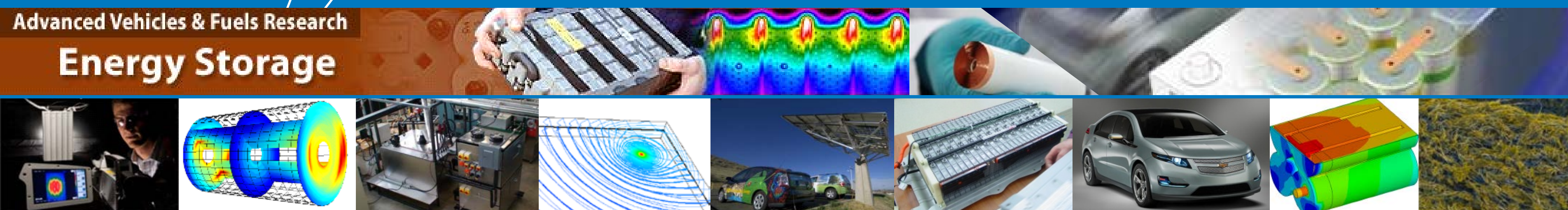
Mechanical-Electrochemical-Thermal Simulation of Lithium-Ion Cells



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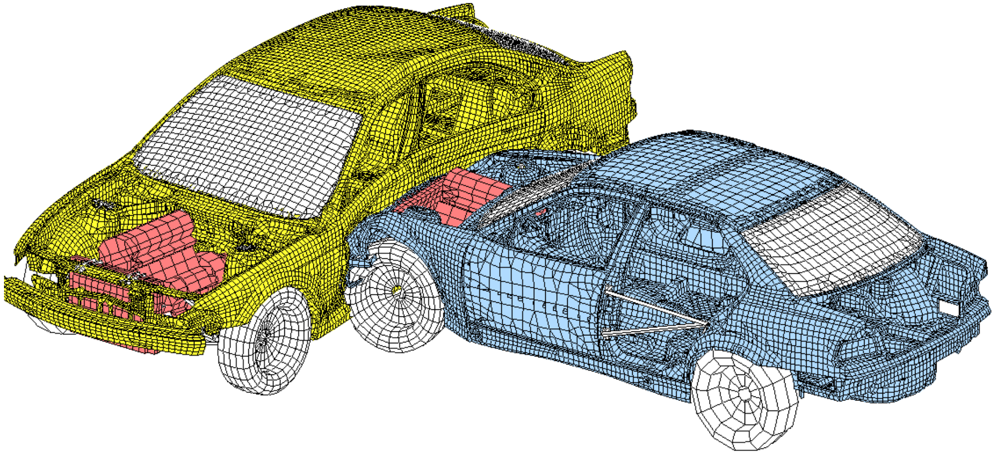
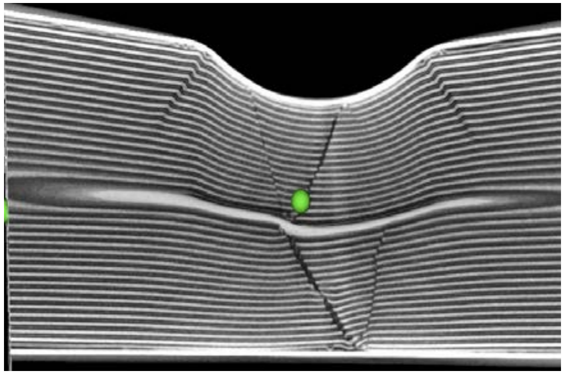
Introduction

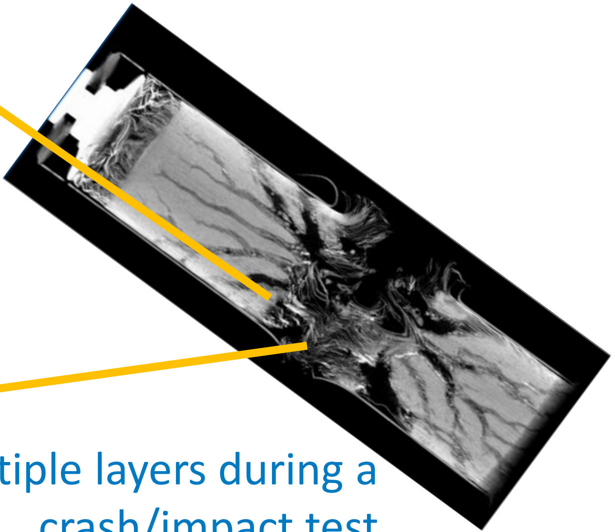
- Battery performance, cost, and **safety** must be further improved for larger market share of HEVs and PEVs
- Significant investment is being made to develop new materials, fine tune existing ones, improve cell and packs design, and enhance manufacturing processes to increased performance, reduce cost, and make battery **safer**
- Modeling, simulation, and design tools can play important roles to provide insight on how to address issues, reduce the number of build-test-break prototypes, and accelerate the development cycle of producing products.



