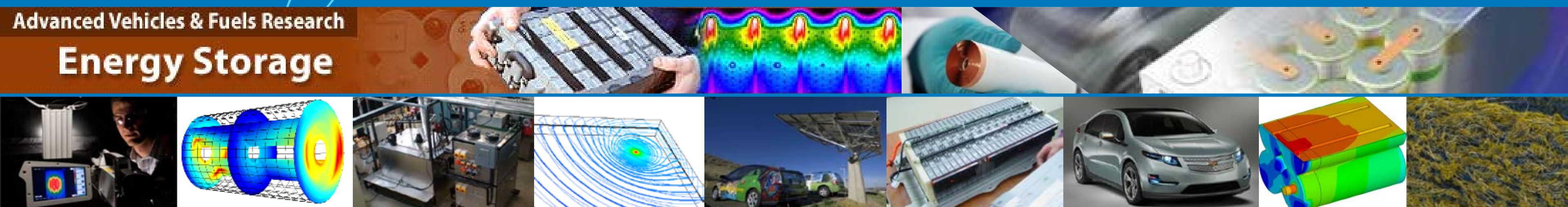
Coupling of Mechanical Behavior of Lithium Ion Cells to Electrochemical-Thermal (ECT) Models for Battery Crush



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NREL/PR-5400-66961

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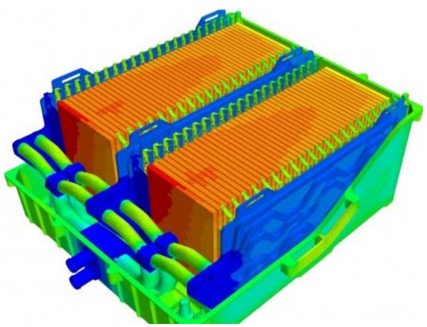
Introduction

- Battery performance, cost, and **safety** need to be further improved
- Modeling/design tools play important roles to achieve these goals
- DOE CAEBAT-1 activity has resulted in ECT CAE simulation tools



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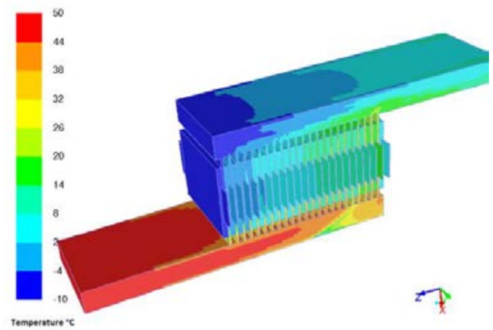
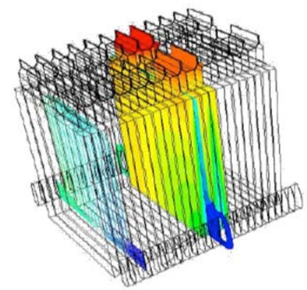
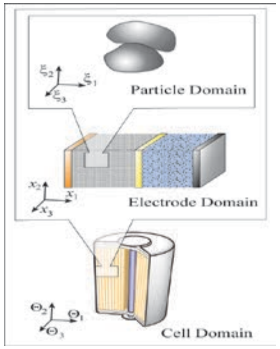


EC Power



ANSYS



NREL MSMD

- In CAEBAT-2, mechanical modeling is being added to ECT tools to simulate cell response after a crash-induced crush

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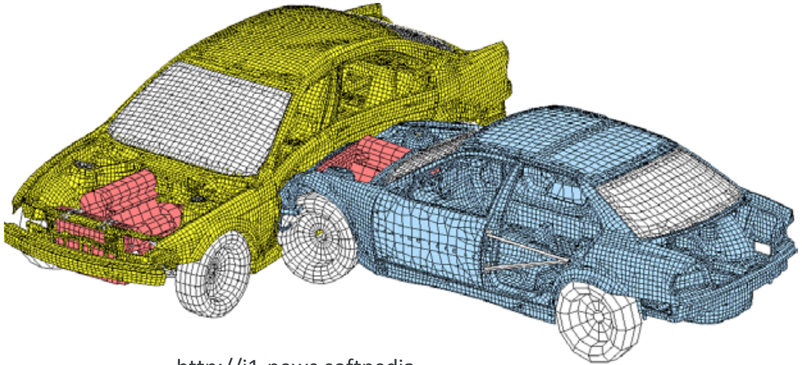


http://i1-news.softpedia-static.com/images/news2/BMW-and-Audi-Are-Using-Linux-2.png

