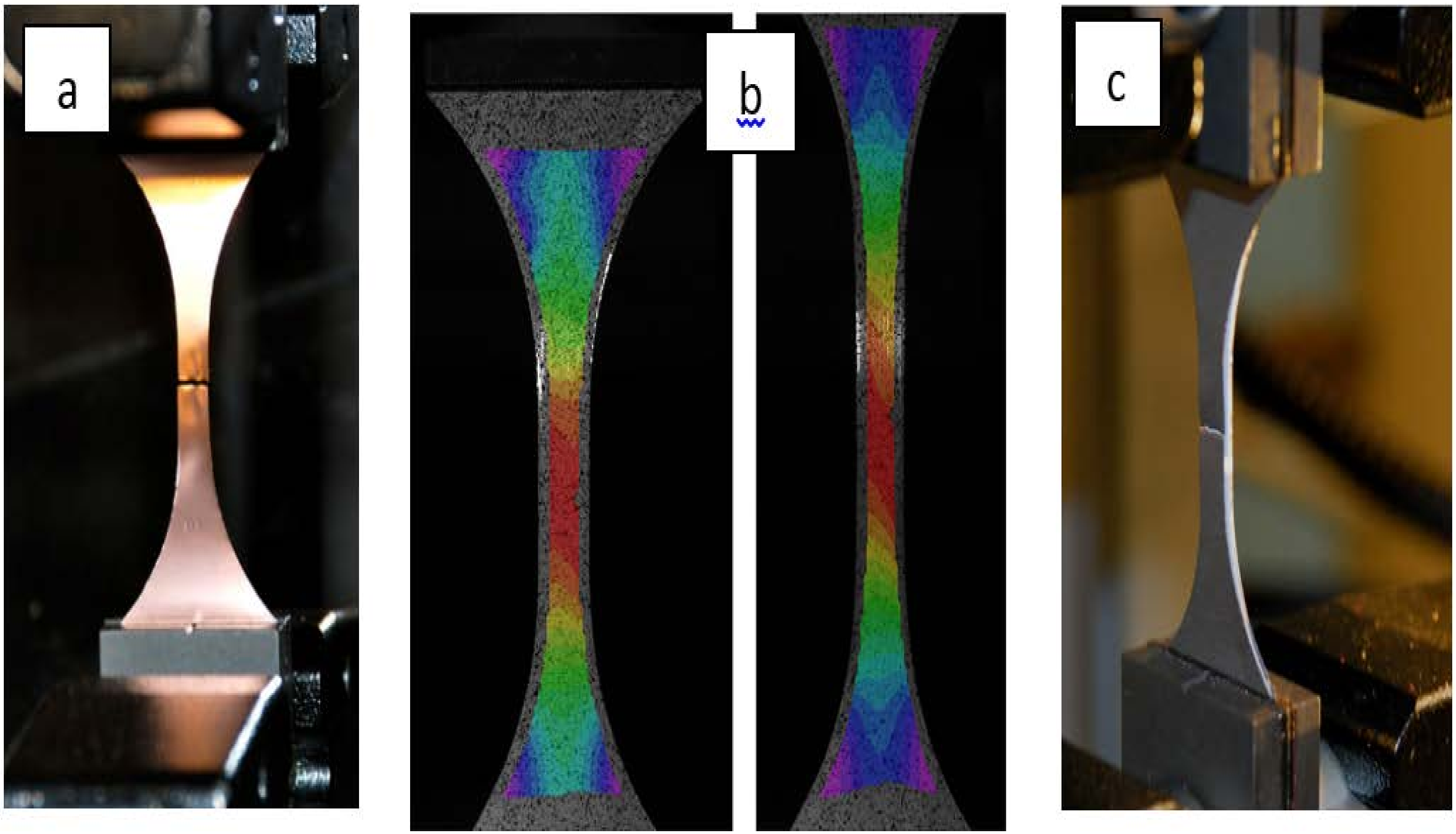


Component level information used to build constitutive cell-model

MECT Model: Mechanical Properties Measurements

- **Mechanical properties of individual components**
  - Digital Image Correlation (DIC) assisted tensile tests