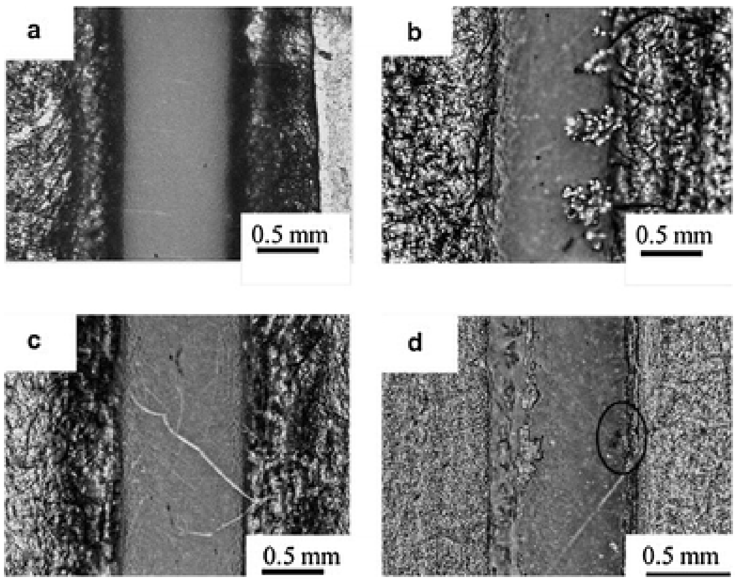
Mechanical Failure in Cell Components



Crack in active material coatings



Fracture of multiple layers during a crash/impact test

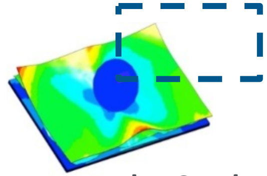


Dendrite penetrating separator films

Slow crush of a battery module

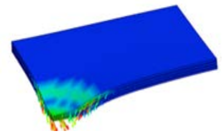
Approach

Start with Cell-Level Test Results as Input

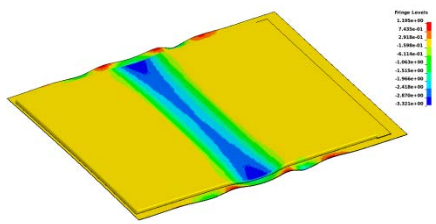


Displacement under Crush

Parameterize material response

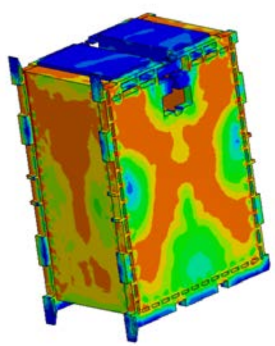


Current density under short-circuit



Simulate Cell-Level Response for Multiple Cases

Validate against Module-Level Data



Scale to Module-Level

Import Initial Geometry

⇩

Crush + Electrical Simulations in LS-DYNA

⇩

Compute individual ‘resistance’ Vs deformation

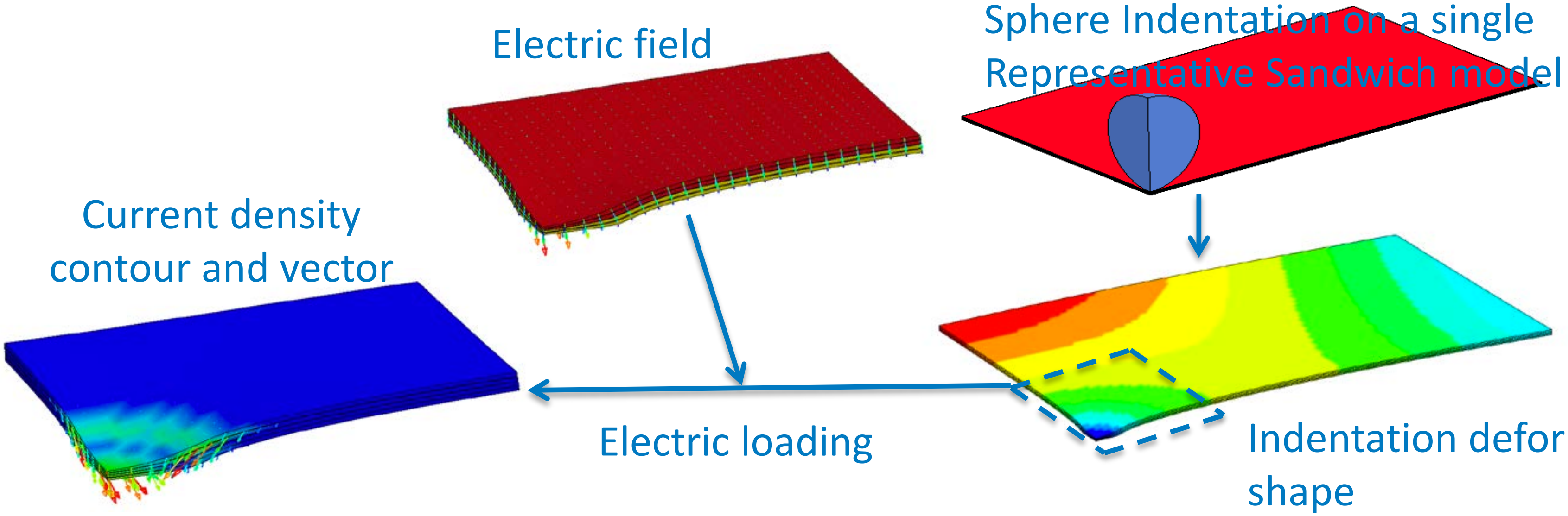
⇩

Feed Mesh and Resistance to ANSYS

⇩

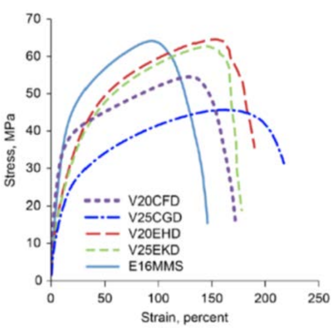
Echem + Thermal Simulations in ANSYS

MECT Models in CAEBAT



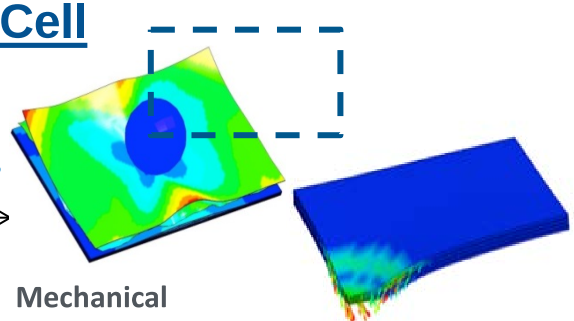
Zhang et al. Journal of Power Sources, 2015

Component



Interaction of Mechanical/Electrical/Thermal effects

Cell

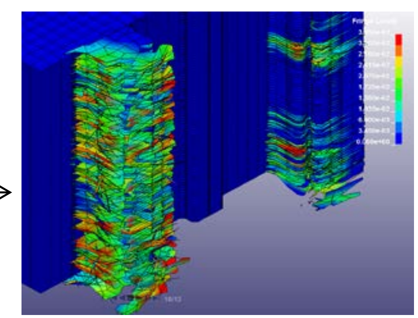


Mechanical Displacement under Crush

Current density contour and vector

Module

Propagation phenomena under crush



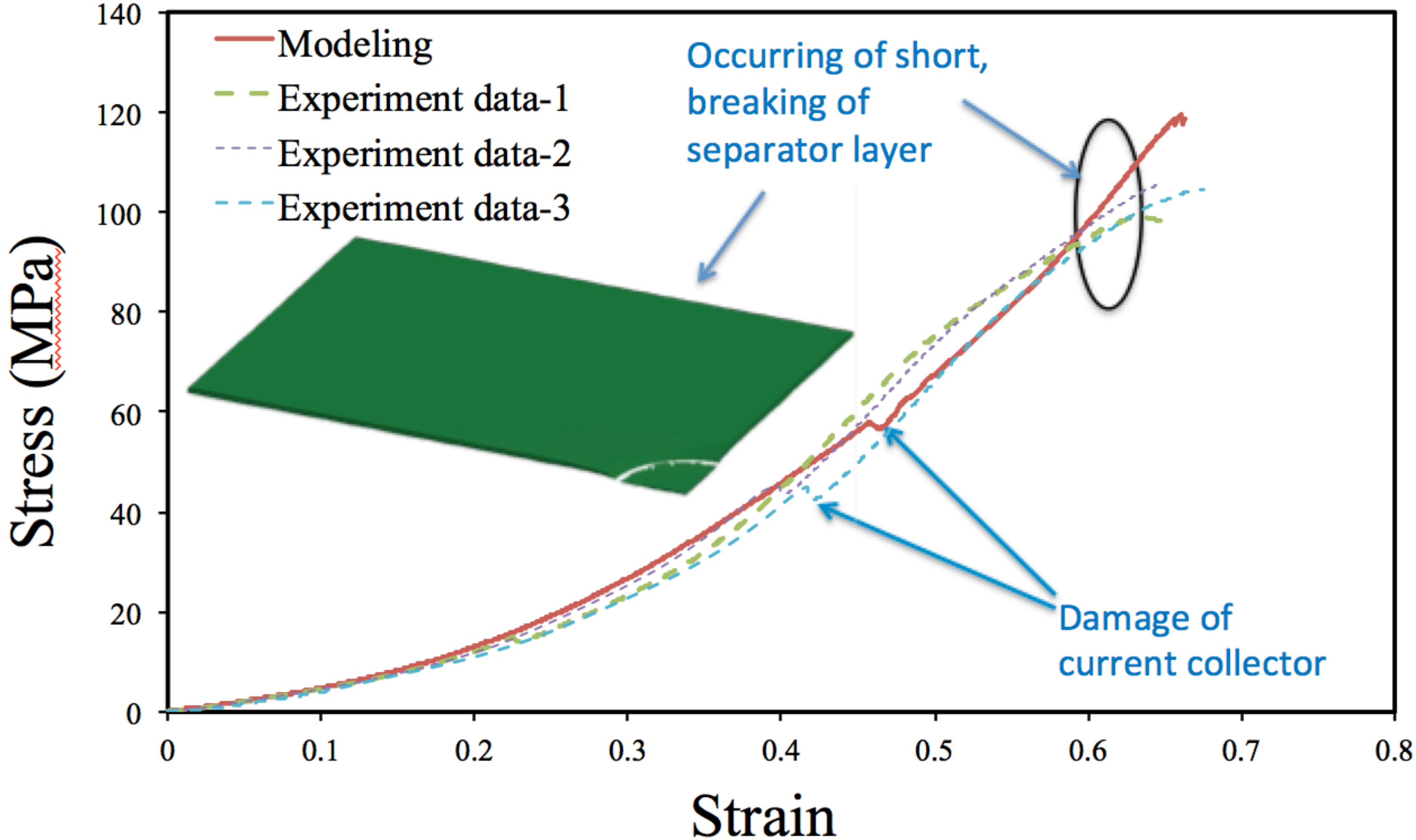
Displacement from crush response of a multi-layer stack