Battery MECT Modeling After Crash

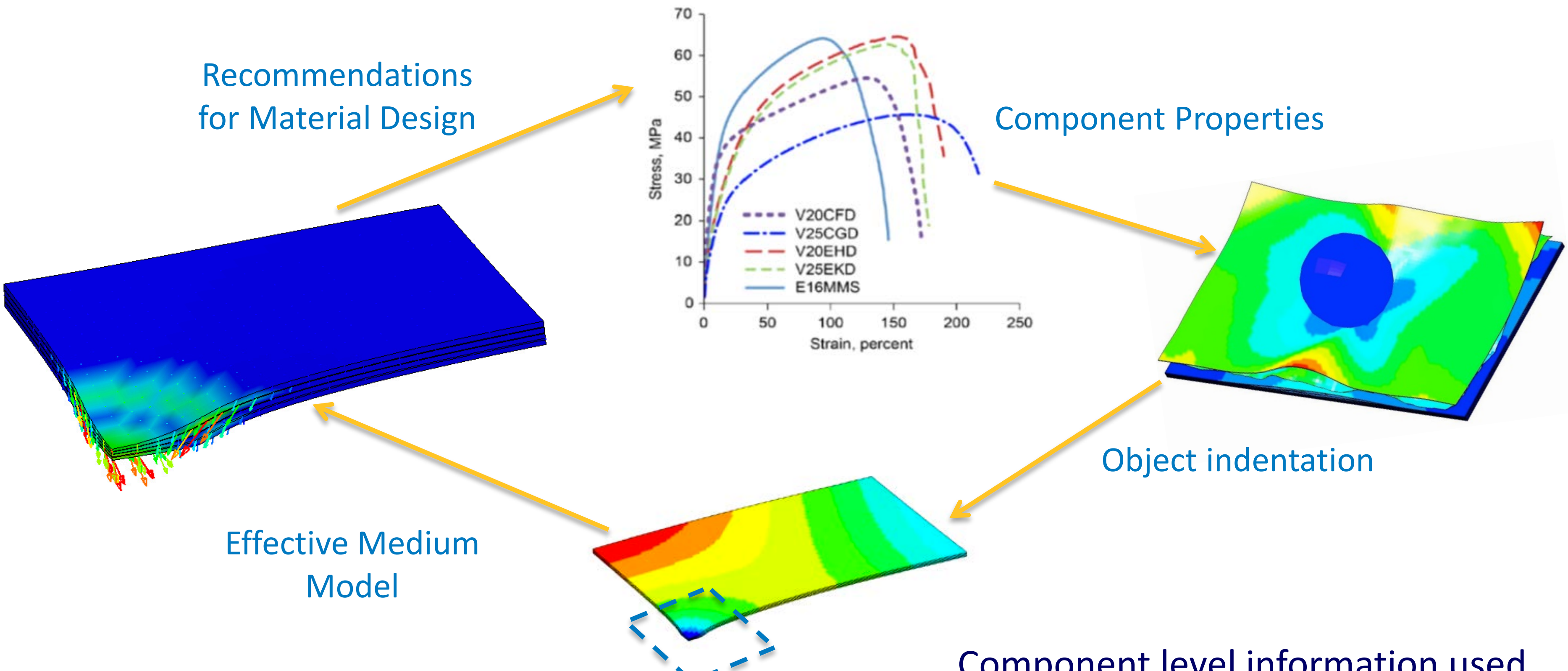
- Vehicle crash → battery crush → cell damaged zone → separator failure → electrode contact → local short → current flow → heat generation → insufficient heat rejection → *temperature* increase → *onset* temperature reached → spontaneous reactions → thermal runaway → smoke and fire

→: may lead to (depending on many factors)

- Simulating all physics and geometries at the same time is challenging and takes a lot of efforts; simplifications are needed
- Our approach:
  - Decouple structural behavior from ECT interactions
  - Simplify and use **LS Dyna** to simulate structural changes after crush
    - Need to obtain structural/mechanical material properties of cell components
  - Then, capture characteristics of damaged zone and transfer to ECT
  - Finally, use data for electrochemical and thermal modeling

MECT Model: Coupling Methodology

- As crash-induced mechanical crush is a much faster process than electrochemical and thermal response, our initial approach was to develop a **sequential one-way coupled** modeling approach
- Conducted electrochemical and thermal modeling on top of a mechanically-deformed geometry



Component level information used to build a constitutive cell-model

MECT Model: Mechanical Properties Measurements

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

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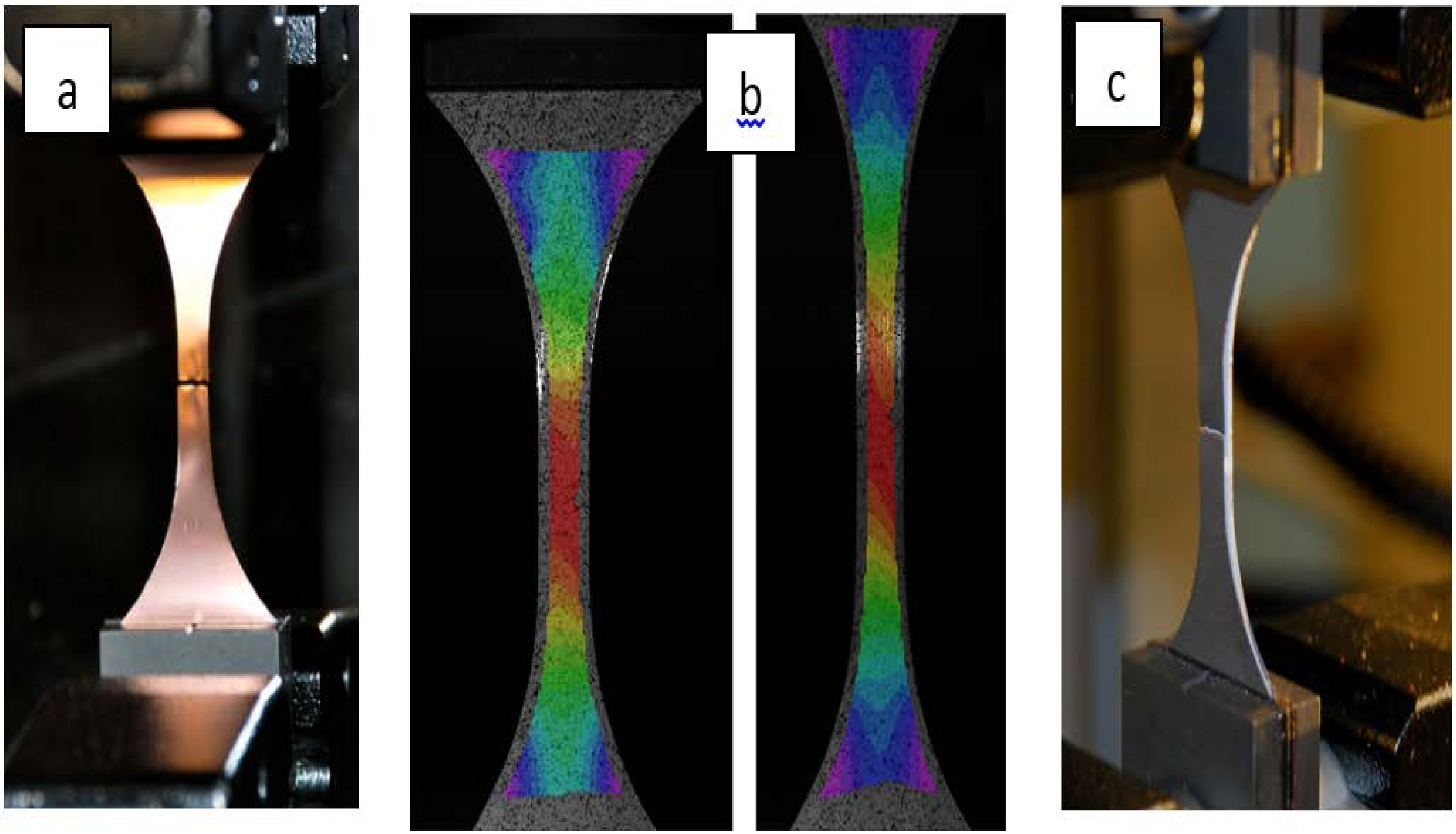


