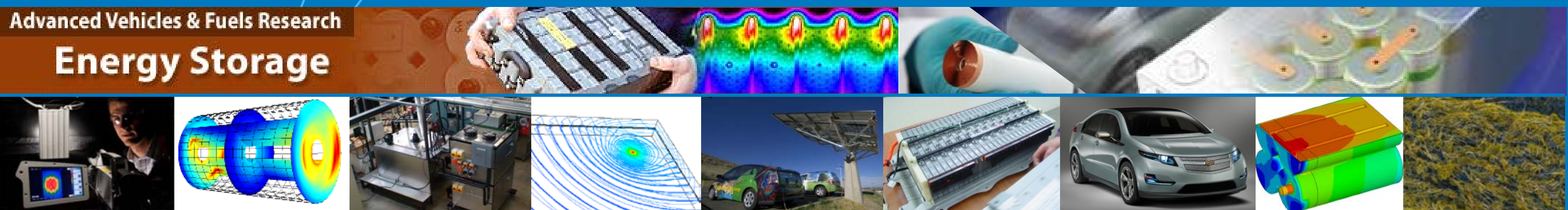
Multi-physics Modeling for Improving Li-Ion Battery Safety



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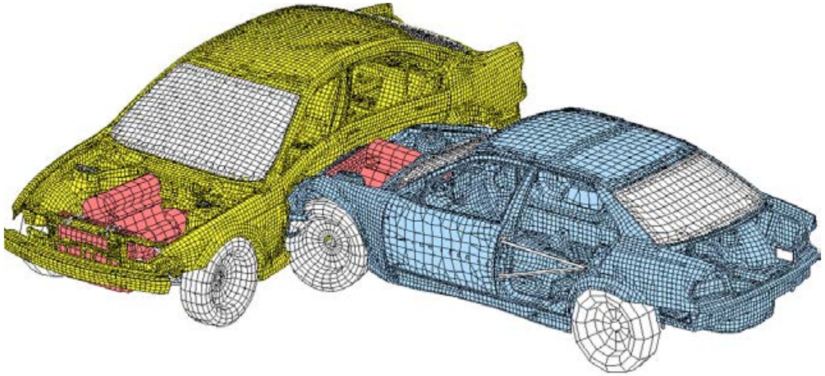
Outline

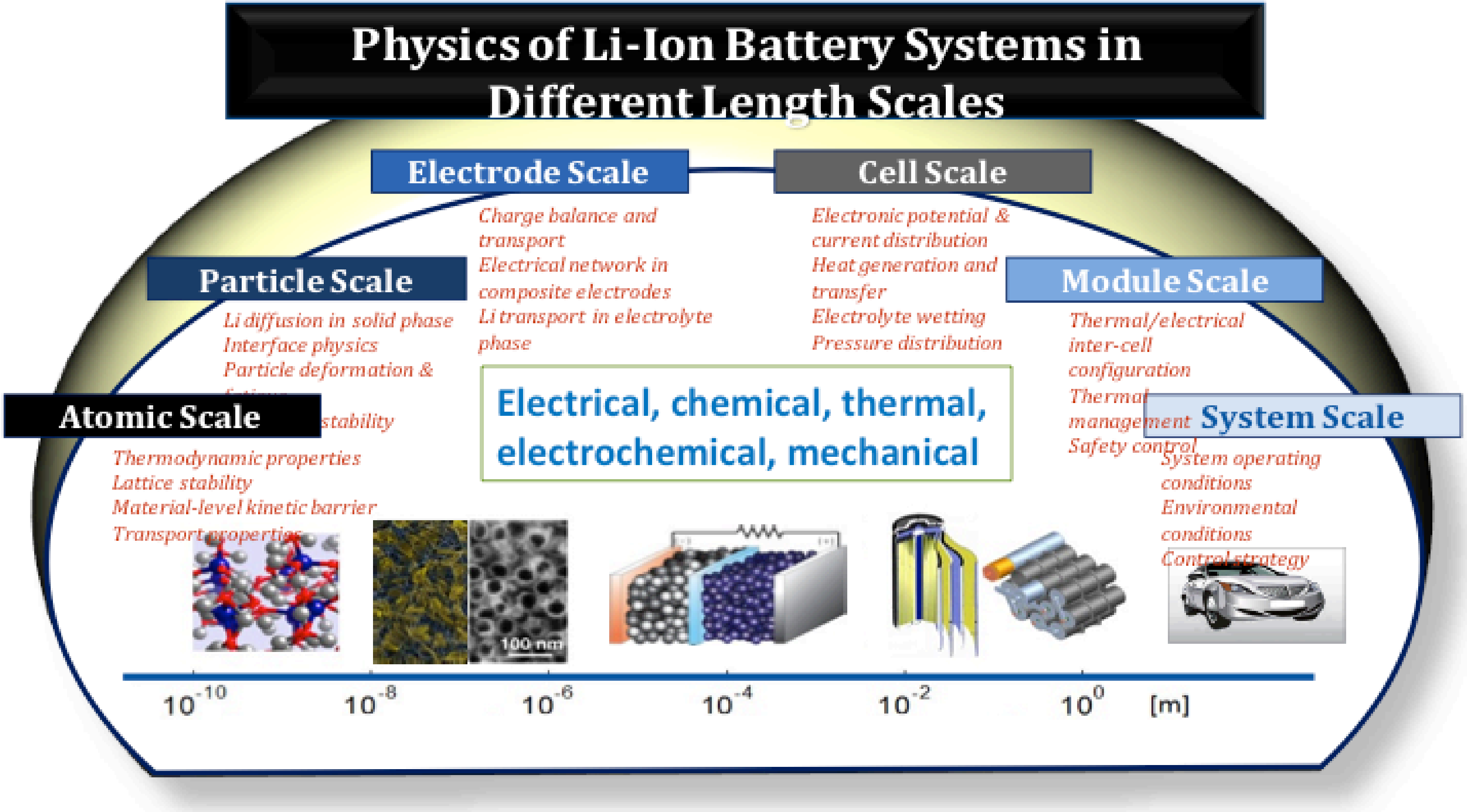
- Introduction
- Multi-physics Modeling of Batteries
- Safety/Abuse Modeling
- Examples of How Safety Modeling Could Lead to Improvements
- Summary

Introduction

- 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, improve cell and pack designs, and enhance manufacturing processes 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 of generating products.



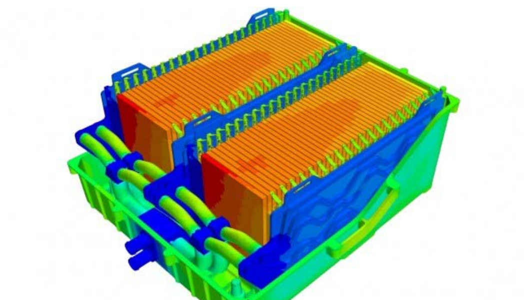
Multi-physics and Multi-Scale Phenomena Make Battery Modeling Complicated



- Electrochemical (e.g., anode-cathode interactions)
- Electrical (e.g., electron moving in the current collectors)
- Thermal (e.g., heat release due cell inefficiencies)
- Chemical (e.g., electrolyte reactions with electrode surfaces)
- Mechanical (e.g., pressure build-up, deformation after a crush)

Current State of Battery Modeling

- US Department of Energy has supported development of lithium ion battery modeling, simulations, and 3D computer aided engineering tools (**Computer Aided Engineering for Electric Drive Batteries**)
- DOE's 3-year funding in CAEBAT activity has resulted in availability of commercial **electrochemical-thermal** design tools



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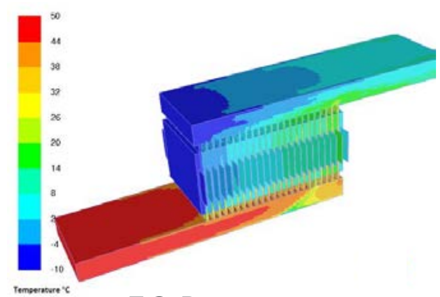
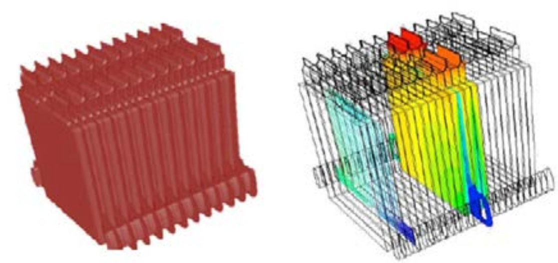


EC Power



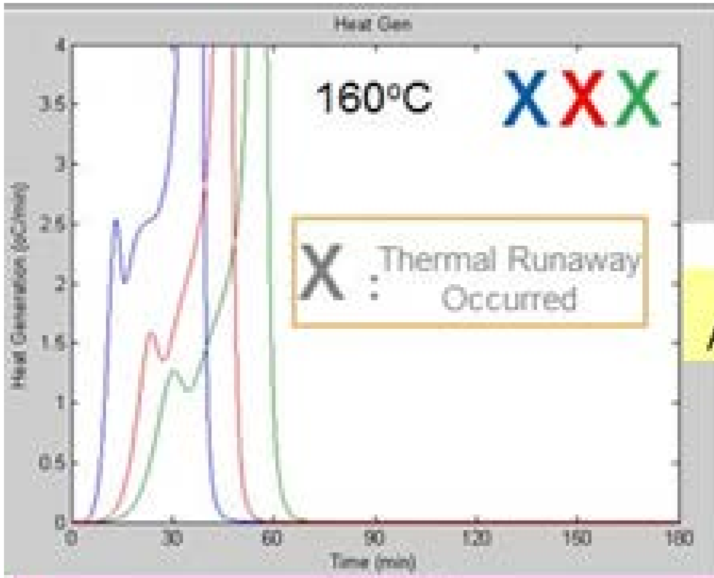
ANSYS

- In addition, DOE funded NREL to develop high-fidelity research tools for electrochemical-thermal, life, and safety modeling
- DOE is currently supporting NREL to further advance its safety models: couple structural models with electro-chemical-thermal models to simulate crash-induce crush and thermal runaways
- NREL safety models are discussed in this presentation.