Massachusetts Institute of Technology



Anode current collector | Separator | Cathode current collector

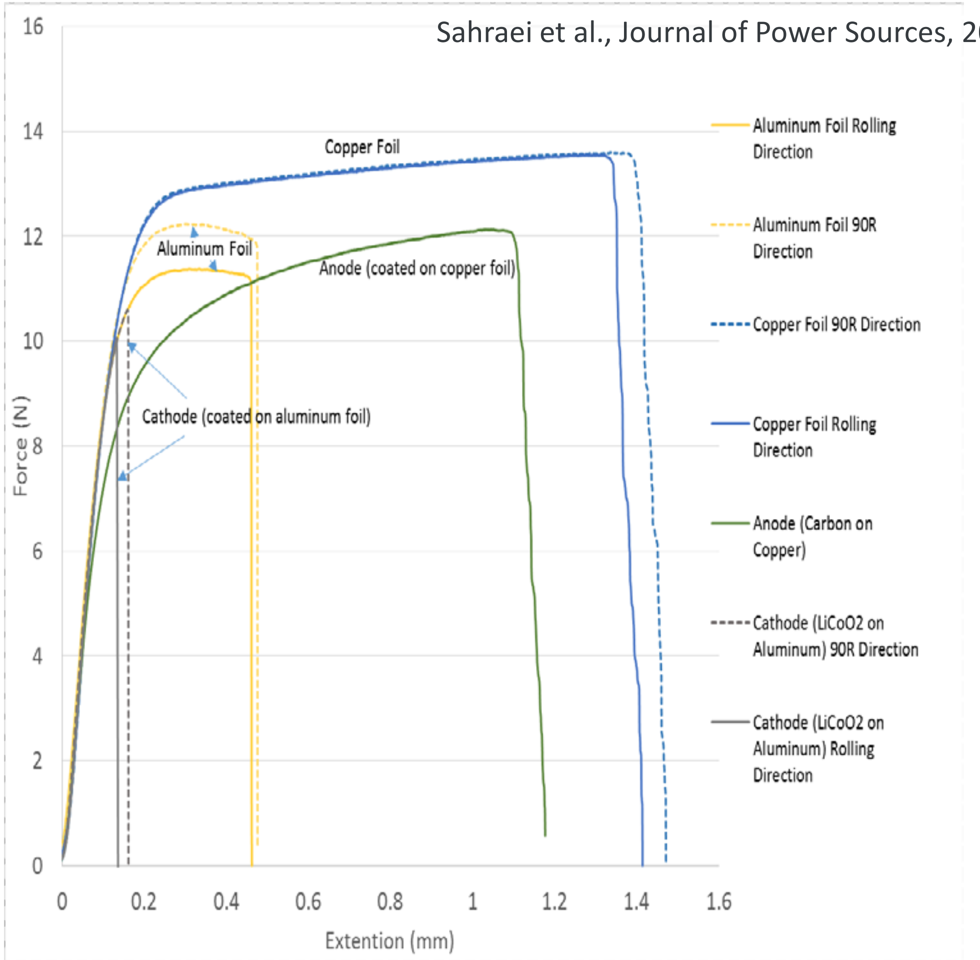
Sahraei et al., Journal of Power Sources, 2015

Tensile Test Results

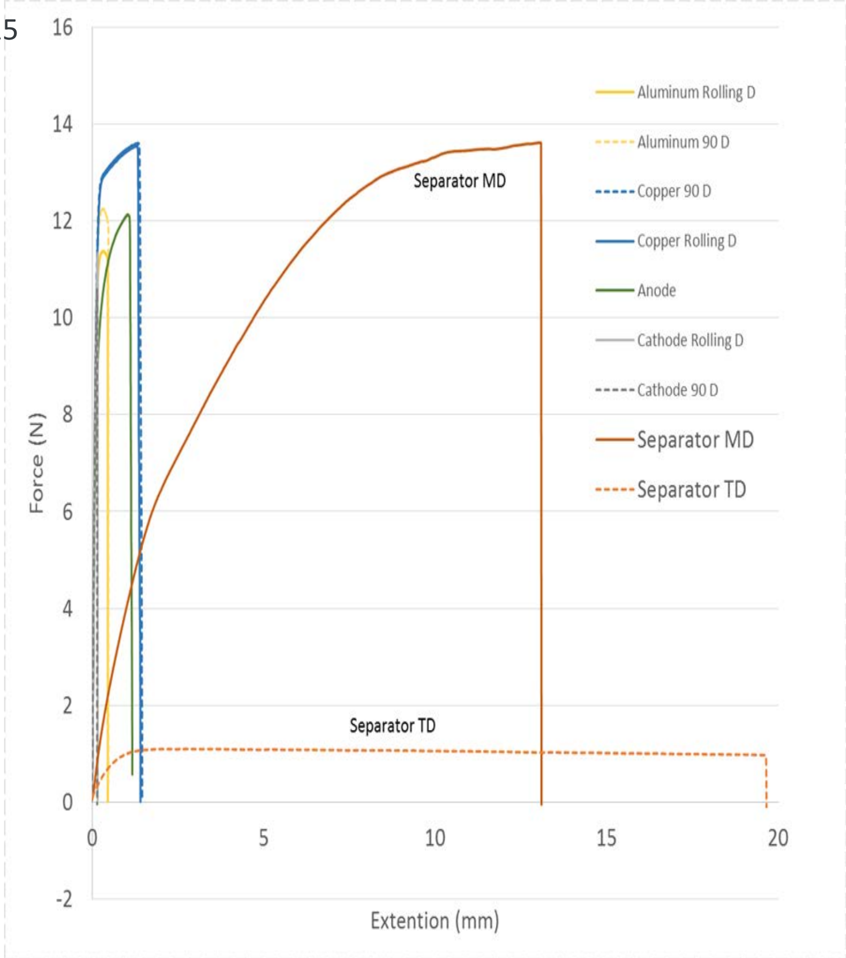
Tensile tests show a typical elasto-plastic response for metallic thin films for the current collectors.

Some anisotropic behavior was observed in the separator tests.