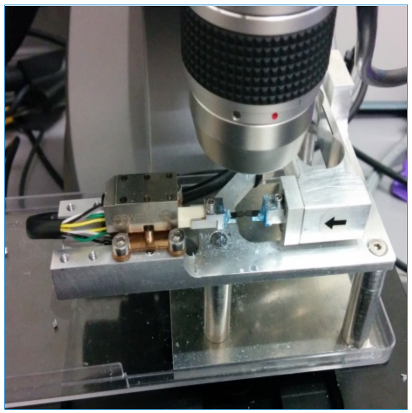
Anode current collector | Separator | Cathode current collector

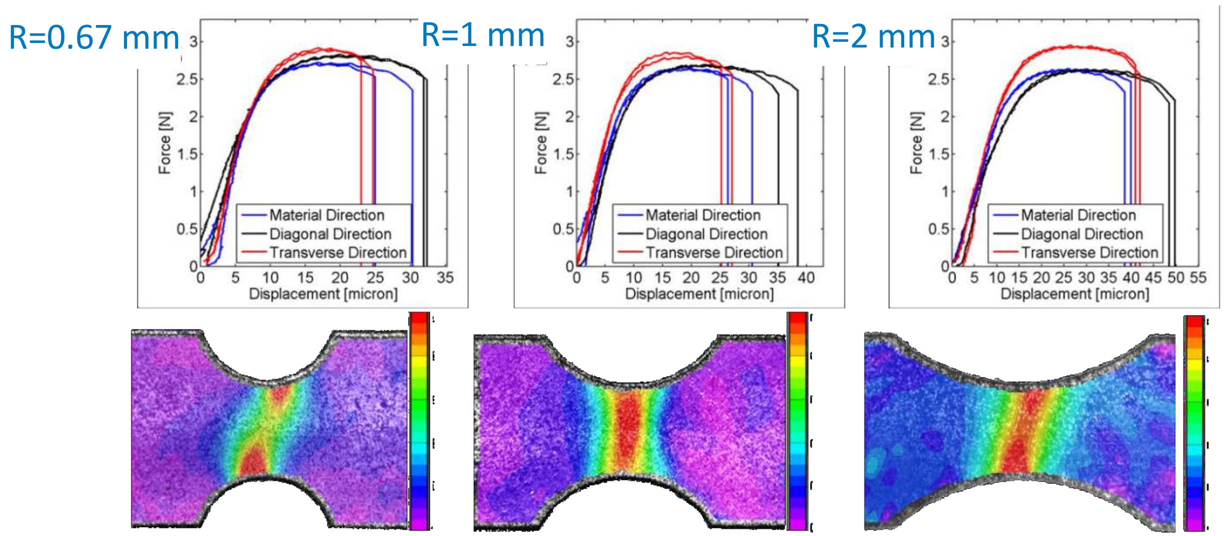
Sahraei et al, Journal of Power Sources, 2015

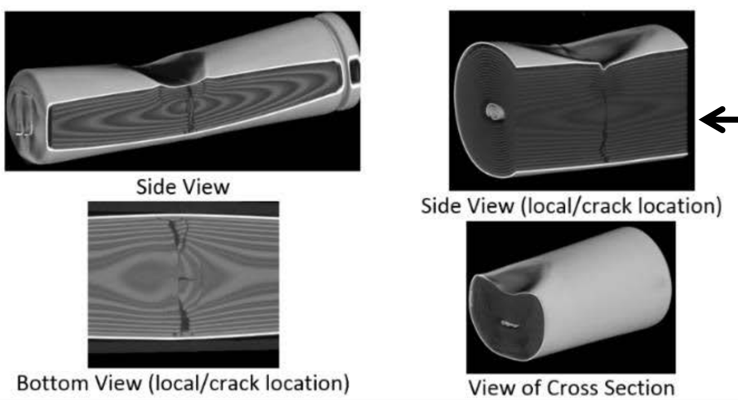
MIT Mechanical Characterization

- **MIT providing experimental and model inputs, to support the mechanical constitutive and fracture modeling of battery cell components**