Aging

Santhanagopalan et al. 228th ECS Meeting, 2015

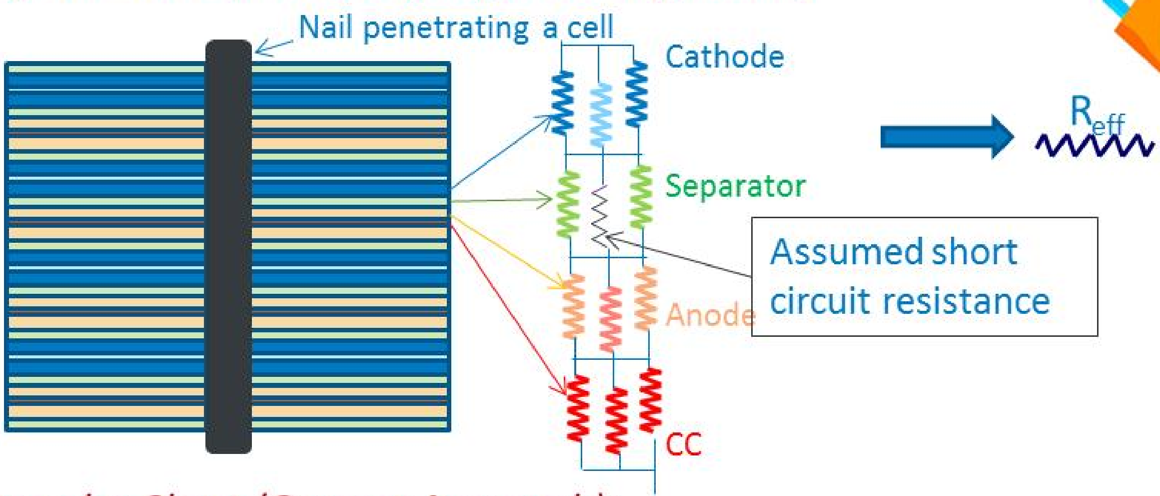
Constitutive Models

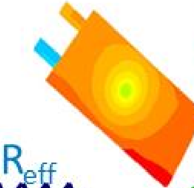
- Constitutive Models are extracted from component-level test data



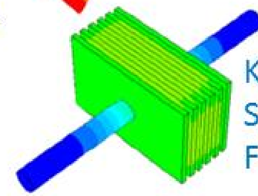
Short-Circuit Resistance

Regular Short (Previously Reported Approach):



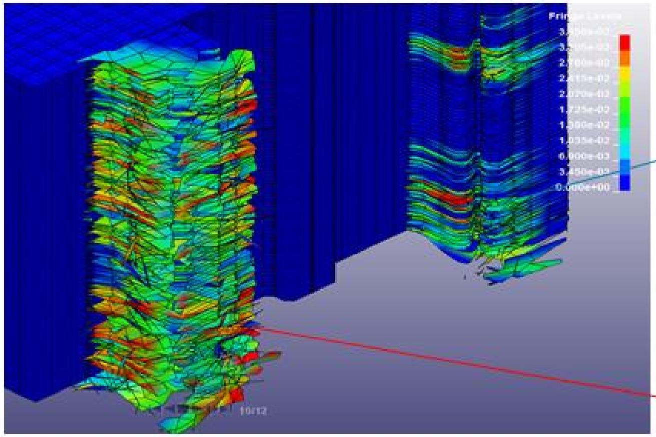


Gi-Heon Kim, 6th Lithium Mobile Power Conference, Boston MA, 2010.

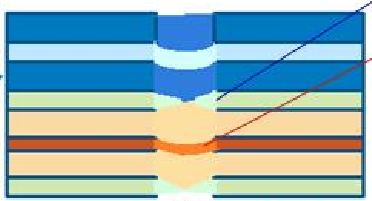


Kalupson et al., ECS Spring Meeting, Orlando FL, April 2014.

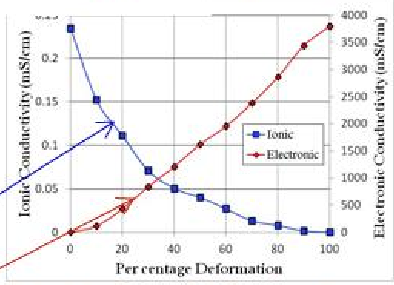
Irregular Short (Current Approach):



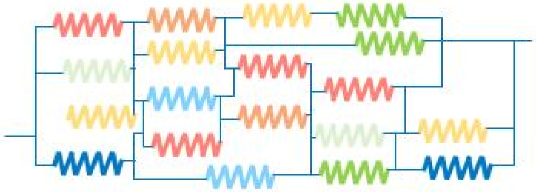
Deformed geometry obtained using CAD geometry of cells subjected to crush in LS-DYNA simulations



Before fracture



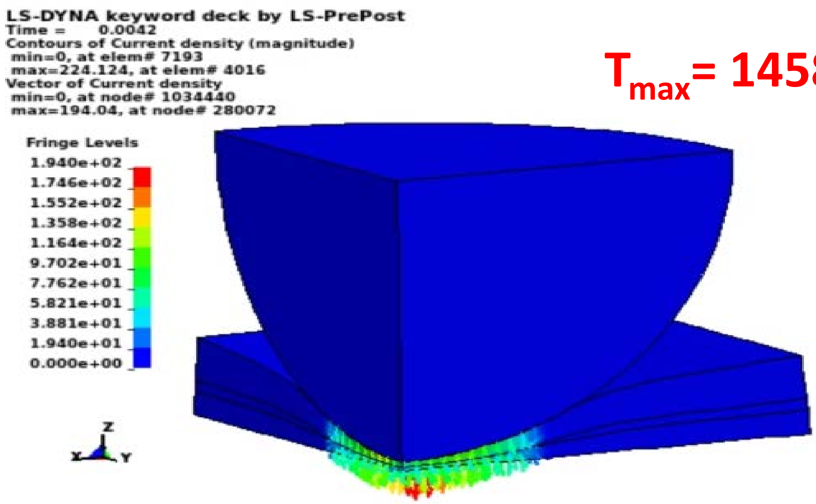
Use ionic and electronic resistivity of the deformed layers change as a function of thickness