Sahraei et al., Journal of Power Sources, 2015



Electrodes and current collectors

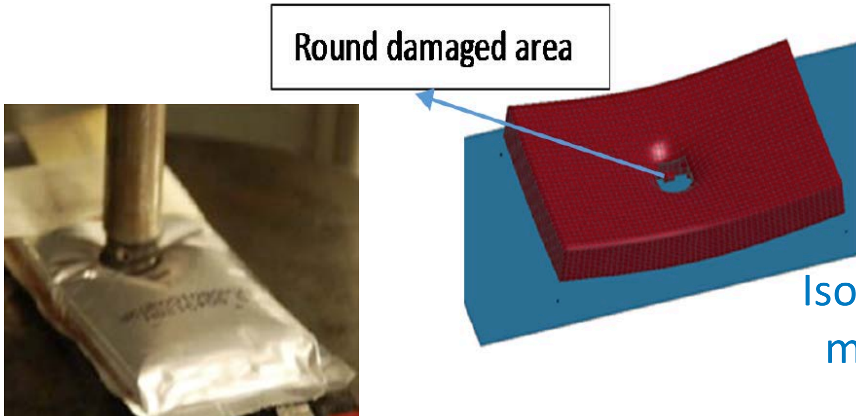


Electrodes and separators

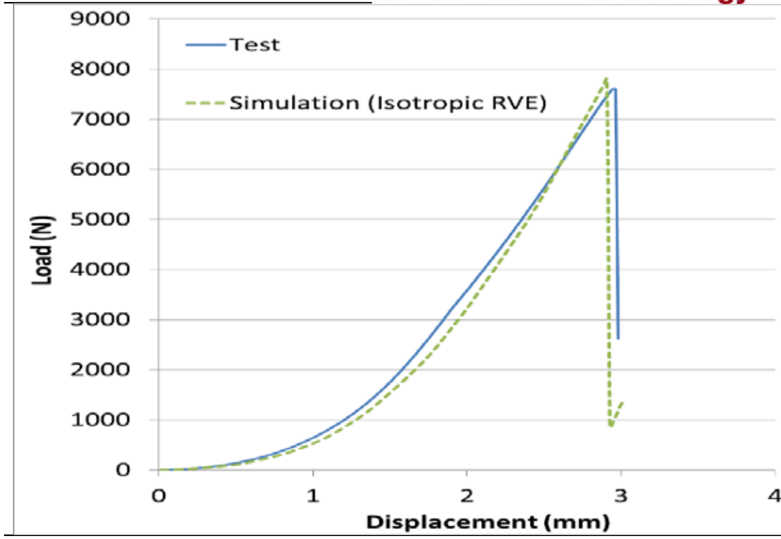
Mechanical Model of a Cell vs. Experiments

- Homogenized model for mechanical simulation at MIT

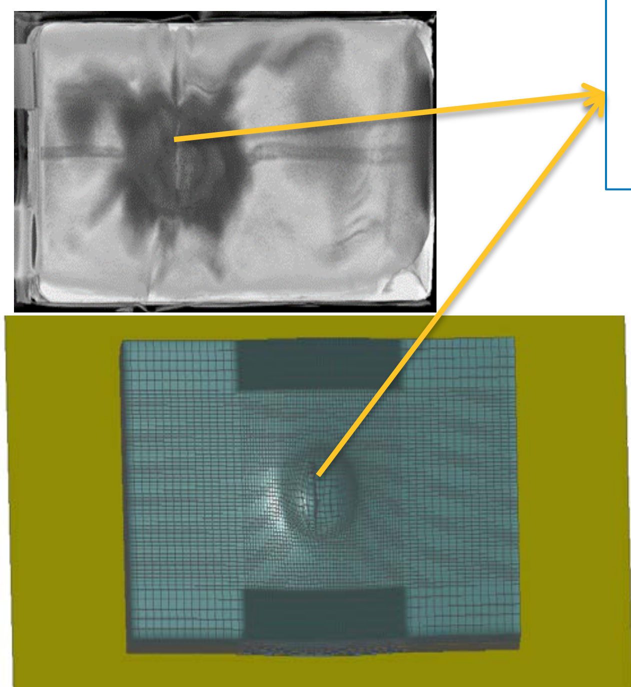
Massachusetts Institute of Technology



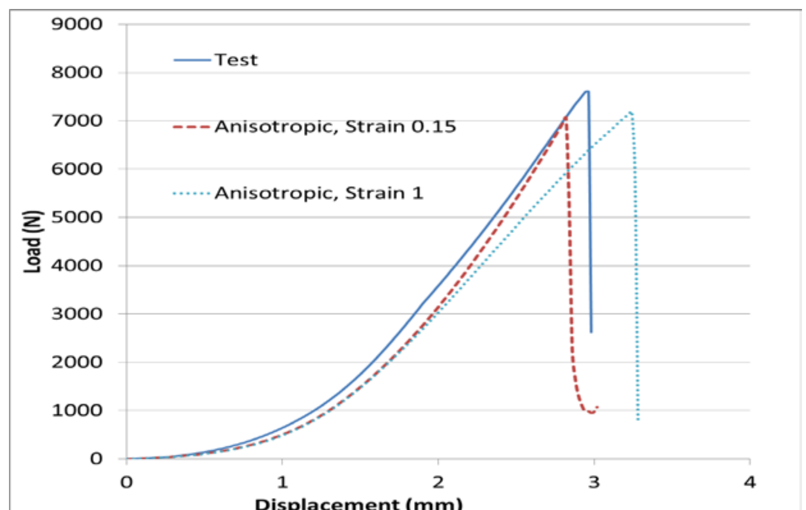
Isotropic model



Crack location and orientation



Anisotropic model



Sahraei et al., Journal of Power Sources, 2015

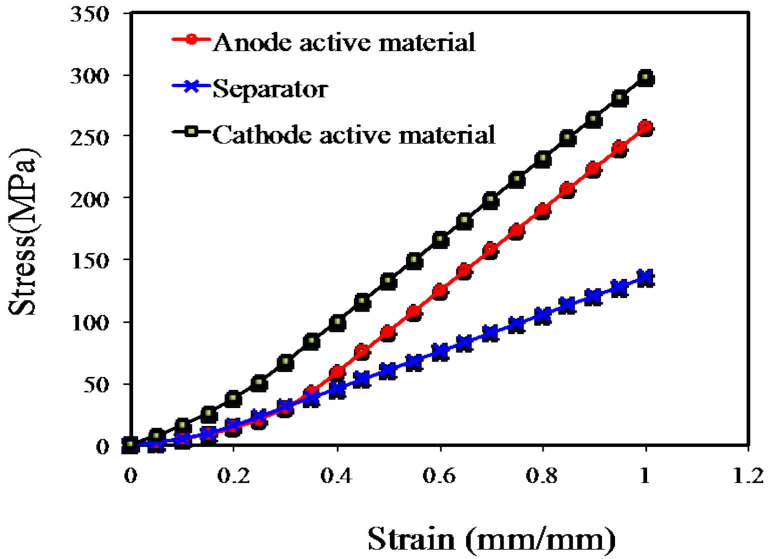
MECT Model: Material Properties for Porous Layers