Micro testing of collectors

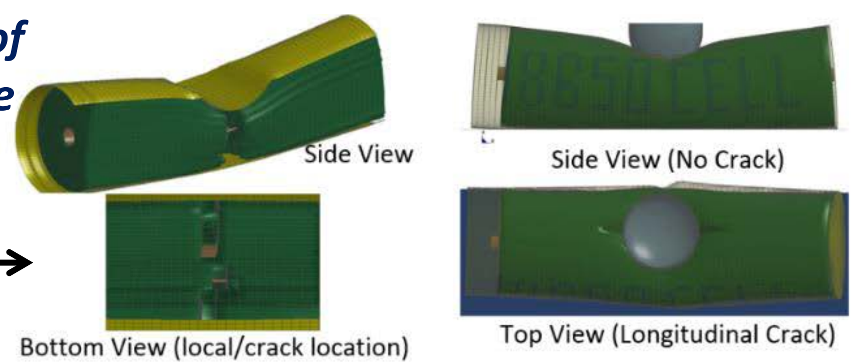






CT images of cell fracture

Fracture modeling



Component Testing: Tensile Test Results

- Tensile tests showed a typical elasto-plastic response for metallic thin films for the current collectors.
- Anisotropic behavior was observed in the separator tests.

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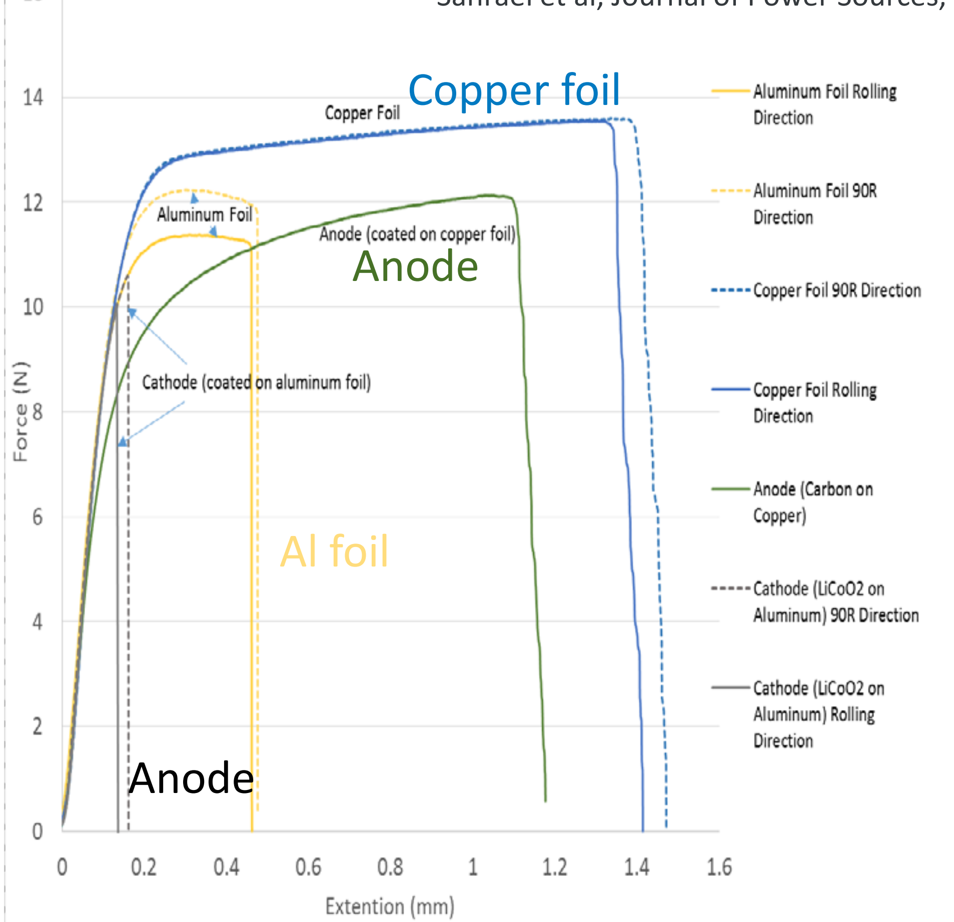
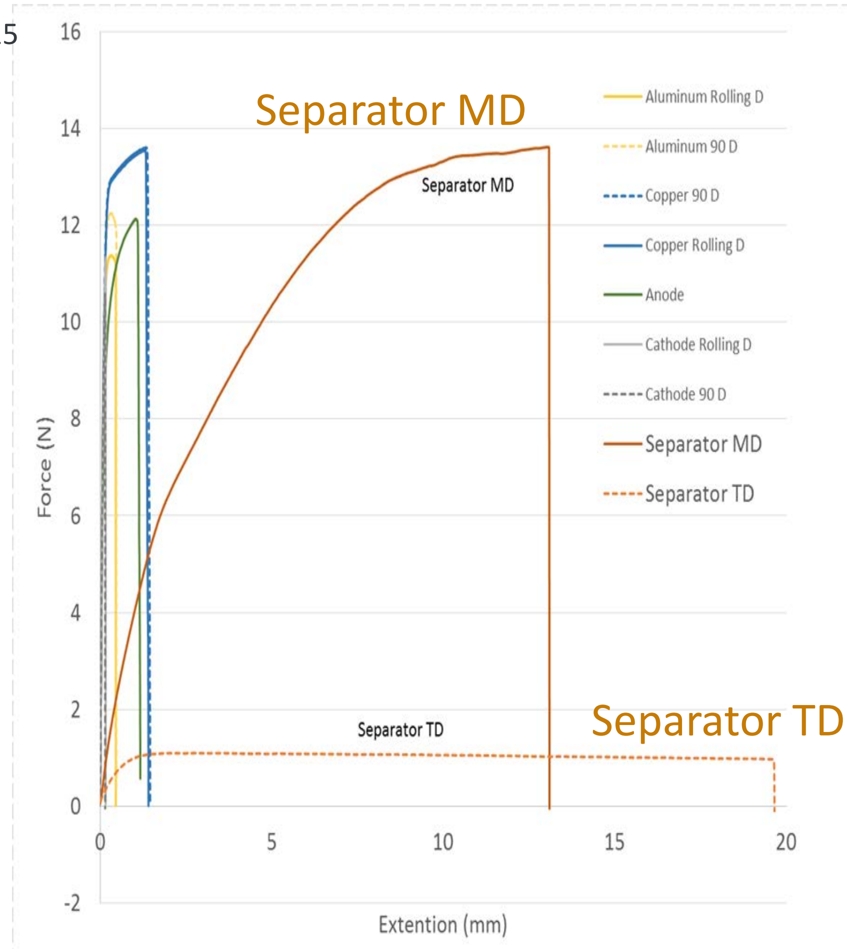
Sahraei et al, Journal of Power Sources, 2015