Calculate short resistance by solving Maxwell's equations in Ansys or DYNA using deformed geometry and properties of individual layers

Santhanagopalan et al. , 228th ECS Meeting, 2015

Component Level Results



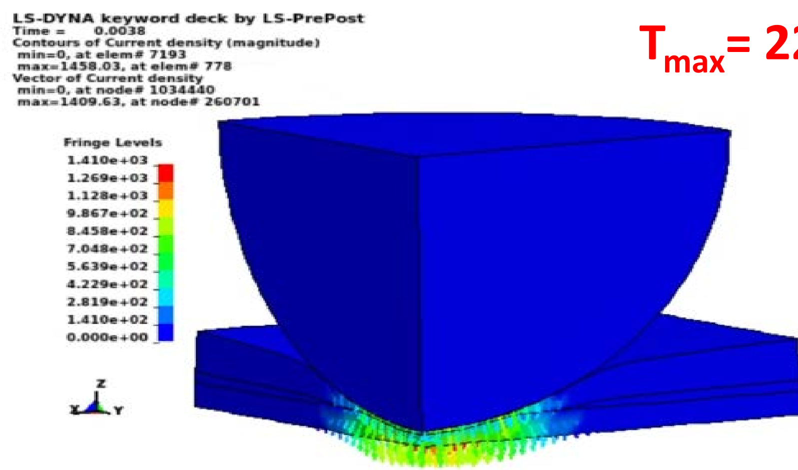
T_{max}= 1458°C

- ❖ Models accommodate detailed description of different heat sources and heat dissipation pathways:
  - Joule heating
  - Reaction heats
  - Properties as functions of temperature

Anode-to-Aluminum Short

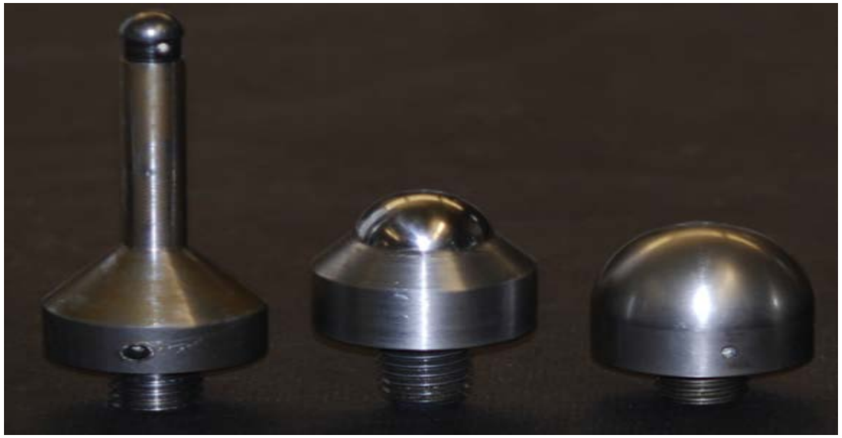
Anode-to-Cathode Short

- ❖ Models can distinguish different types of short circuit
- ❖ Short areas for in-plane versus through-plane failure of cell components are different
- ❖ Propagation pathways in modules and packs depend on types shorts, electrical pathways and heat dissipation rates