- Properties of the porous layers cannot 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

Stress-strain relationships

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

$$\varepsilon_{eff} = v_{actives}\varepsilon_{actives} + v_{collectors}\varepsilon_{collectors} + v_{separator}\varepsilon_{separator}$$



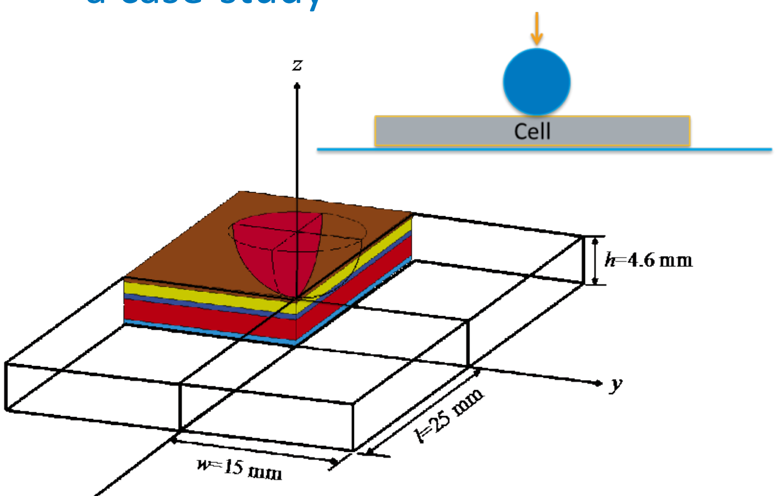
Analytically derived compressive responses

- The tensile test data of each component are directly implemented into the materials models to describe tensile responses; the current model is able to take into consideration the anisotropic mechanical properties

Zhang et al., J Power Sources 2015

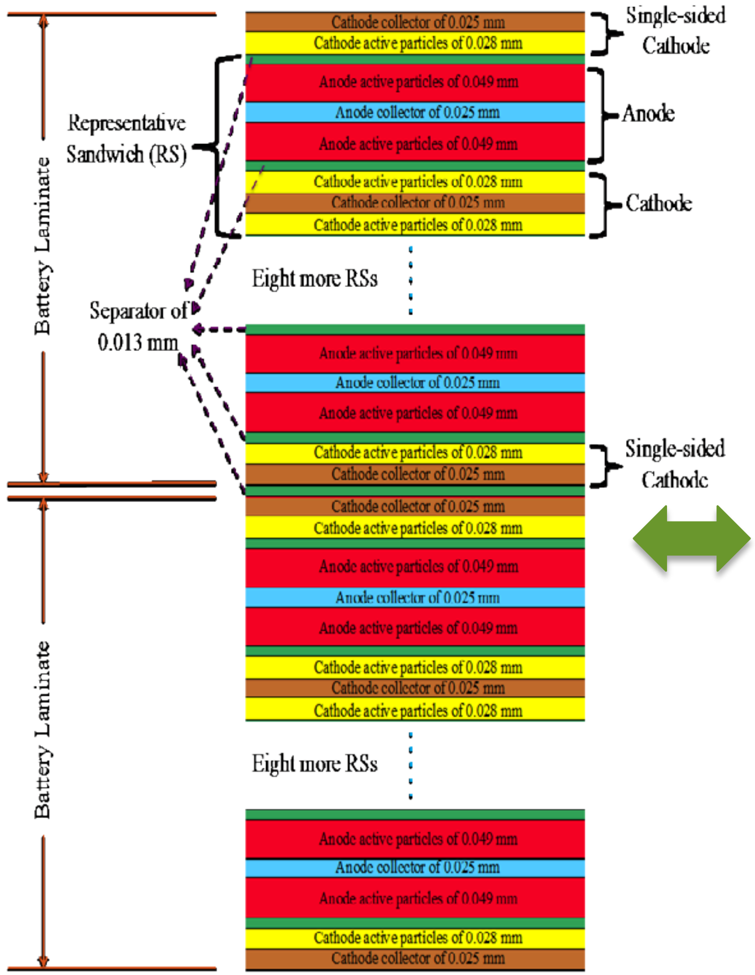
Mechanical-Electrochemical-Thermal (MECT) Modeling