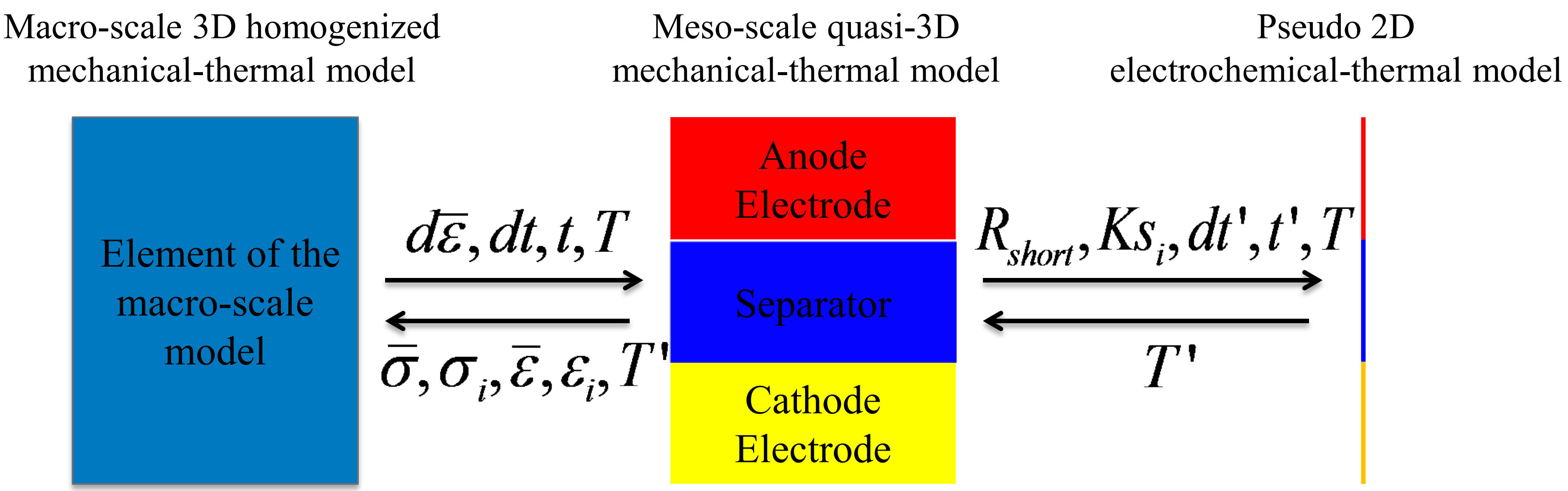


Electrodes and current collectors



Electrodes and separators

NREL Multi-scale Simultaneously Coupled MECT Model



- Short Resistance ($\Omega \bullet m^3$)

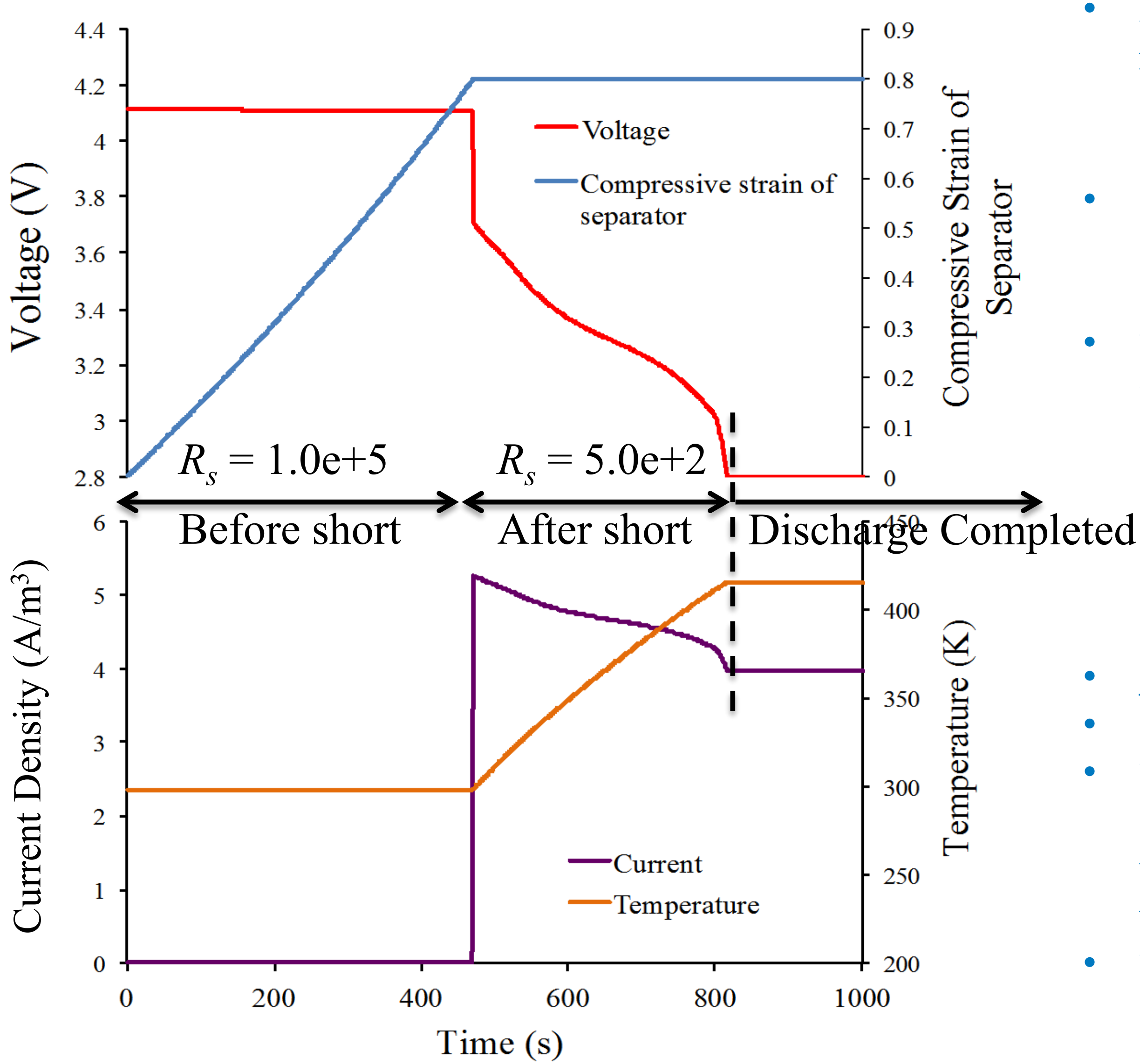
  Different type of shorts can be distinguished by the short area for the different failure modes of separator layer, e.g. tensile failure or shear failure.