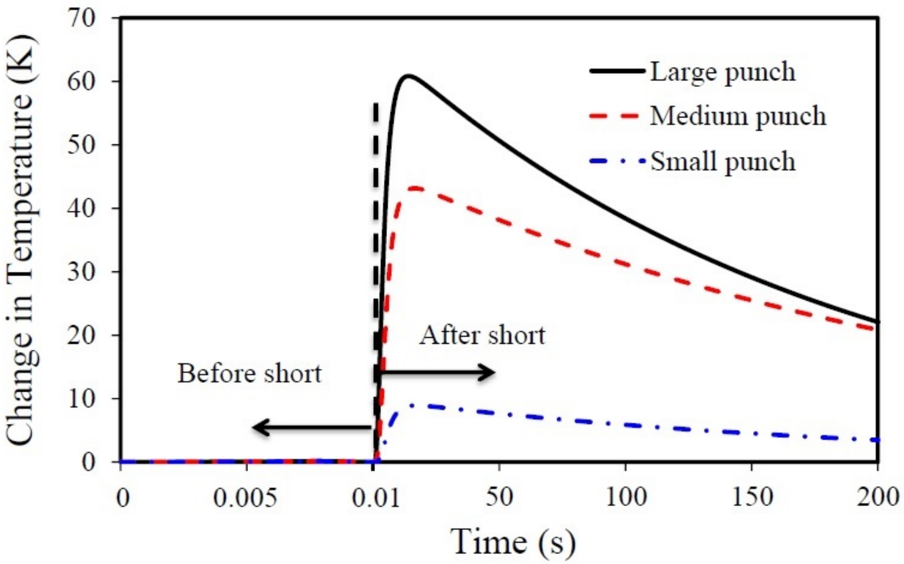


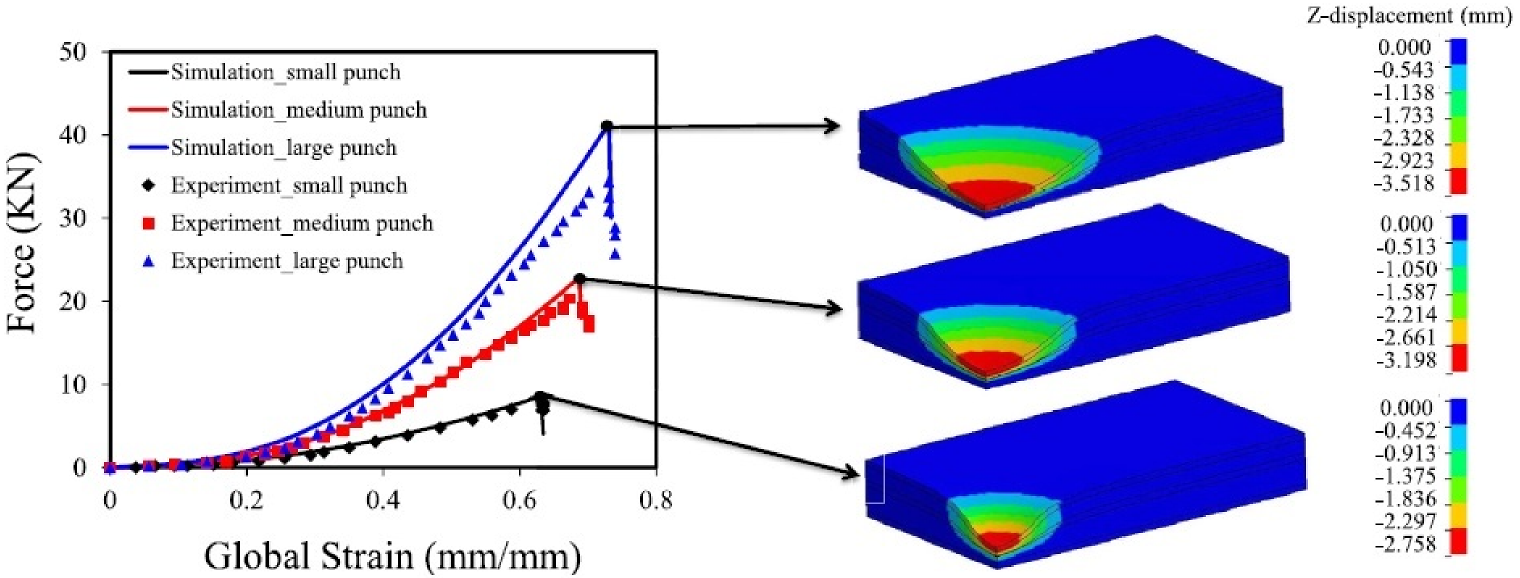
T_{max}= 224°C

Designing Test Methods



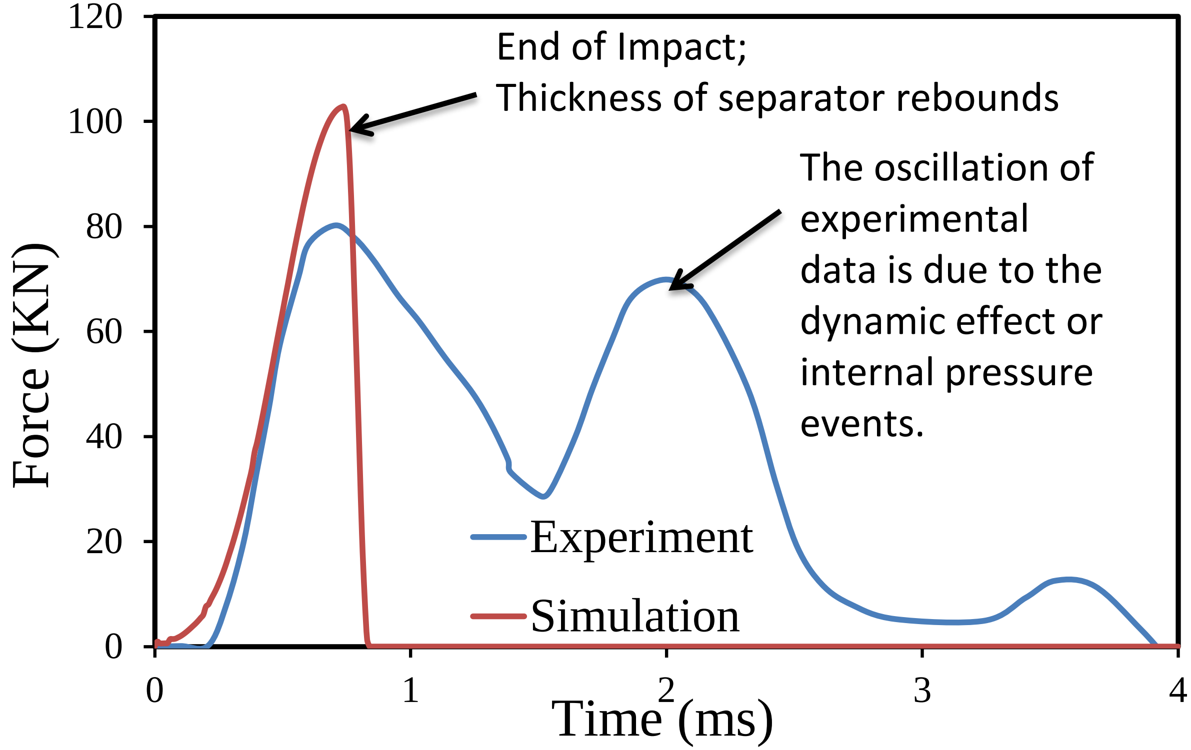
Sahraei et al. Journal of Power Sources, 2014

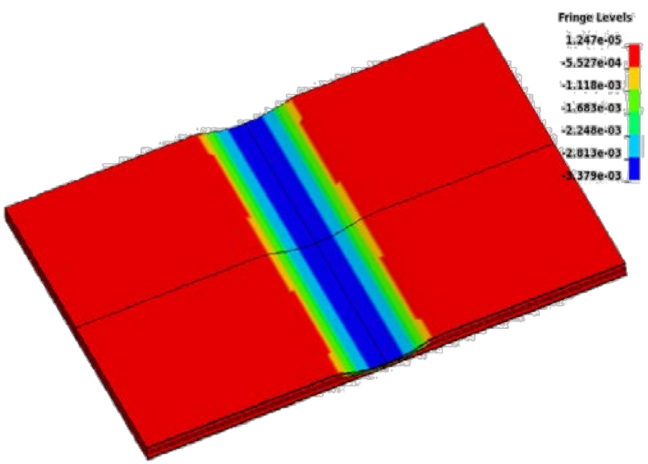




Crash Response – Mechanical Results under Cell Impact

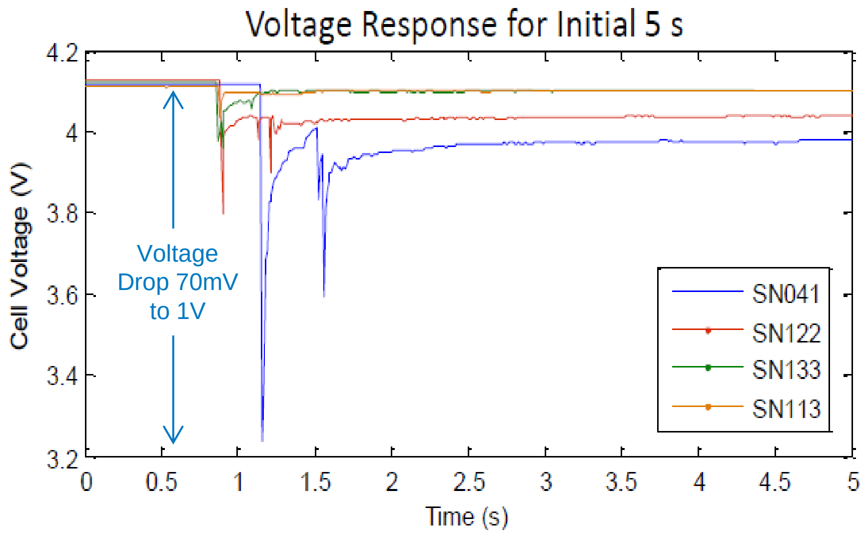
Comparison of experiment vs. simulation results