- 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

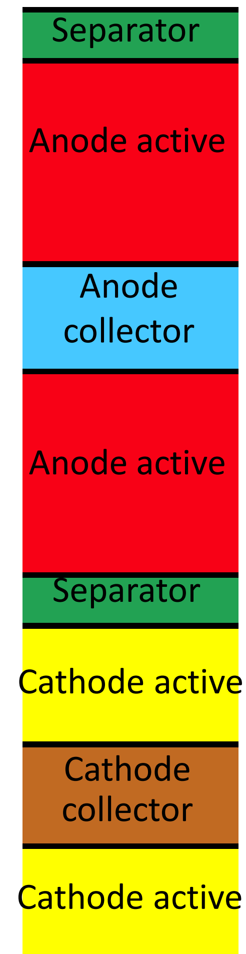


Schematic representation of a indentation test and dimensions of the RS model

Representative-sandwich model



Full pouch cell layout



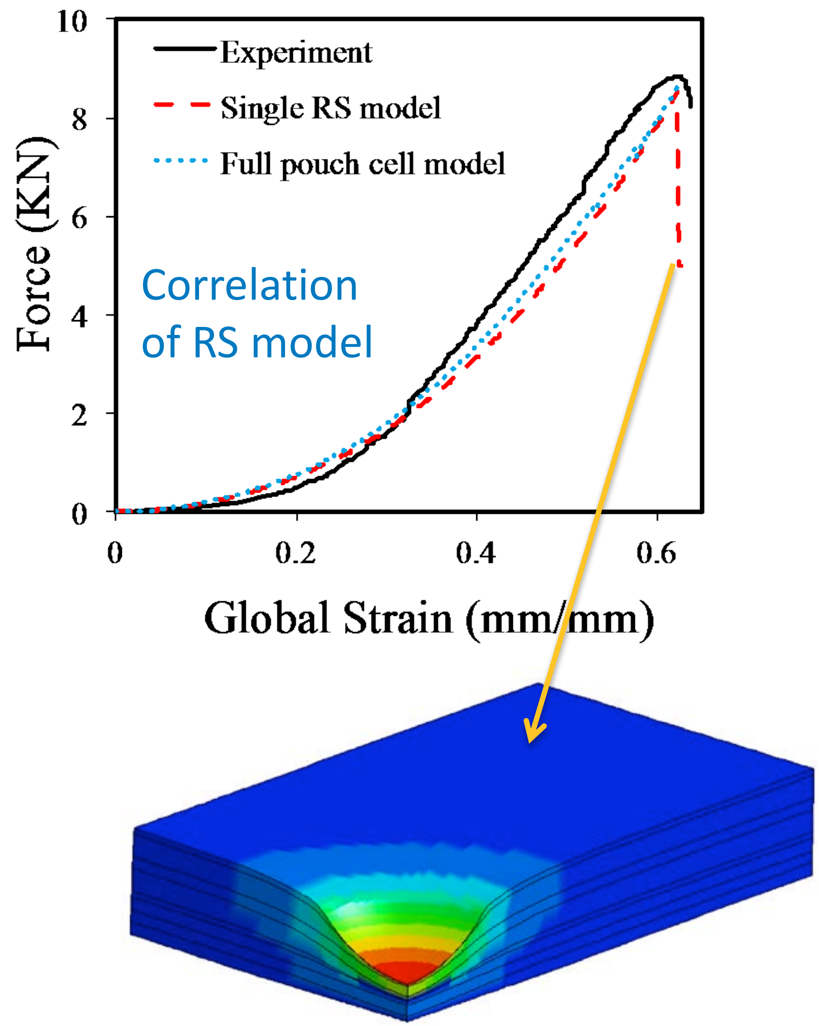
Single RS

MECT: RS Model Vs. Experiments

Representative-sandwich model

- The single RS model correlated well with experiments in predicting global effective response and fracturing of battery structure

- The RS model can be used to:
  - Conduct electrical-thermal simulation on geometries with different extent of deformation
  - Predict onset of short circuit during mechanical crush
  - Investigate the effect material properties of individual components have on the safety behavior of the battery
  - Integrate with ANSYS ECT model to study electrochemical responses