NREL Battery Safety/Abuse Modeling Portfolio

- **Abuse Reaction Kinetics**
  - Simulates the response of the cell after on-sent TR temperature
- **Internal Short Circuit**
  - Simulates the 3D behavior of a cell due to internal shorts
- **Nail Penetration (static and dynamic)**
  - Simulates response of cells to various nail penetration conditions
- **Cell Structural Deformation Response**
  - Simulates thermal response of cells to various mechanical deformations
- **Module Crush Response**
  - Simulates the thermal response of a module due to impact
- **Cell-to-Cell Propagation in a Module or Pack**

NREL Abuse Reaction Kinetics Model



Oven Temperature & Size Impact Onset of Events

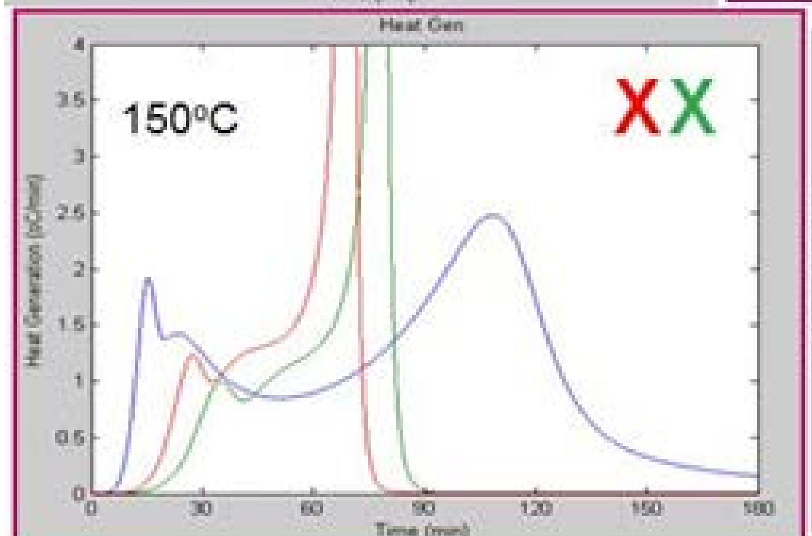
Color Key

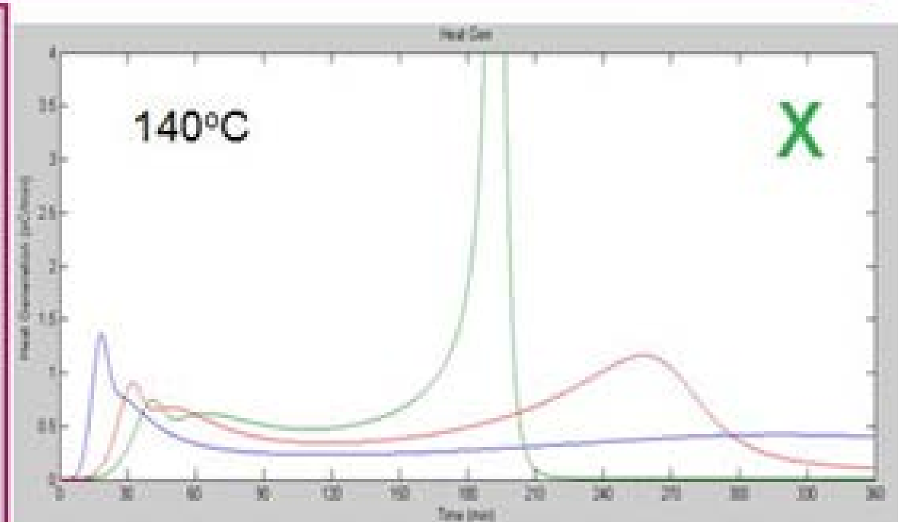
	18650 Cells	Oval Cell	50900 Cells
Vjr (cc)	10.52	157.1	157.1
A/Vjr (1/m)	48.37	29.14	25.01

V_{jr}: Jelly Roll Volume

A/V_{jr}: Heat Exchange Area per Volume

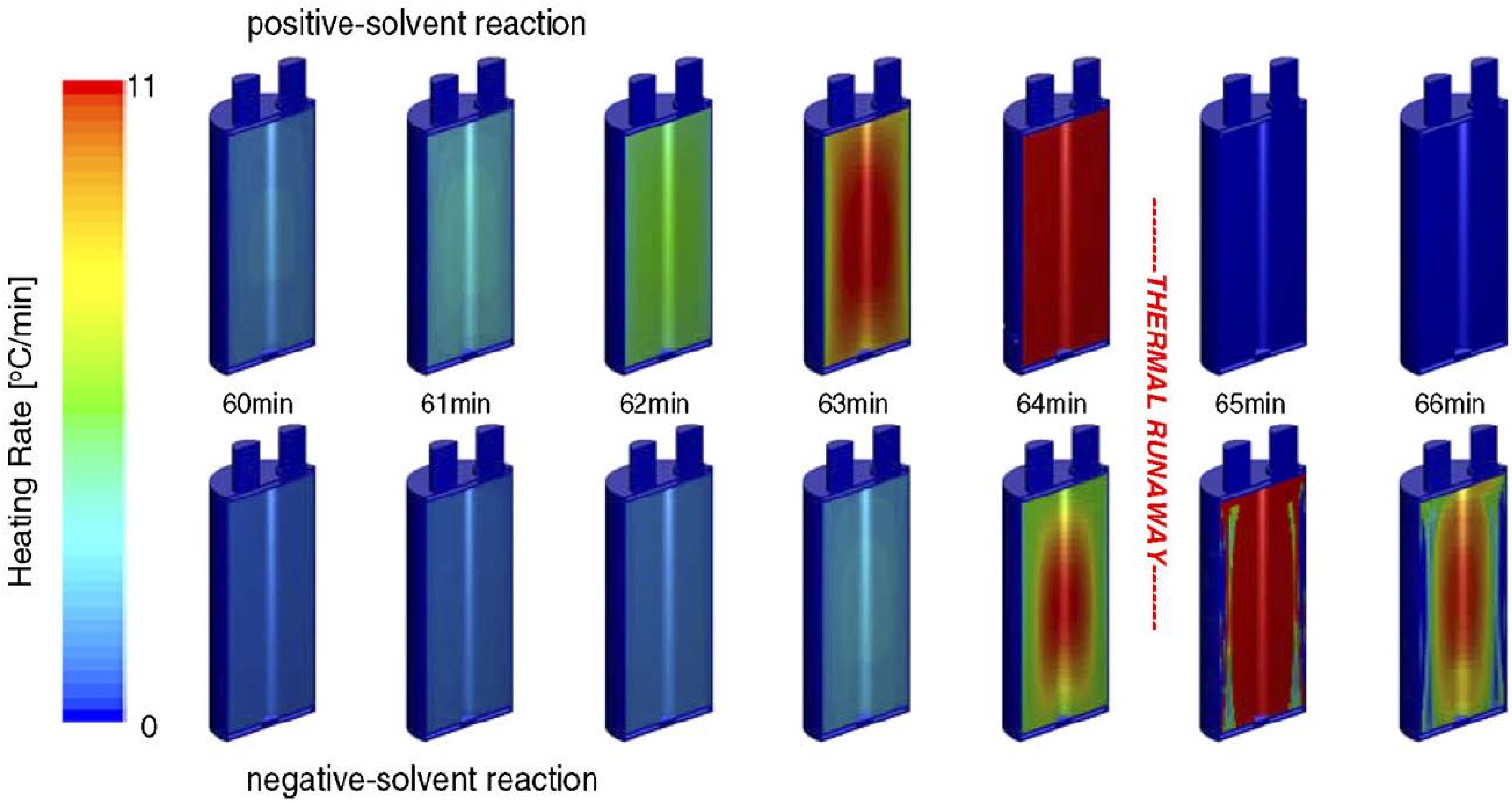
Small cell did not go into thermal runway at 150°C