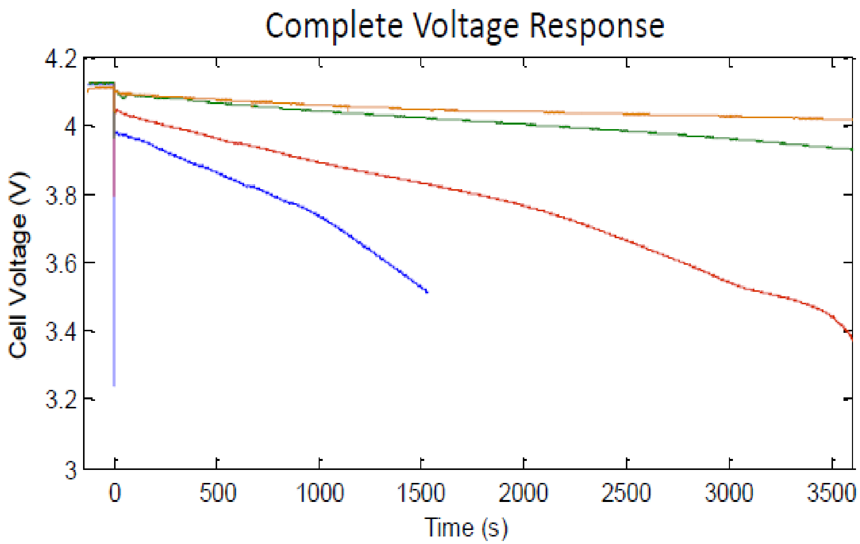


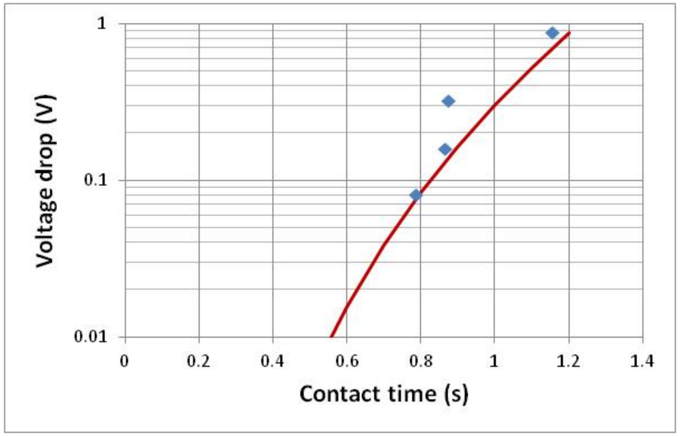


- Cell level mechanical simulations predict no breach of the packaging; this is in line with the experimental observations.
- The maximum force during the impact test is captured to within 20% of the experimental value in the simulation results.

Crash Response – Electrical Characteristics





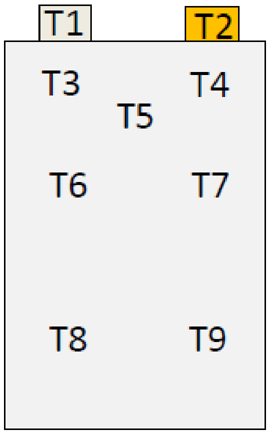


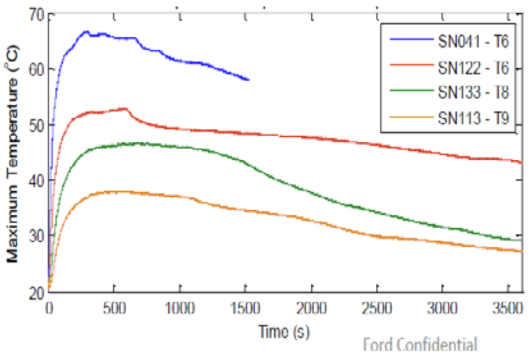
Model predictions (solid line) versus experimental data from high-speed imagery (dots): Consistent with the model predictions, the initial voltage drop varies directly as a function of contact time with the load.

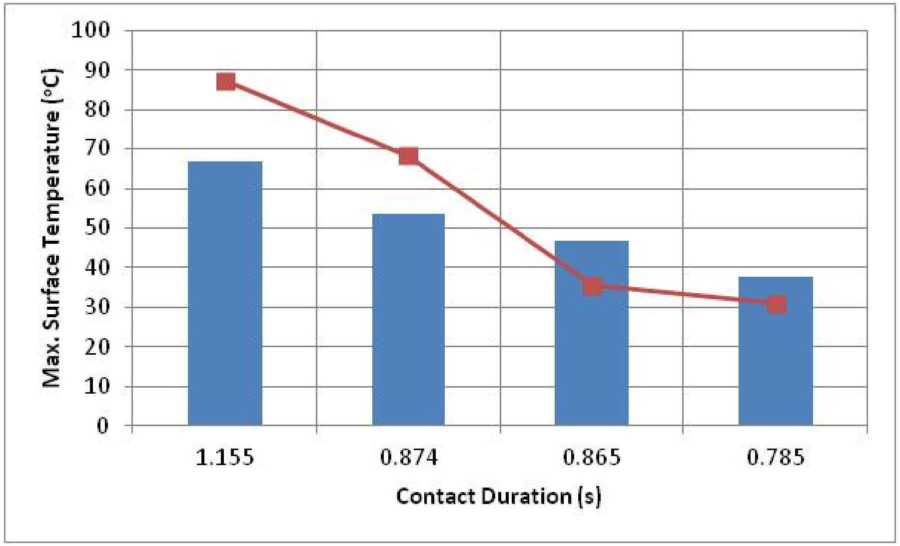
- Different contact times between the impact-load and the cells used to capture different extents of voltage drop.
- Resistance of short varies with the duration of contact.
- This metric is predictive – and can be used as an indicator of the remaining energy in the battery at any given time after the crash. This result has significant implications towards safety assessment of battery packs after crash.

Single Cell Thermal Response

- Cells were out-fitted with 9 thermo couples at locations shown in the figure alongside.
- Unlike previous results that show a continuous evolution of temperature and heating-up of the tabs, the thermal simulations for crash-induced temperature rise, show localized heating.
- The temperature subsequently drops in the simulation results, due to the change in the contact resistance during a mechanical crash.
- Previous models assuming constant resistance throughout the short-circuit predict propagation along the current collectors 25s into the short.
- Evolution of resistance with mechanical deformation predicts localized thermal events within the first few seconds of impact.
- The simulation results capture the trend from the experiments, that the maximum temperature rise is proportional to the duration of contact of the impactor with the cell.

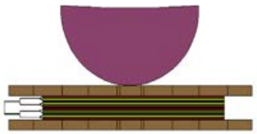






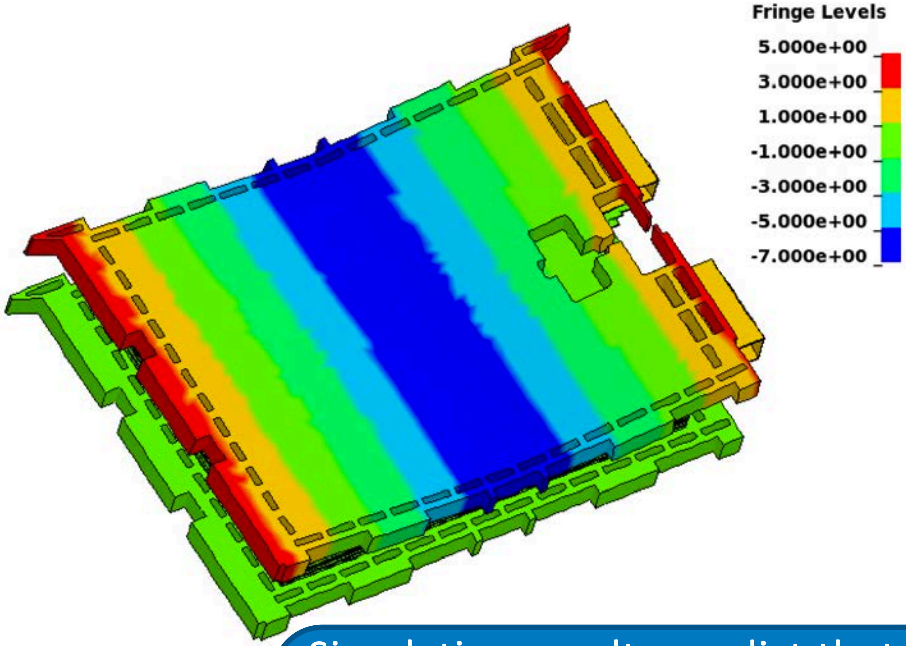
Max. temperature proportional to contact time