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

- 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.

NREL Single-Element Demonstration of MECT Model

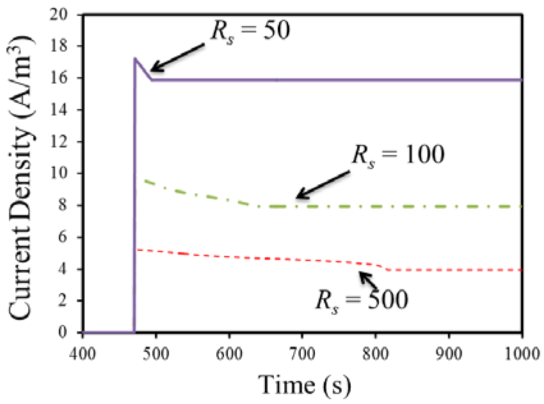


- Linear elastic mechanical response for electrodes and separator were used for demonstration purposes.
- Strain based failure criteria for separator was used to simulate short-circuit.
- The current shows an instant increase and then starts drop due to the decrease in the cell voltage.

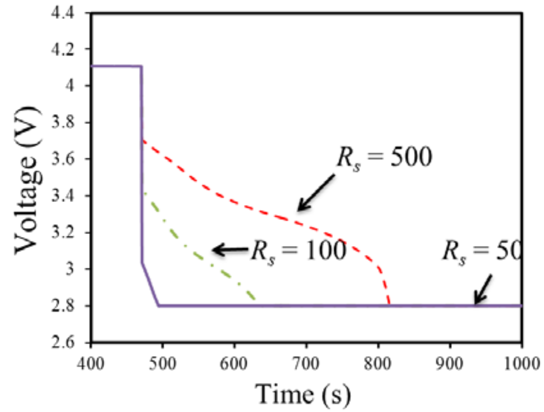
- Simulation Conditions:
- 5 Ah $LiCoO_2$/graphite cell
- The cell voltage of fully discharged is set to 2.8V and the battery model stops after that.
- The model uses 2 minutes for 10^6 time steps.

NREL Numerical Study on the Effect of Short Resistance

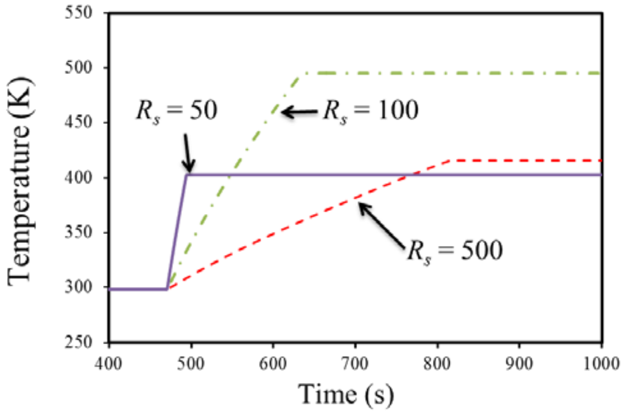
- **The developed MECT model is further utilized here to investigate the effect of short resistance on the battery cell performance**