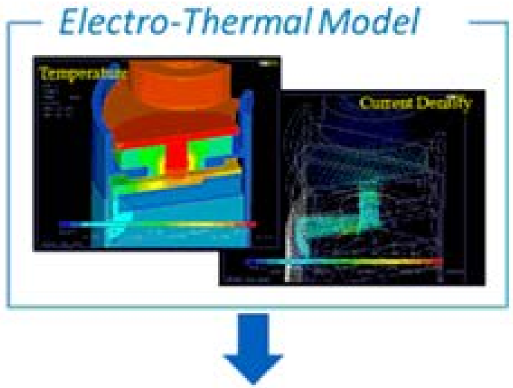


Typical Results of NREL Chemical Kinetics Reaction Model

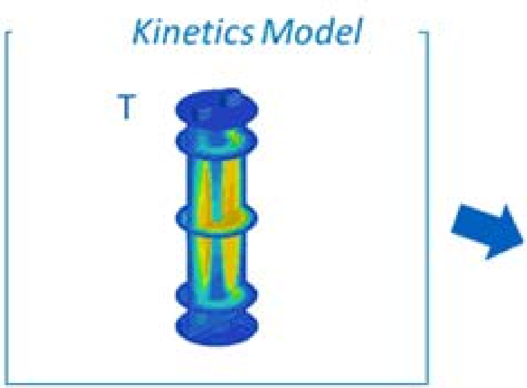
Electrode active material/solvent reactions trigger thermal runaway in a $LiCoO_2$/graphite cell

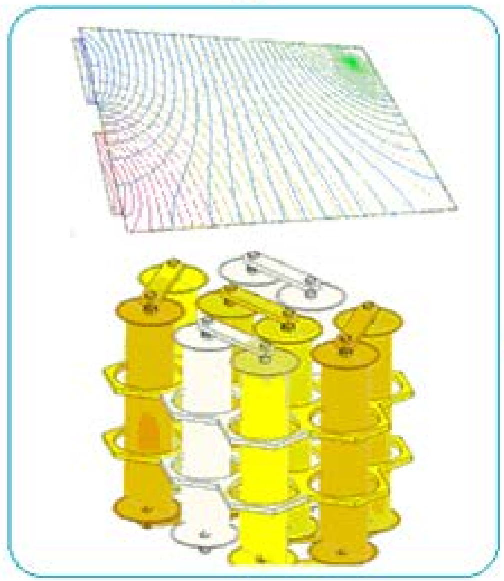


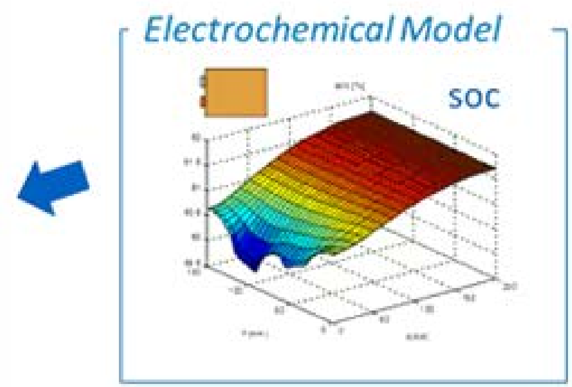
Internal Short Circuit Model



- MSMD upper level
- Cell/pack potential fields
- Short current Joule heating



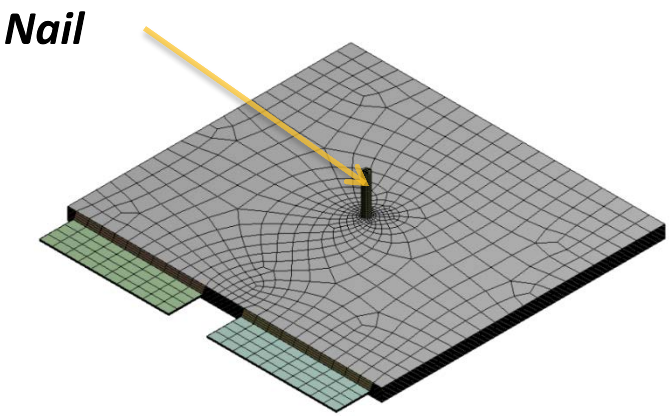


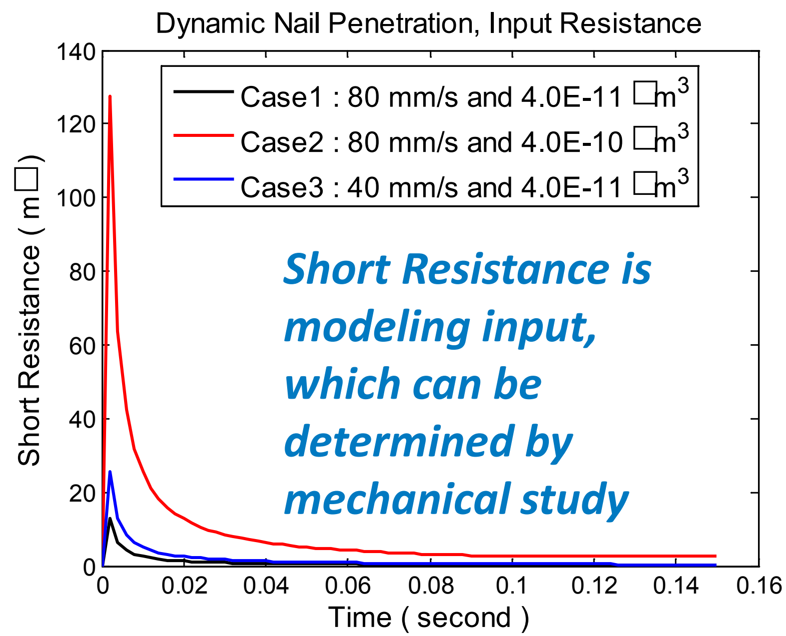


- Abuse chemical Reactions (thermally triggered)
- Produce abuse reaction heat
- Top-down approach

- Electrode pair/particle level
- Distributed 1D ECM model Electrochemical responses

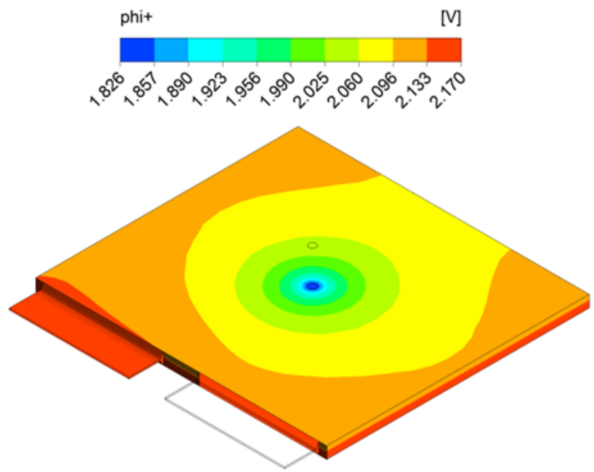
Dynamic Nail Penetration Modeling



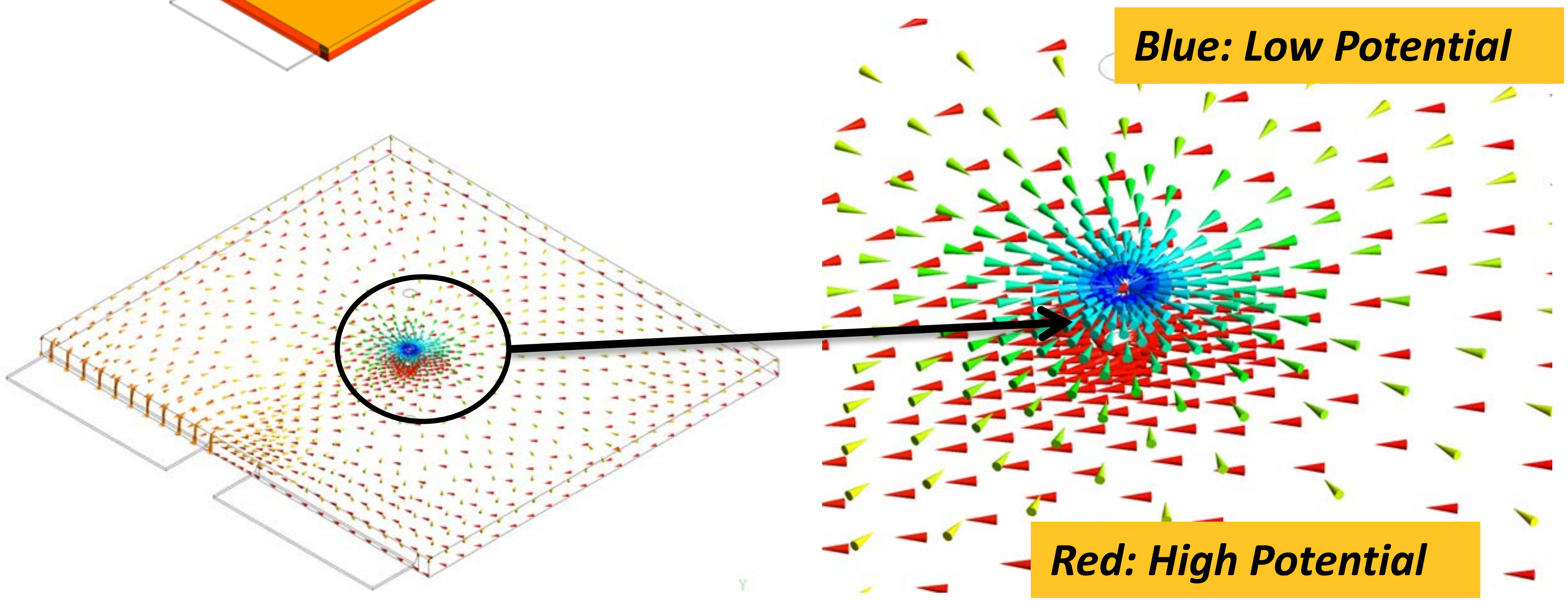


- In this example, assume nail penetration results in uniformly internal short circuit; Once created, internal short circuit remains during modeling
- Short resistance in Ohm is the volumetric short resistance (Ωm^3) divided by shorten volume