1S4P Cell-String – Mechanical Results

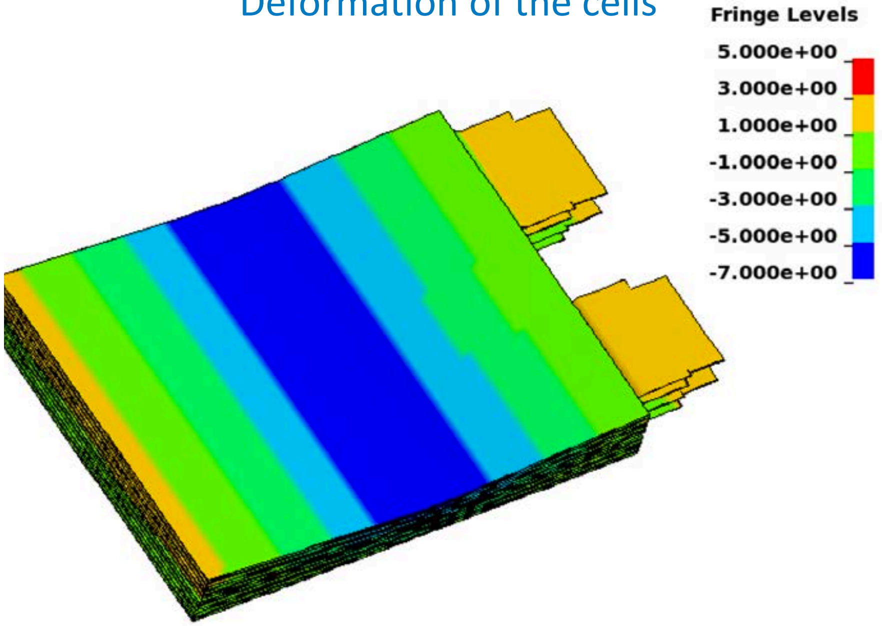


Simulation Results - Displacements

Deformation of packaging material



Deformation of the cells

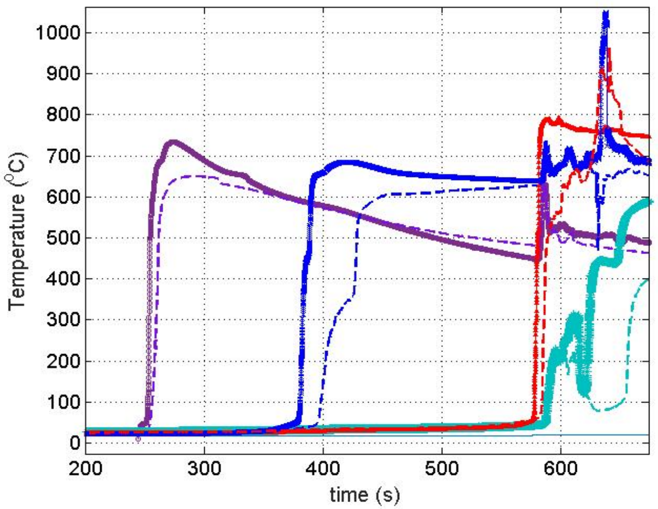


Simulation results predict that:

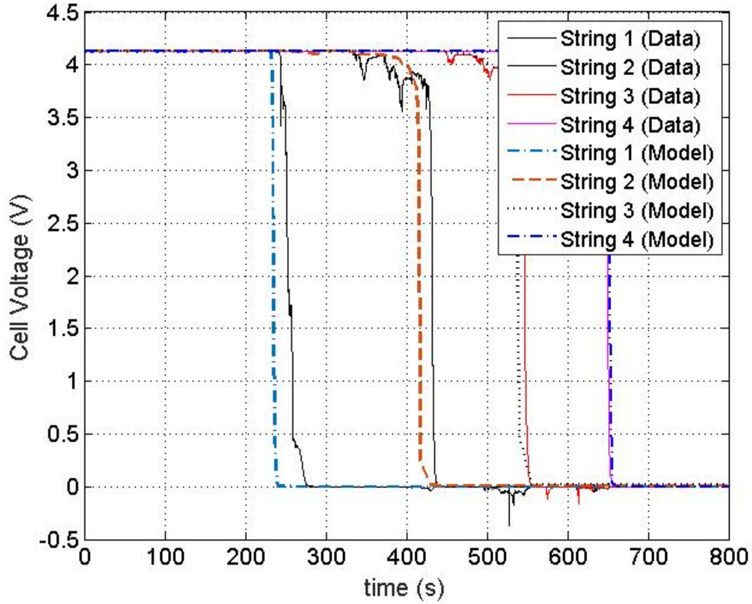
1. The packaging can prevent deformation of the cells by as much as 50% under these crush test conditions.
2. There is a significant scope to light-weight the pack, even after the safety threshold is met.

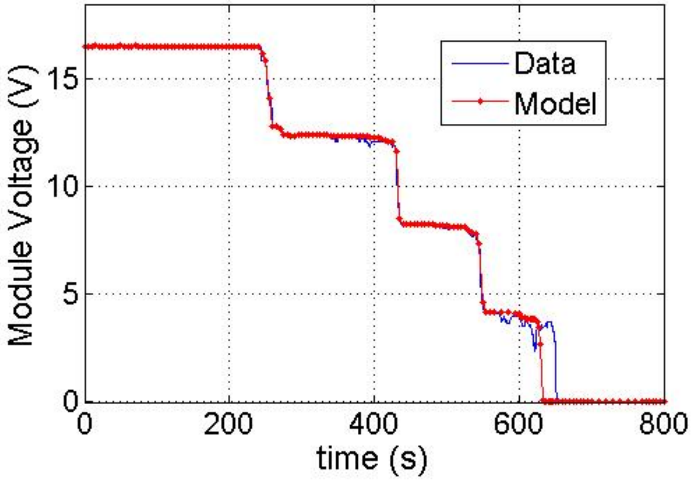
4S5P Module – ECT Response

- Utilizing cell and string-level outcome as inputs, the module-level model was able to capture the voltage drop across each string with good accuracy.
- The thermal parameters for the packaging material are the biggest unknowns. So, the temperature data was not a good match.
- The simple model was not able to capture the multiple step-rise in temperature due to the different reactions.