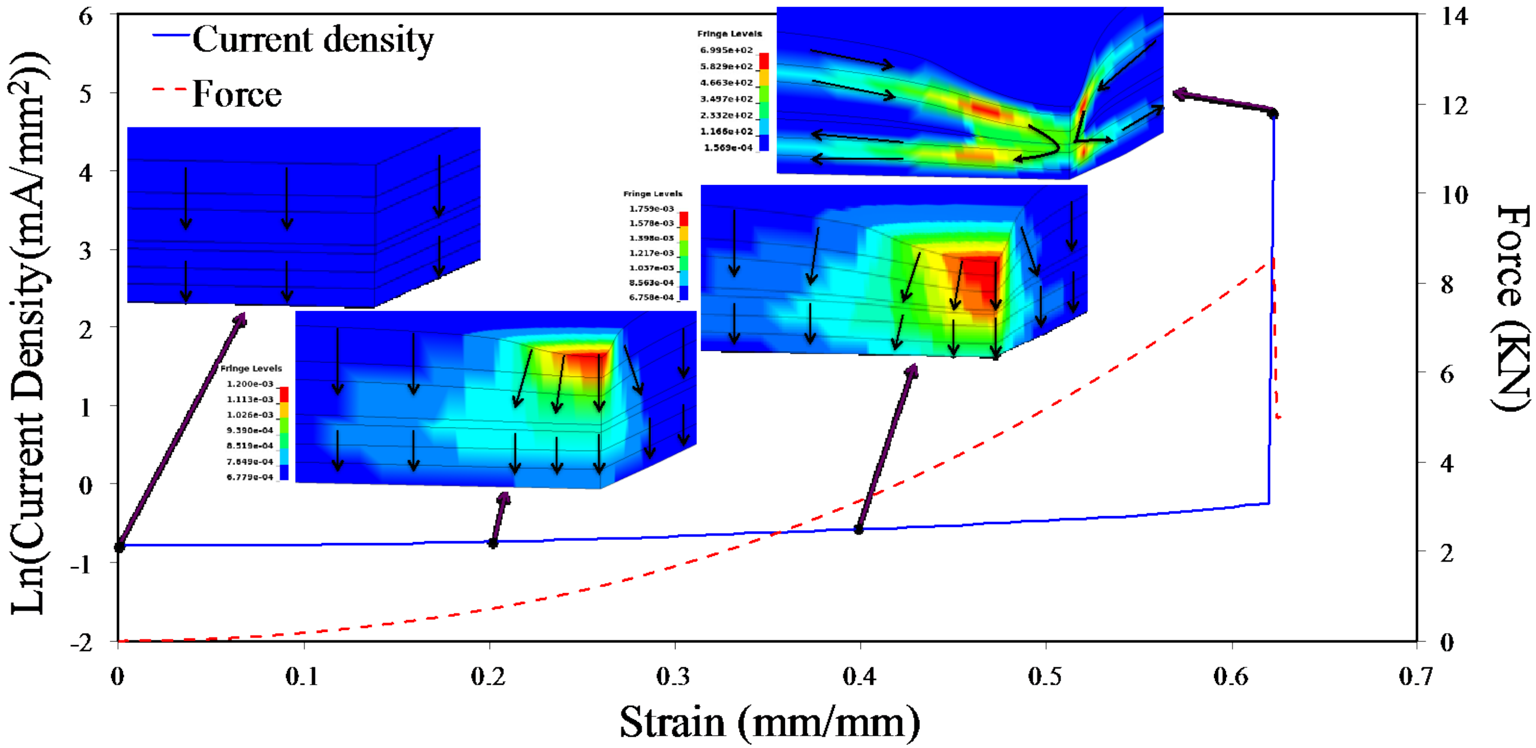


Numerically predicted deformed geometry at the moment of mechanical failure

Zhang et al., J Power Sources 2015

Mechanical Failure-Induced Short Circuit

- In the results shown below, short circuit initiates upon failure of separator and electrical contact between positive (Cathode) and negative (Anode) active layers
- Onset of short circuit is predicted, which occurs simultaneously with mechanical fracture of battery structure



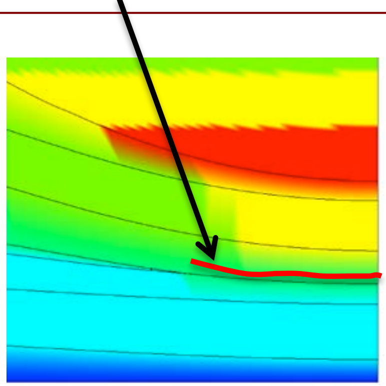
Evolution of current density during mechanical indentation test

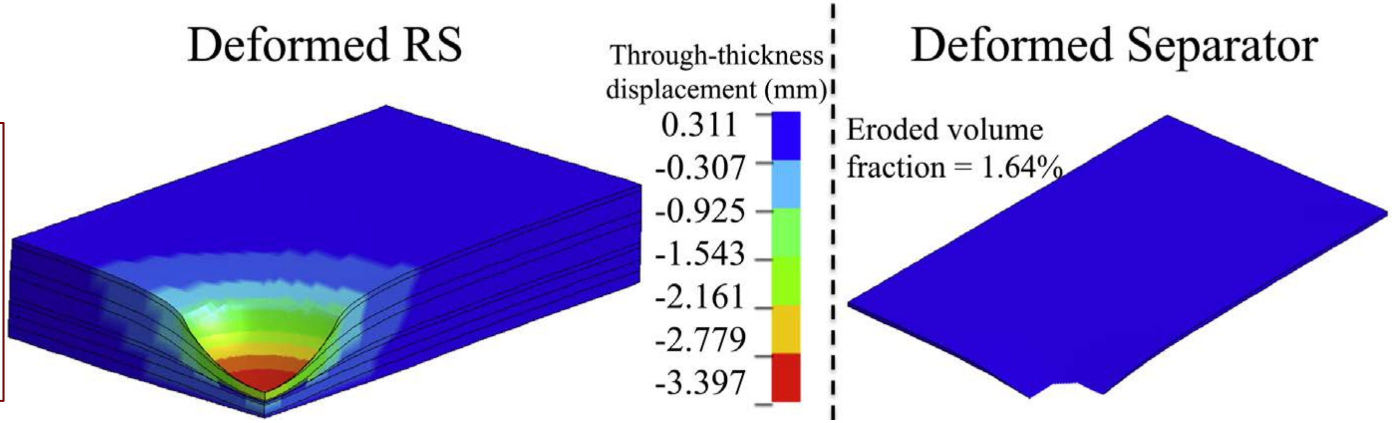
Zhang et al., J Power Sources 2015

Magnitude and Location of Short-circuit

- Failure criteria are specified for individual cell components; elements that meet mechanical failure criteria are deleted, resulting in physical contact
- An electrical simulation is run on deformed geometry by imposing an arbitrary voltage across the terminals and monitoring current distribution across the different layers to obtain the magnitude of the short

Location of Short: the red line highlights the electrical contact surface of short circuit, where separator layer failed