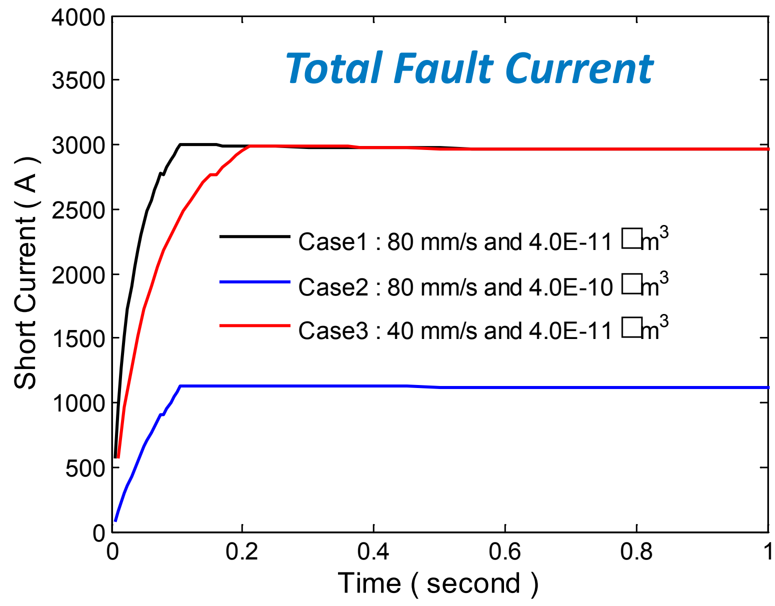
3D Illustration of Potential and Current

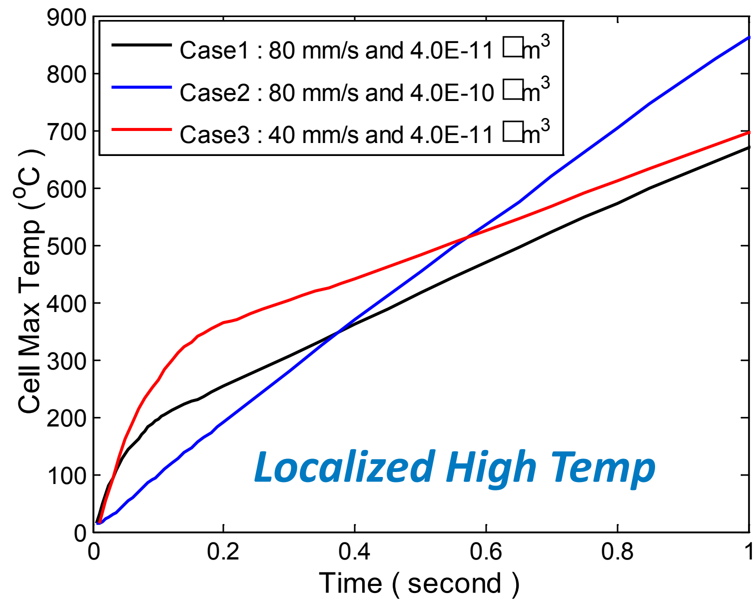


- The approach captures the difference between penetrated and un-penetrated layers along penetrating direction
- Current from un-penetrated layers went through battery tab and feed into shorted layers



Current and Temperature Predictions

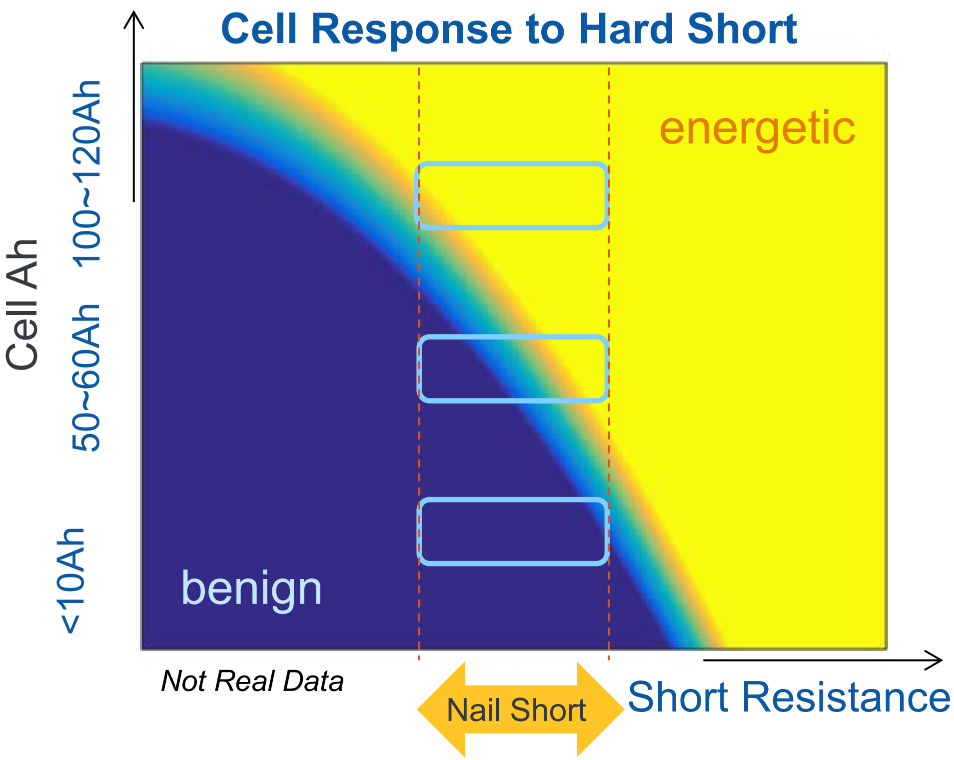


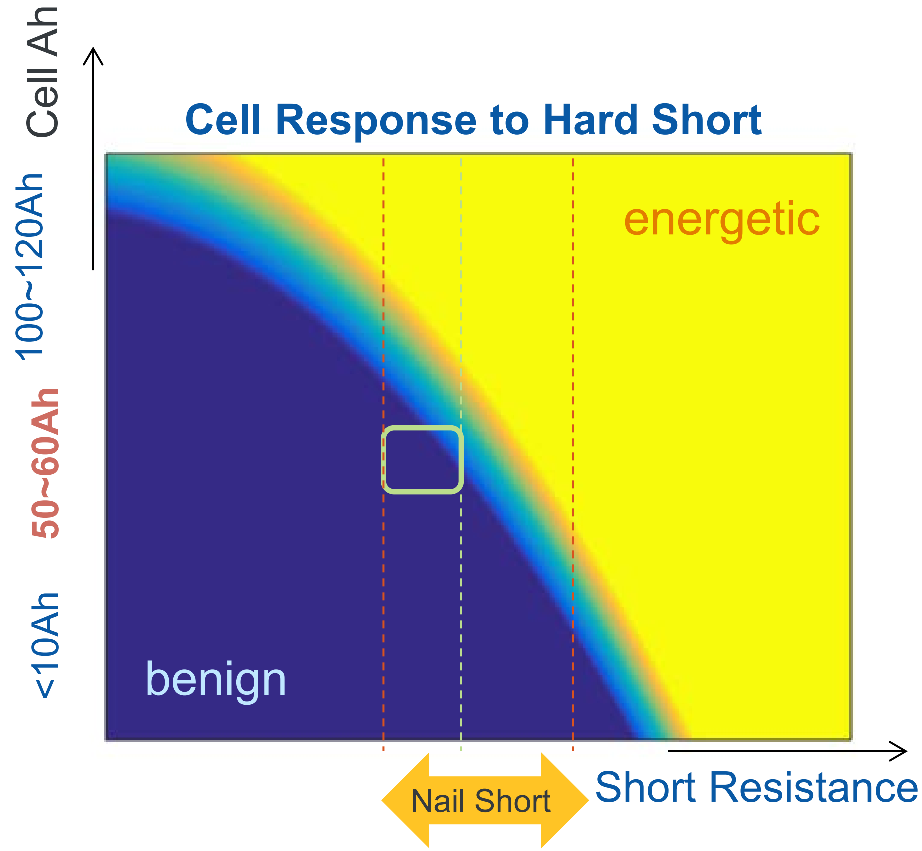


- **The model reasonably predicts the current and thermal response**
- **Case 2 has a larger short resistance; as such, the short current is relatively low**
- **In case 3, nail speed is slower; it took longer time to reach quasi-steady states**
- **The maximum temperature was determined by both short current and short resistance; in case 2, though short current was relatively low, its short resistance is larger; as such, its maximum temperature can be low during nail penetration, and became higher after nail penetration**