Current Profile



Voltage Profile

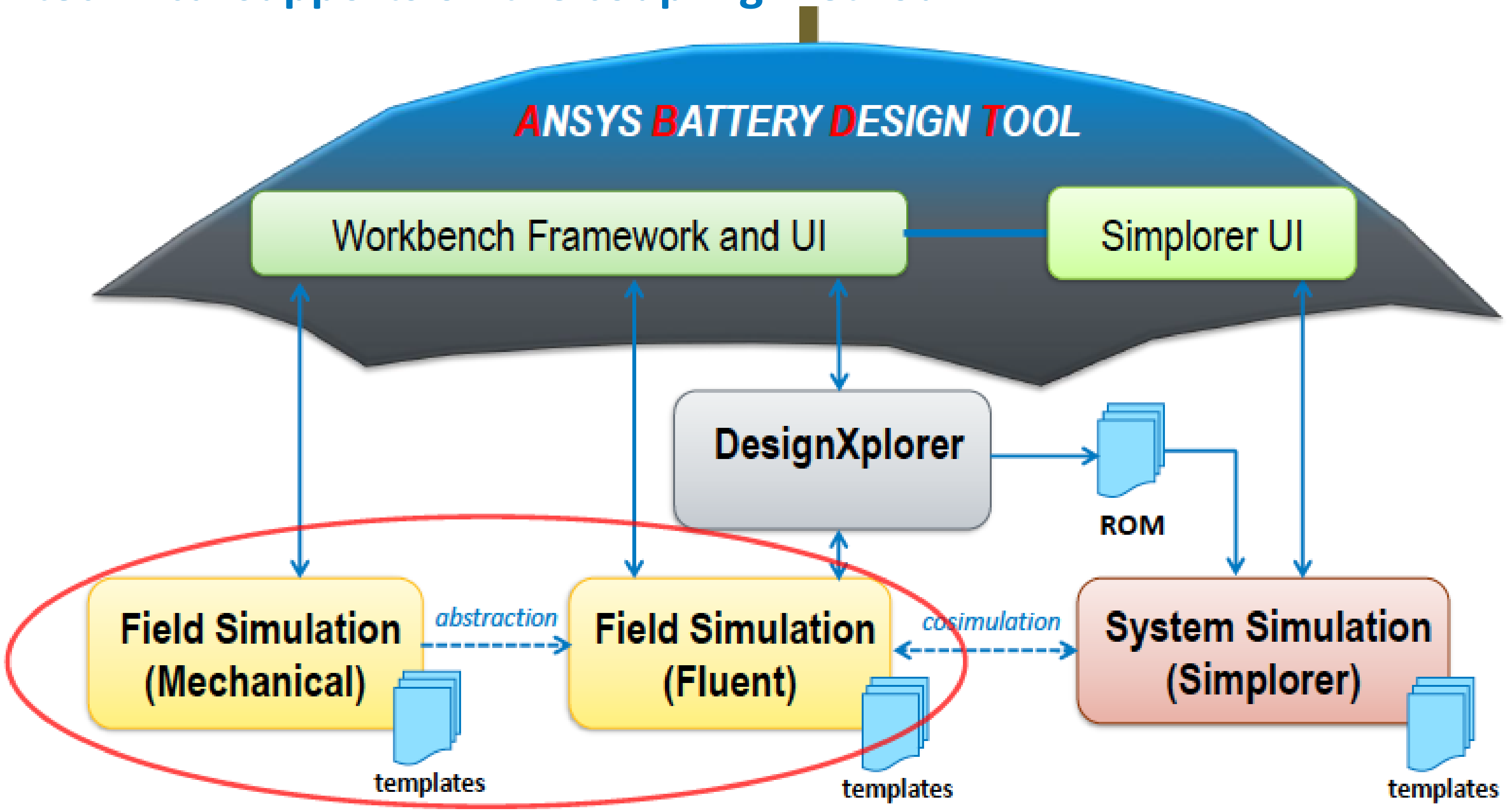


Temperature Profile

- The model captures the effect of short circuit resistance on the subsequent electrical response.
- 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.

ANSYS Integration of Mechanical - ECT Coupling

- **ANSYS implementing the developed MECT model in ANSYS products, providing technical supports on the coupling method**

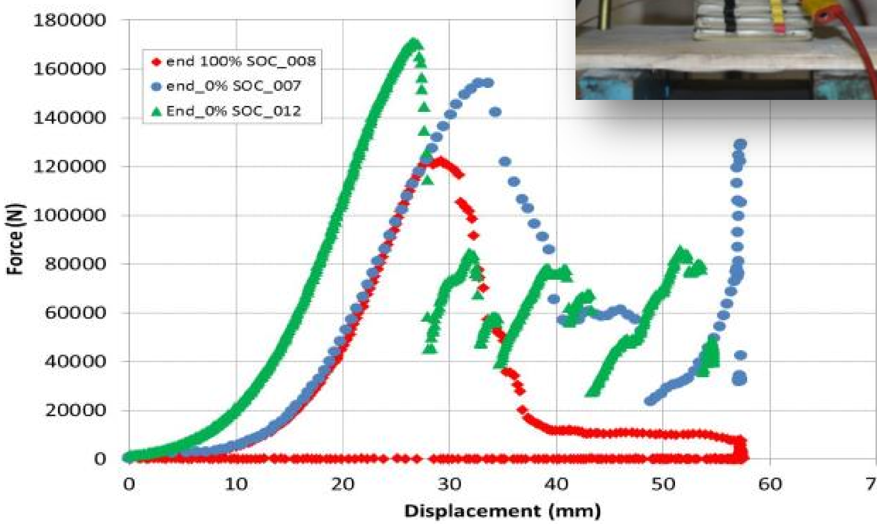


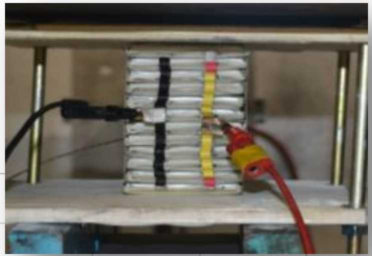
- Convenient "vertical app" around standard ANSYS products
- Plug-and-play with other products via open-standard interfaces