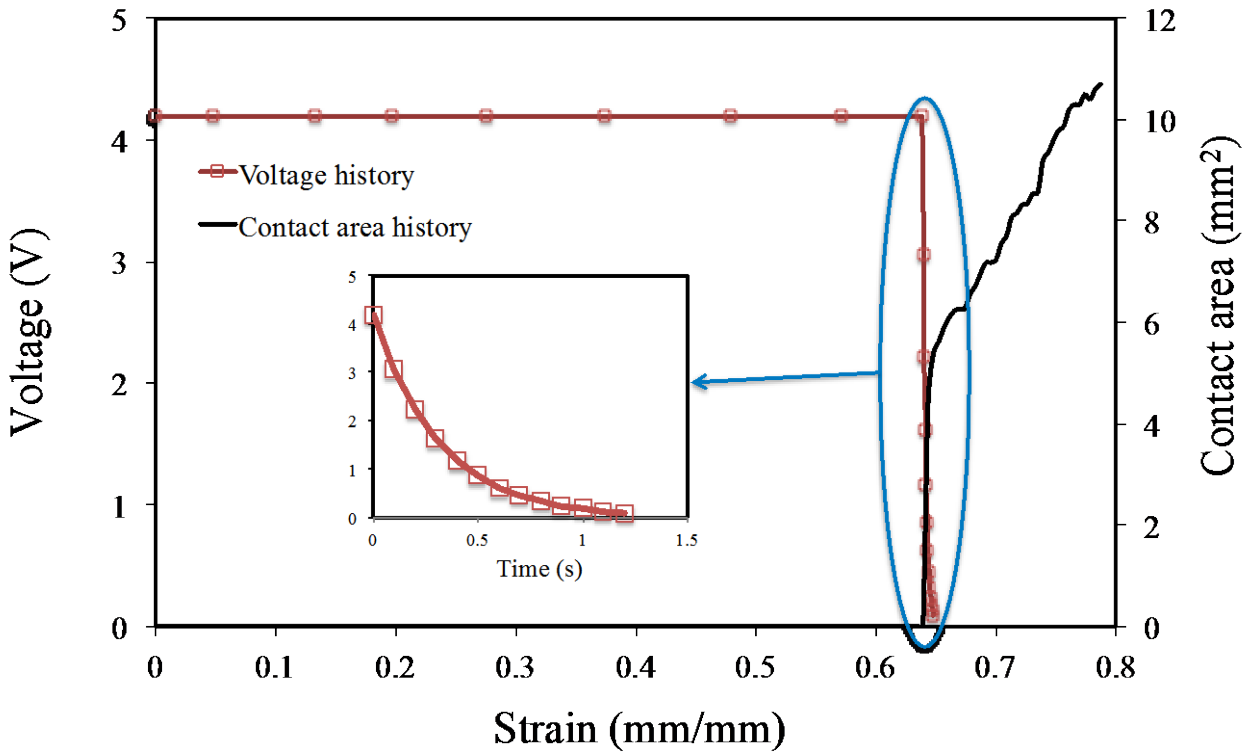




Failure criteria used to determine location and magnitude of short-circuit within the cell

Electrical-Thermal Responses after Short Circuit

- 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



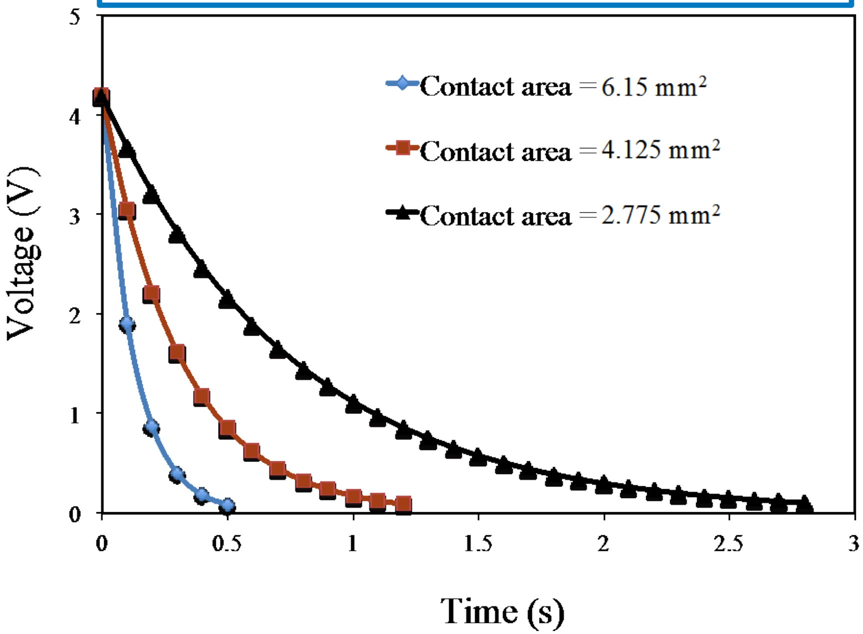
Evolution of voltage and short-circuit area before and after short circuit

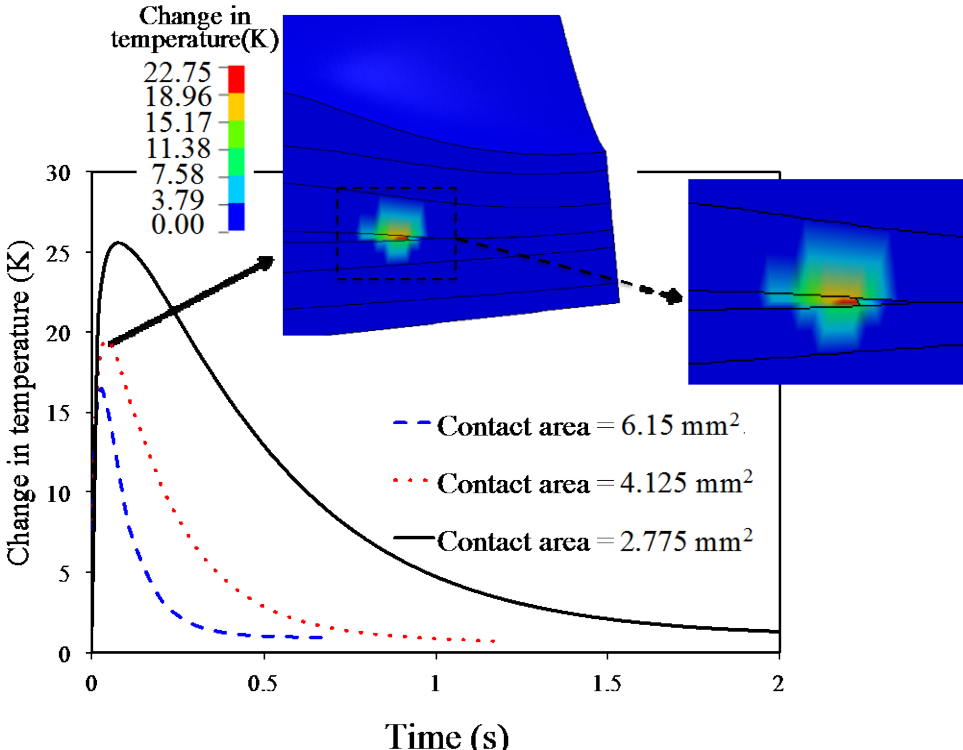
Zhang et al., J Power Sources 2015

MECT Model: Parametric Studies

- Thermal ramp after short circuit can also be predicted using the coupled modeling approach
- 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 response