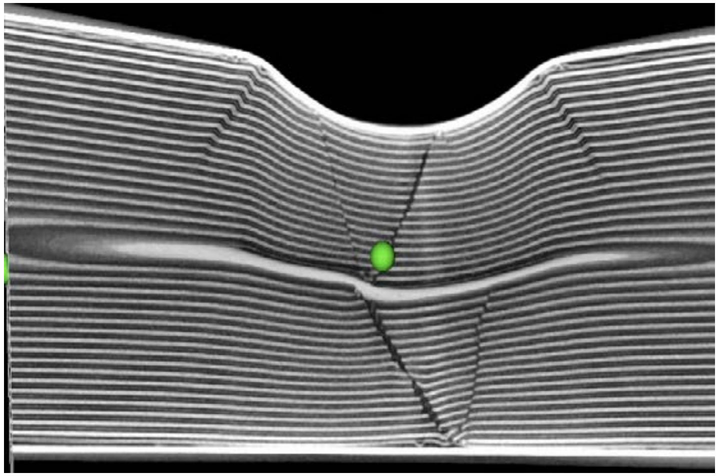
Why Does Nail Penetration Response Vary?

To understand and improve the nail penetration test response of cells





Battery Crush Modeling



Origin of mechanical failure within the active material

Crack orientation

Deformed geometry of the fractured region

Battery Crush M-ECT Modeling

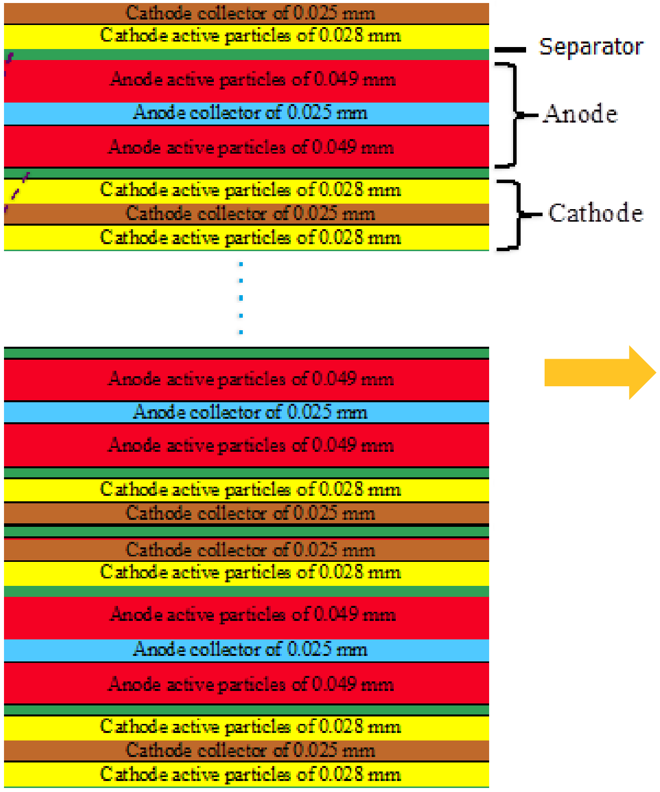
- **Battery crush → damaged zone → failure of separator → electrode contacts →local short → current flow → heat generation → Heat generation without rejection →*temperature* increase →*reaching above onset* temperature → spontaneous reactions → thermal runaway → smoke and fire**

→: may lead to (depending on many factors)

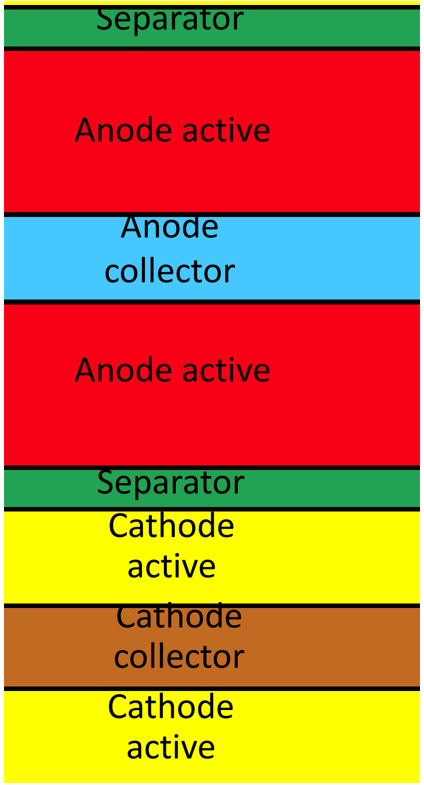
- **Simulating all physics and geometry is very challenging; need simplifications**
- **Our approach:**
  - Decouple structure from ECT interactions
  - First, model structural changes after crush
  - Capture the characteristics of damaged zone
  - Use it for electrochemical and thermal modeling

Cell-Level Structural Modeling Simplification

- **Structural modeling of many thin layers of electrode requires significant computational time**
- **Structural simplification to capture deformation of layers upon crush to predict short circuit**
- **Combine individual layers of current collector, anode, cathode, and separator into representative sandwich (only for structural)**

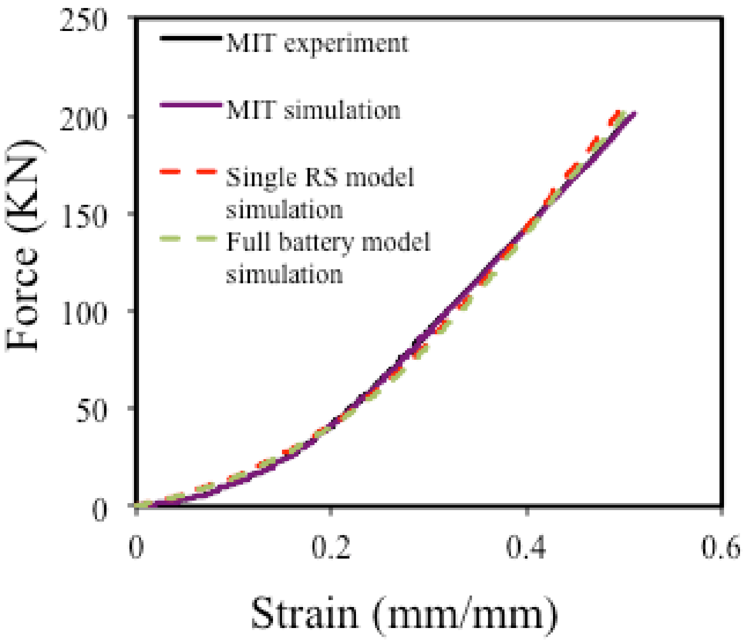


Through-thickness architecture Multiple layers in a cell

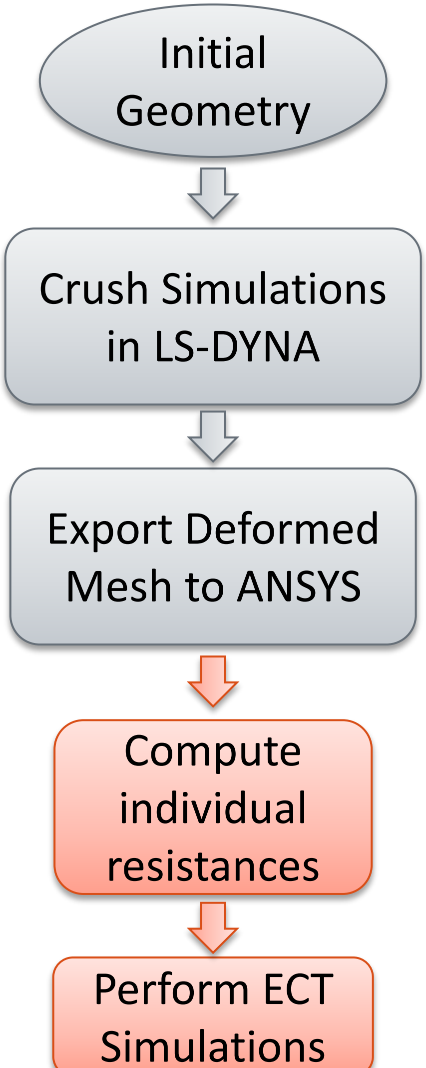


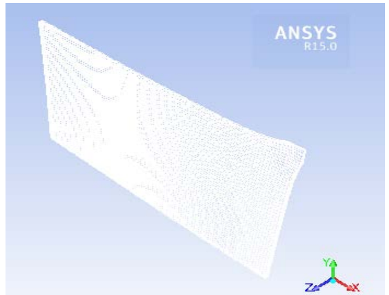
Simplified representative sandwich (RS) with equivalent mechanical properties