Max. Module Temperatures during Propagation





Multi-cell Validation: Model vs. Data for Cell and Module Voltages

Next Steps: Physics-based Material Models

Mechanical Models

Step 1. Develop physics-based models

$$\sigma_{ij,j} + \rho f_i = \rho u_{i,tt}$$

$$\sigma_{ij} = C_{ijkl}\gamma_{kl}$$

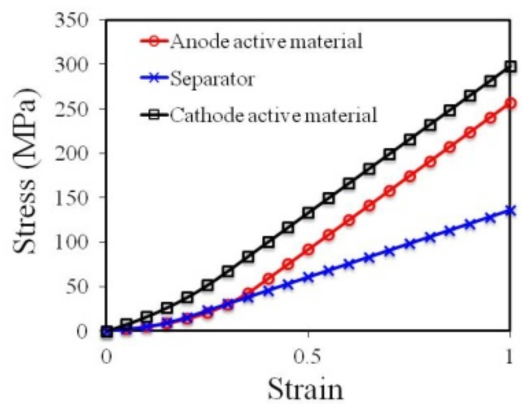
$$E = \begin{cases} E_{max} e^{\beta(\varepsilon - \varepsilon_p)} & \varepsilon < \varepsilon_p \\ E_{max} & \varepsilon \geq \varepsilon_p \end{cases}$$

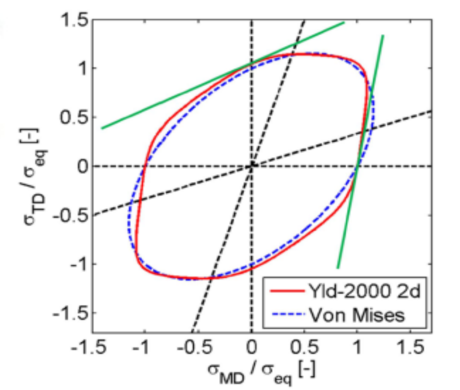
Step 2. Obtain model parameters

Approach a:
Calibrates parameters out of component level stress-strain data from MIT

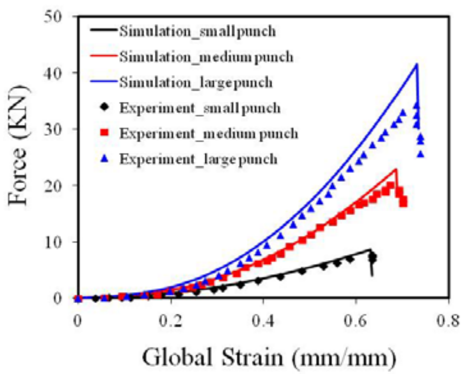
Approach b:
MIT's 8-par. model for aluminum

$$\bar{\sigma}(\sigma) = \bar{\sigma}(\sigma_{xx}, \sigma_{yy}, \sigma_{xy}) = \frac{1}{2^{1/a}}\left(|S'_I - S'_{II}|^a + |2 \cdot S''_I + S''_{II}|^a + |S''_I + 2 \cdot S''_{II}|^a\right)^{1/a}$$





Step 3. Validate against independent dataset



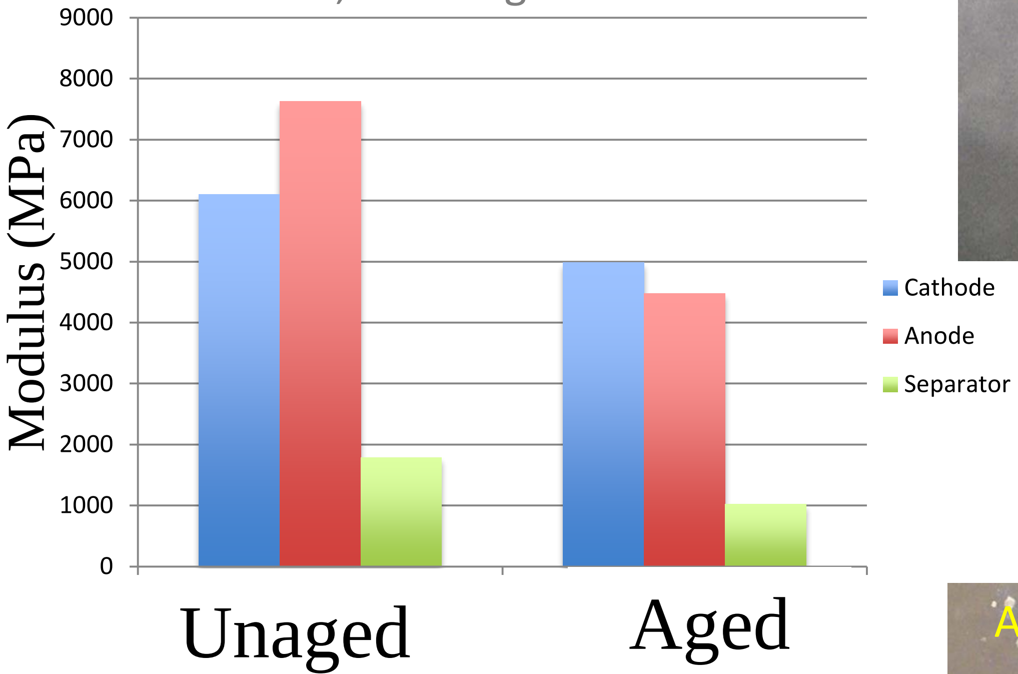
Cell-level data vs. Model

Under CAEBAT-III, we are working on:
- enhance predicting ability of mechanical models
- tighter coupling of the ECT models

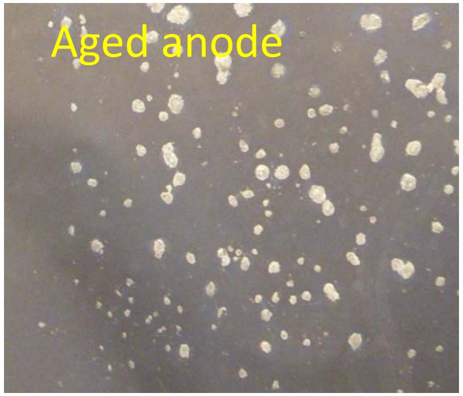
Next Steps: Effect of Cell Aging on Battery Safety

❖ Aging Effect on Modulus

L. Cao, 229th Meeting of the ECS, San Diego 2016



There is a decrease of tensile modulus due to aging, indicating the change of chemical composition or microstructure for electrodes and separator.



Summary

- For the single cell and cell-string levels, the models capture the force response to within 15-20% accuracy; and predict the location for the origin of failure based on the deformation data from the experiments. At the module level, there is some discrepancy due to poor mechanical characterization of the packaging material between the cells.
- The thermal response (location and value of maximum temperature) agree qualitatively with experimental data. Quantitative comparisons are shown where appropriate in this report. In general, the X-plane results agree with model predictions to within 20% (pending faulty thermocouples, etc.); the Z-plane results show a bigger variability both between the models and test-results, as well as among multiple repeats of the tests.
- The models are able to capture the timing and sequence in voltage drop observed in the multi-cell experiments; the shapes of the current and temperature profiles need more work to better characterize propagation.
- The cells within packaging experience about 60% less force under identical impact test conditions: so the packaging on the test articles is robust. However, under slow-crush simulations, the maximum deformation of the cell strings with packaging is about twice that from cell strings without packaging.

Acknowledgements

The NREL Team

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