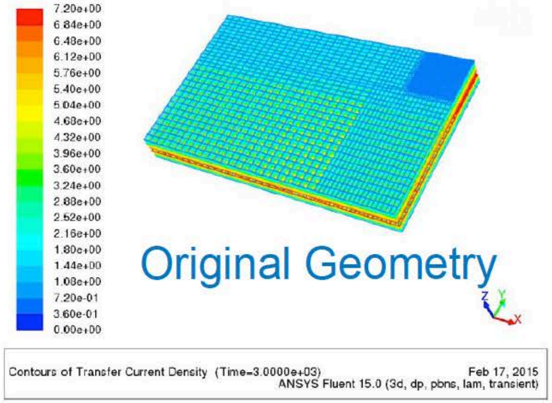


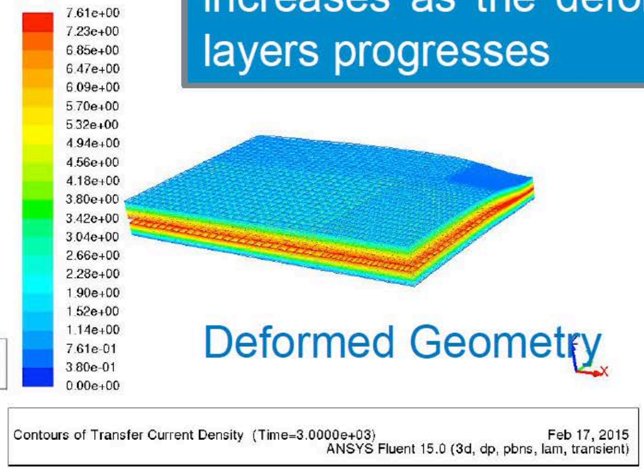
Zhang et al., J Power Sources 2015

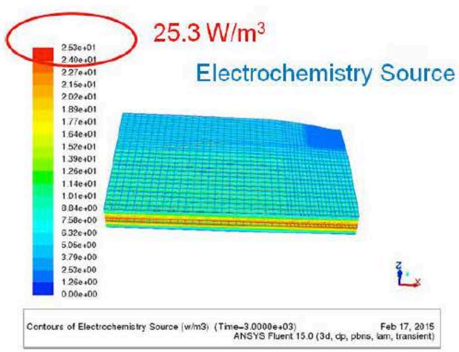
Highlights of location and value of maximum temperature

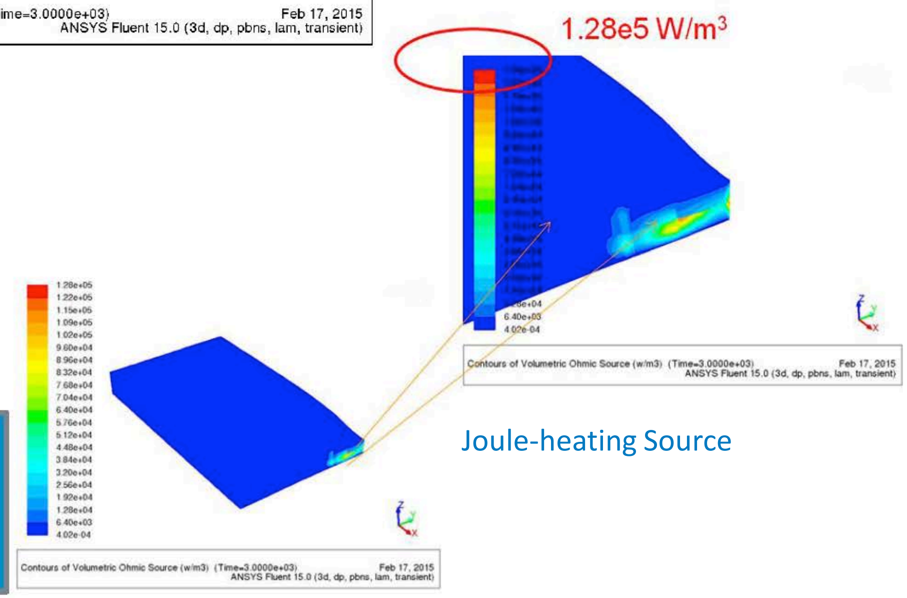
MECT Model: Electrochemical Response

Evolution of Current Density: The current density increases as the deformation of the electrode-layers progresses









Contribution of different Heat Source Terms: Joule heating is localized; but orders of magnitude higher than the entropic heats.

Summary

- We developed a unique sequential approach for coupled mechanical-electrochemical-thermal simulation of lithium-ion batteries
- We conducted a series of tests to characterize the mechanical properties of each component (current collector, active materials and separator), and investigate mechanical failure behavior of a battery cell under external crush
- A single representative sandwich (RS) model was developed, which correlated with experimental results and predicted structural fracture
- Sequential mechanical-electrochemical-thermal coupled simulation was conducted using the single RS model; it predicts initiation of short circuit and consequential voltage evolution and thermal history
- Preliminary results were obtained by linking mechanically-deformed geometry with commercialized ECT model (CAEBAT-1 Achievement)

Future Work

- Simultaneous two-way coupled modeling approach
- Generic material models for battery cells and cell components
- High strain rate impact loading conditions
- Correlate electrical-thermal responses with experiments

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