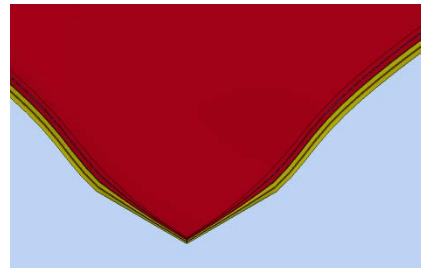
Choice of Model	**Total # of layers**
All-layer model	166
RS model	8

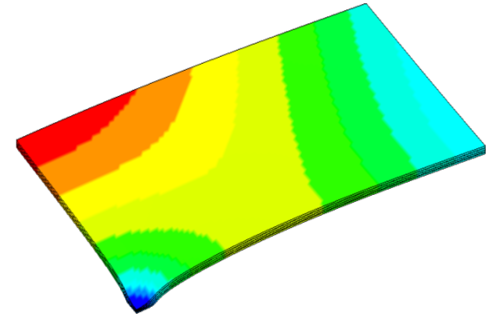


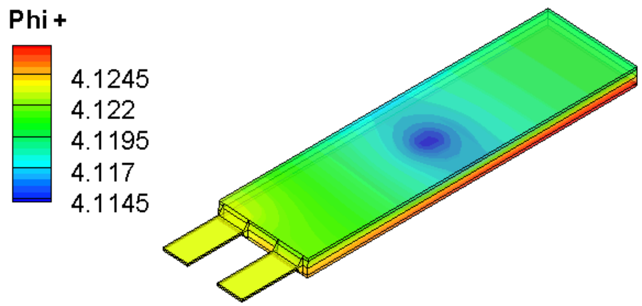
Approach for Linking Mechanical to ECT

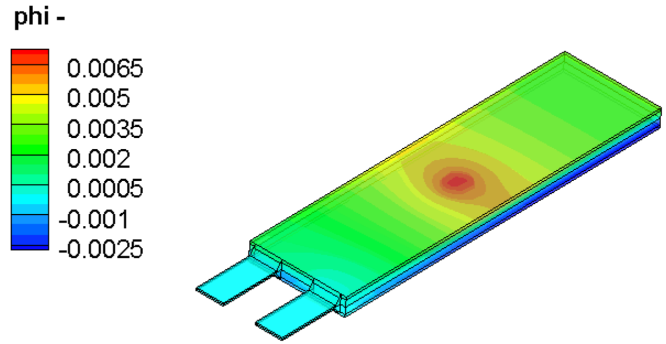












C. Yang et al., 225th ECS Meeting, May 2014, Orlando, FL

Advantage:
Better integration of electrical simulations with existing ECT

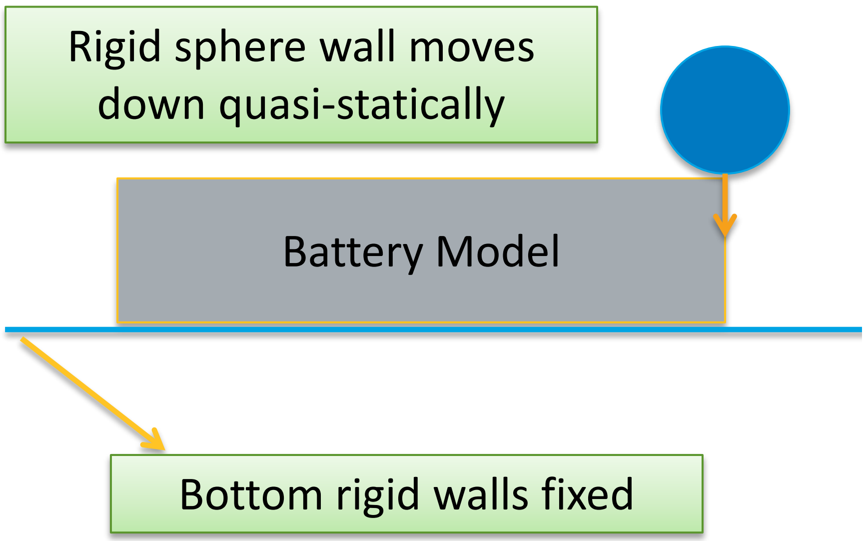
Challenges:

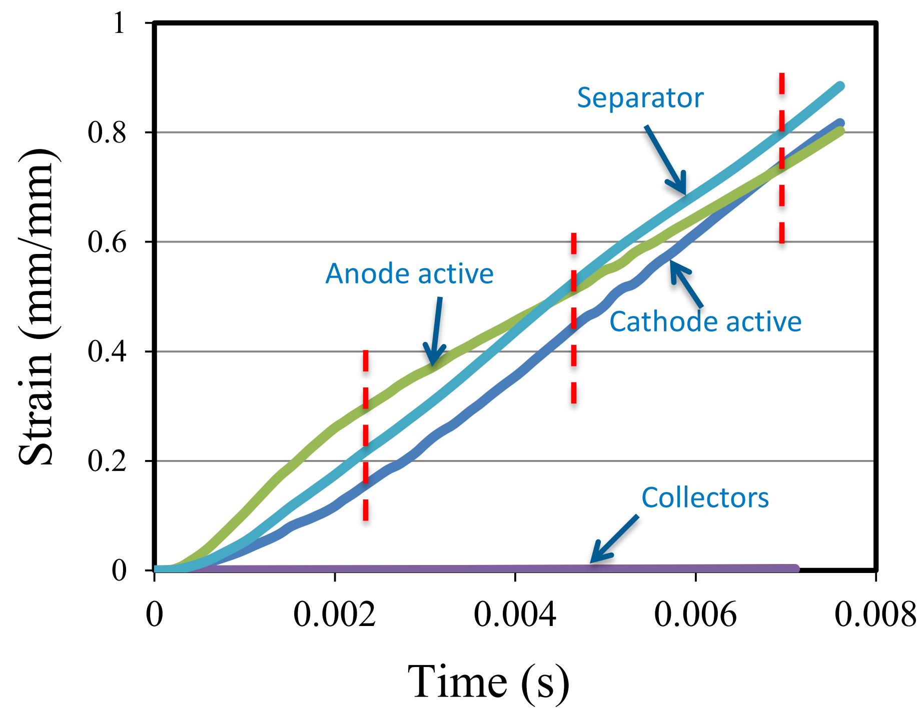
- Performing ECT simulations on the deformed mesh
- Simultaneously solving for resistance distribution and current distribution in Fluent: implications on short-circuit simulations using ECT

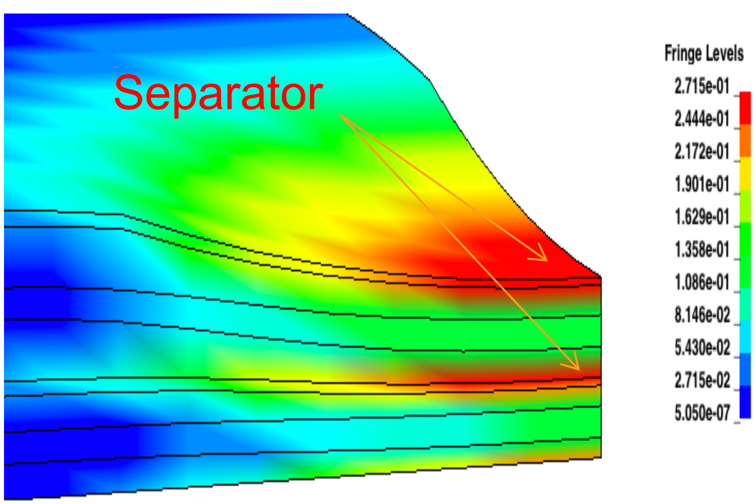
The benefit of this approach used of existing electrochemical-thermal (ETC) in ANSYS/Fluent 15.0/16.0