SNL Battery Abuse Testing for Validation

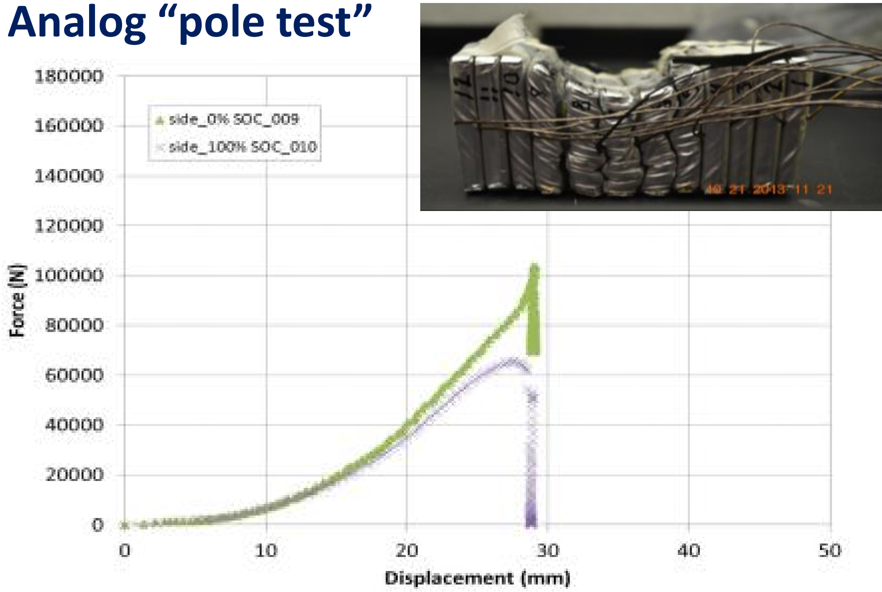
- **SNL providing experimental of abuse test of batteries to support MECT model development**

Module Compression



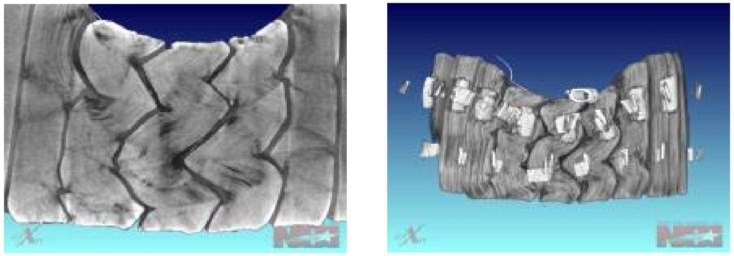


Analog "pole test"



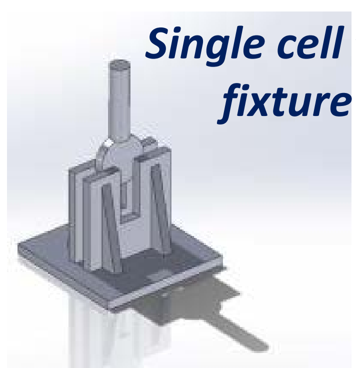
- ***Determining coupled failure behavior of batteries during crush/impact testing***
- ***Providing module level data support for validation of MECT model***

CT image of structural failure



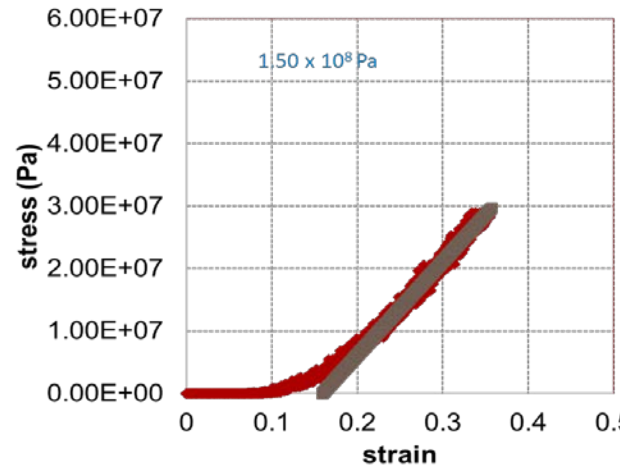
SNL Abuse Testing Planned

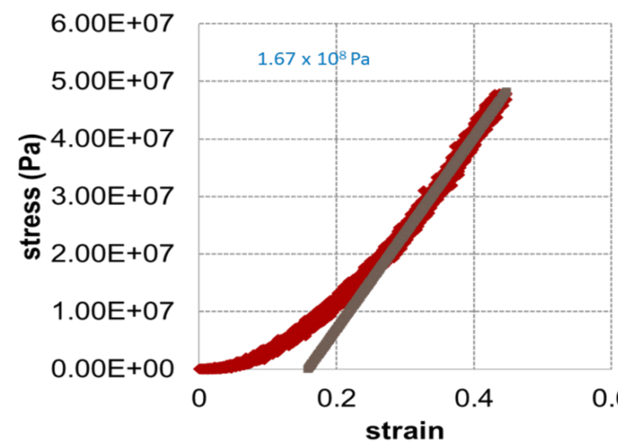
- Single cell end crush – new fixture built for single cell tests
- Failure mode investigation - Crush and CT analysis of charged and discharged packs crushed to predetermined displacement
- Dynamic Testing – drop testing at burn site



Single cell test fixture

Single cell test data





Summary

- Developed a material model for simultaneously modeling of mechanical-electrochemical-thermal behavior
- Predicted the electrical short, voltage drop and thermal runaway behaviors followed by a mechanical abuse induced short
- Studied the effect of short resistance on the battery cell performance
- Demonstrating the applicability of the developed model for full pouch cell abuse simulation
- Received first round of data from SNL on abuse test of battery module
- Implementing ABDT tool into standard ANSYS System in Workbench

Future Work

- Full cell numerical study using the material model presented in this report.
- Verification compared with existing electrochemical models, for example, ANSYS MSMD model.
- Evolve ABDT into standard Analysis System in Workbench
- Work with MIT on fracture modeling of battery cell components.
- Validation against test data from SNL.

Acknowledgements

The NREL Team

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ANSYS

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