LS-DYNA Mechanical Simulation and Results

Indentation Test Simulation





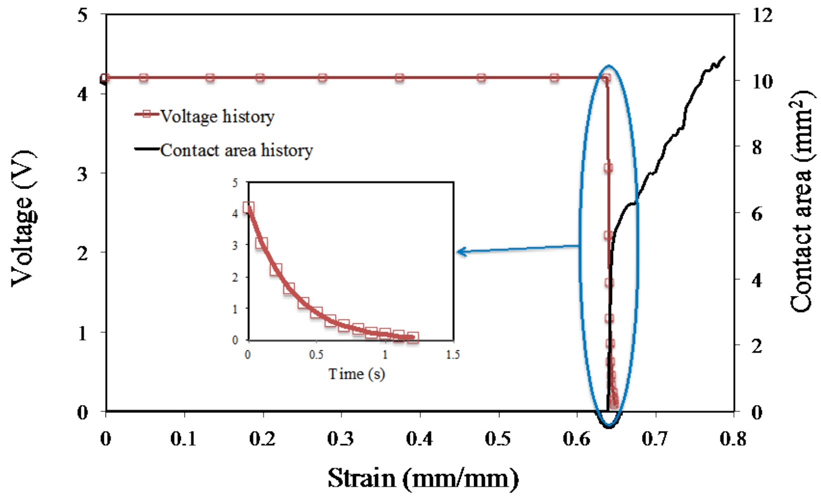


von-Misses Stress Contours

1. Indentation induced damage is localized and complicated
2. Separator is very likely the first to fail

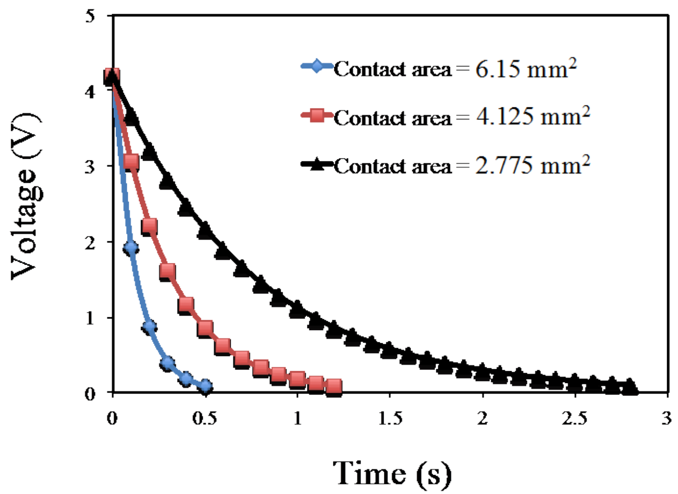
Example 1: Improving Cell Safety Using Models

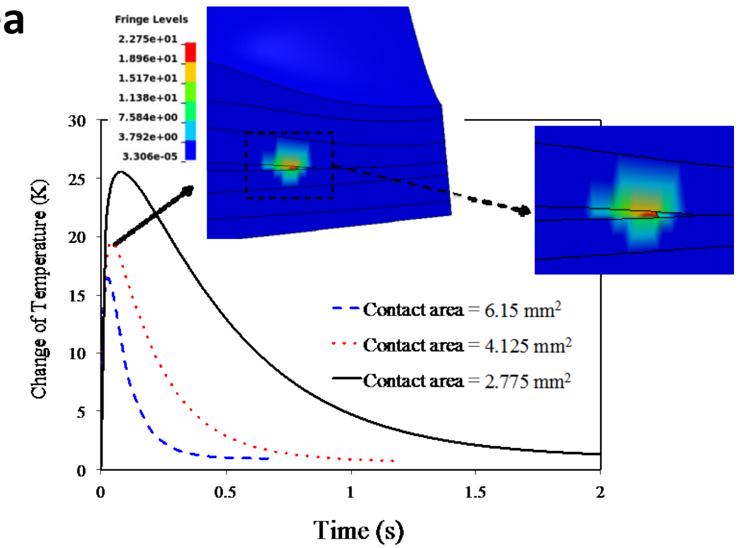
- The voltage and thermal responses before and after short can be predicted using the coupled modeling approach
- The coupled model shows the potential to study different short-circuit conditions, for example, different electrical contact area
- A large short-area implies lower local current density and, thus, lower temperature rise



Understanding parameters that affect short-circuit response leads to design of safer lithium ion cells.

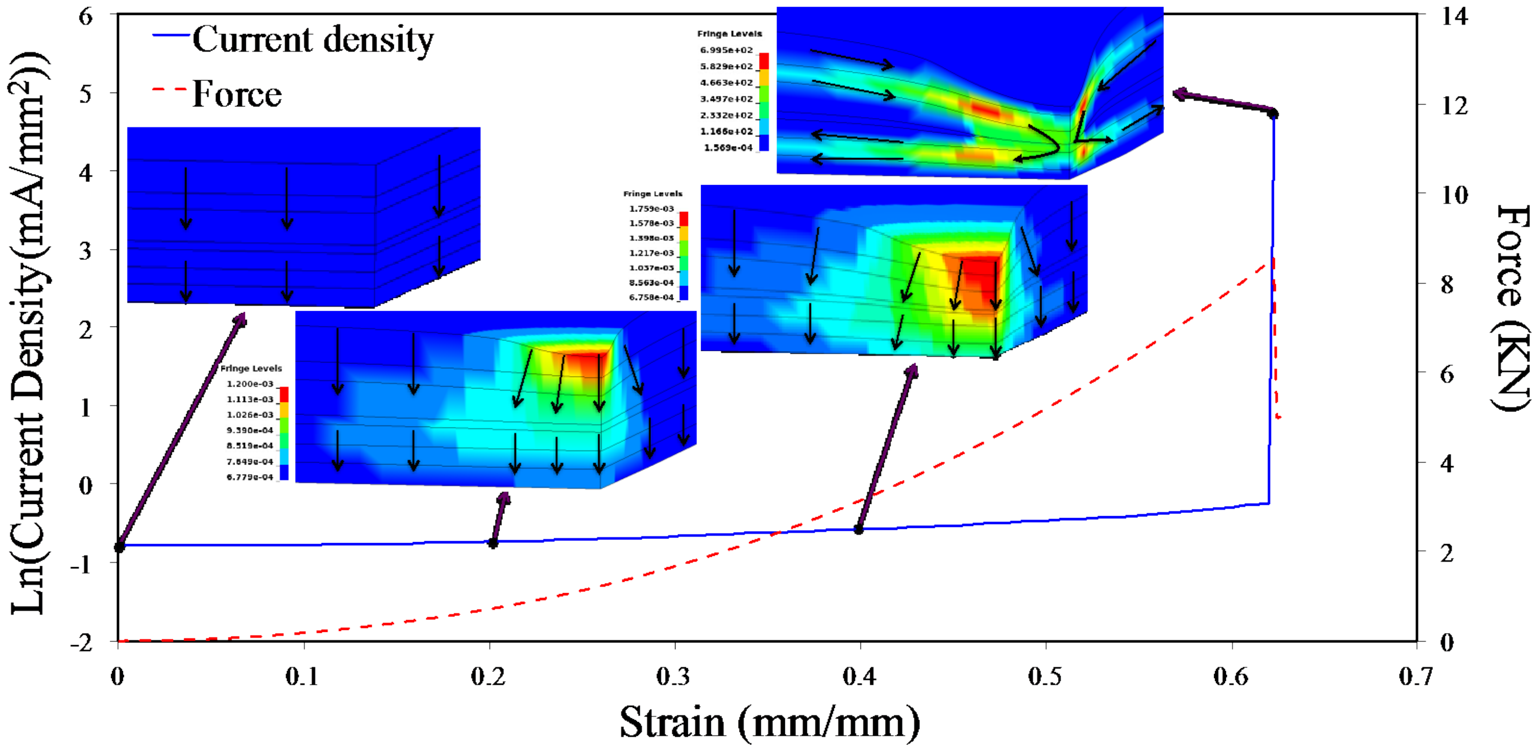
Effect of electrical-contact area





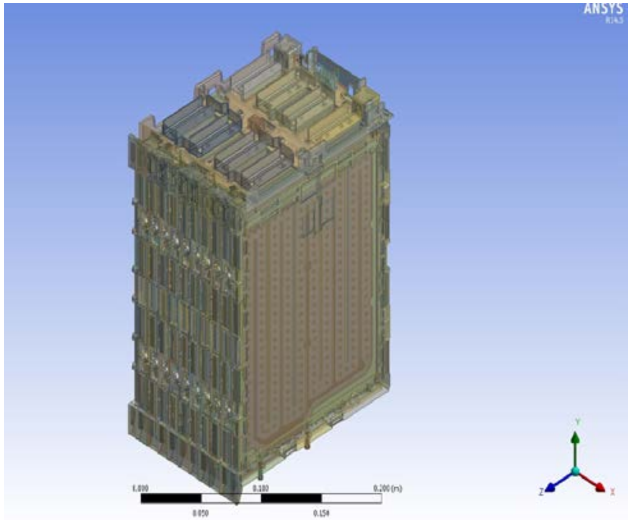
Example 2: Improving Cell Safety Using Models

- **Having separate failure criteria for electrical, thermal, and mechanical responses provides a comprehensive ability to design components that meet or exceed each criterion independently.**
- **For example, we can use these models to verify that a separator with good melt integrity also has the right mechanical properties.**

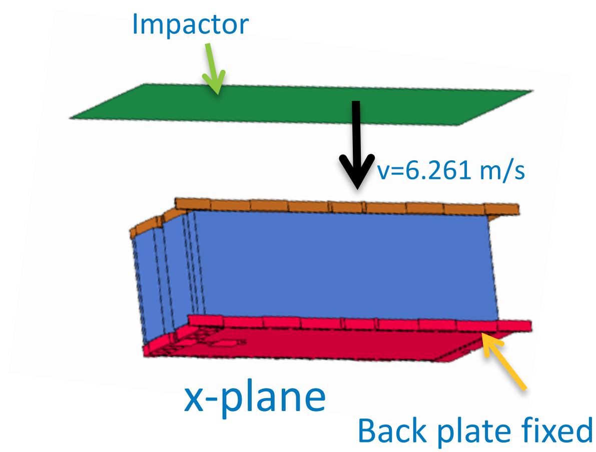


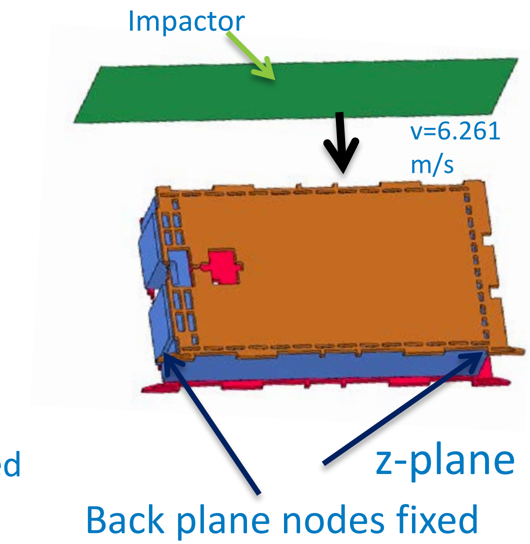
Evolution of current density across the short-circuit area during a mechanical indentation loading condition

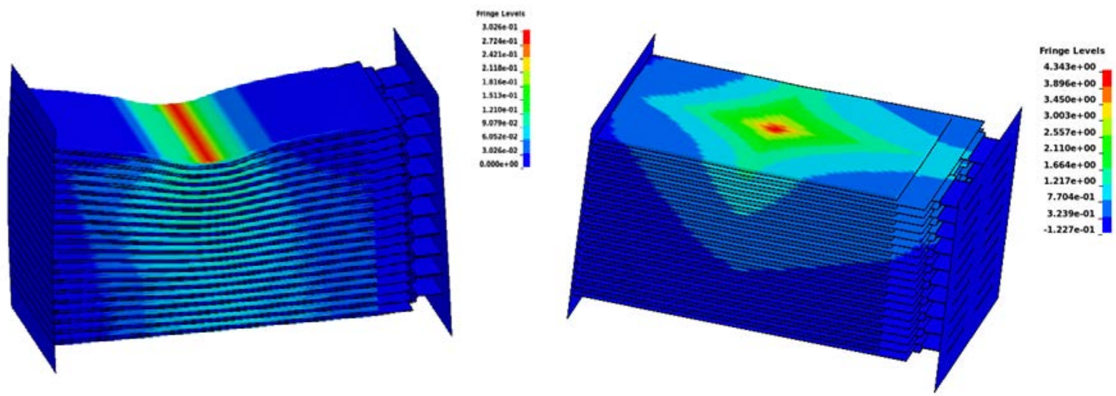
Multi-Cell Simulations



CAD image of a 20 Cell module complete with packaging and heat-exchange

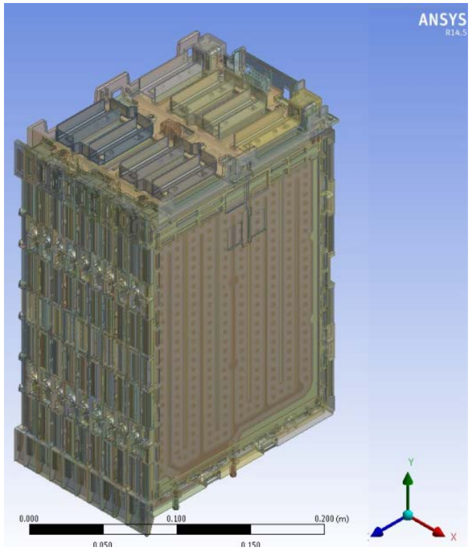






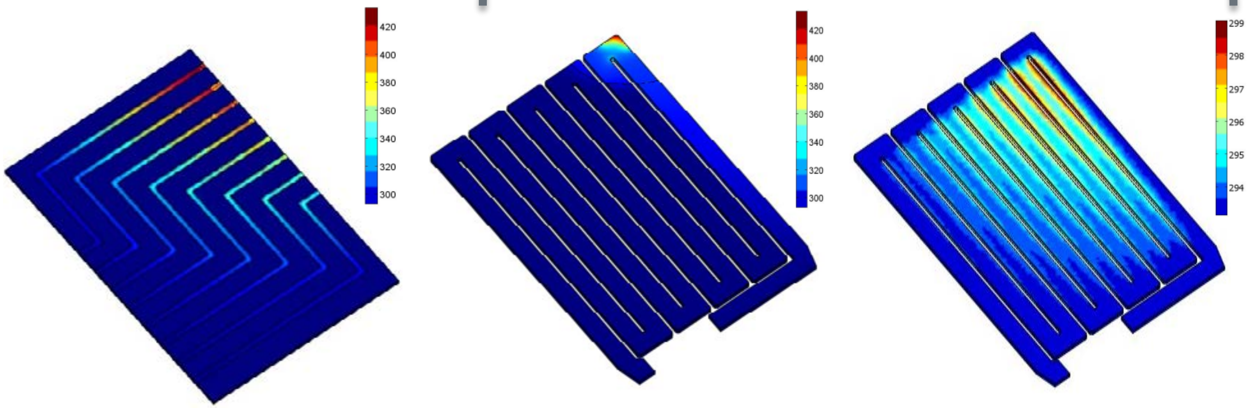
Evolution of mechanical strain in response to different crush tests

Example 3: Improving Pack Safety Using Models



- 20-cell 'test' module
- Comparison of heat generated under different mechanical load conditions
- Comparison of different cooling fin designs on a module comprised of identical cells

Temperature distribution after top vs. side impact



ΔT_{max} = 120°C

ΔT_{max} = 140°C

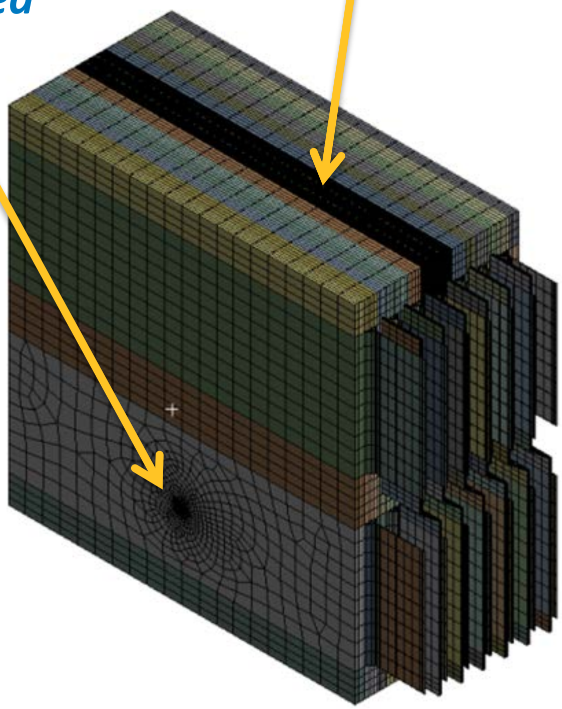
ΔT_{max} = 6°C

Side impact with different cooling channel designs

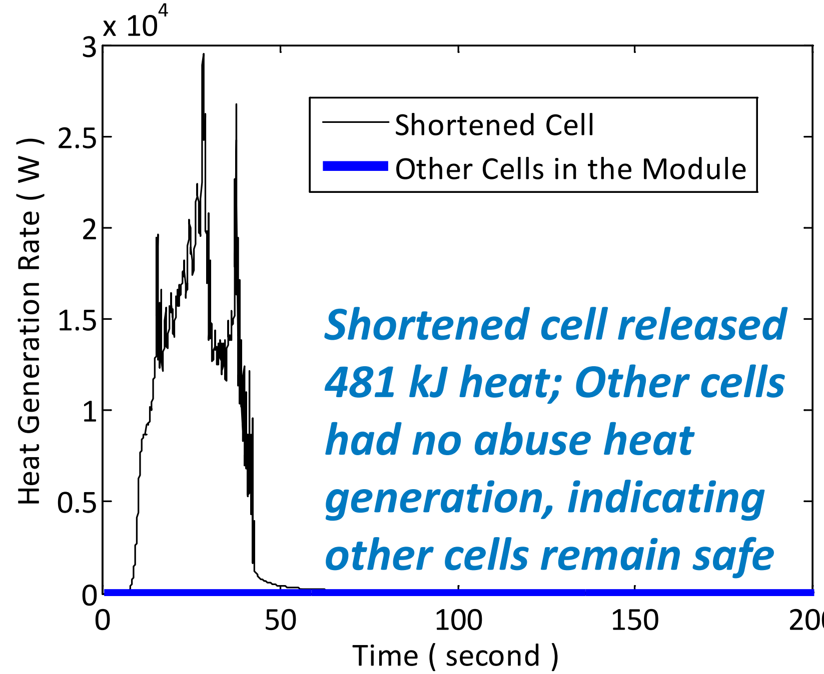
Cell-Cell Thermal Propagation

Initial Shortened Area

Shortened Cell Located at the Middle



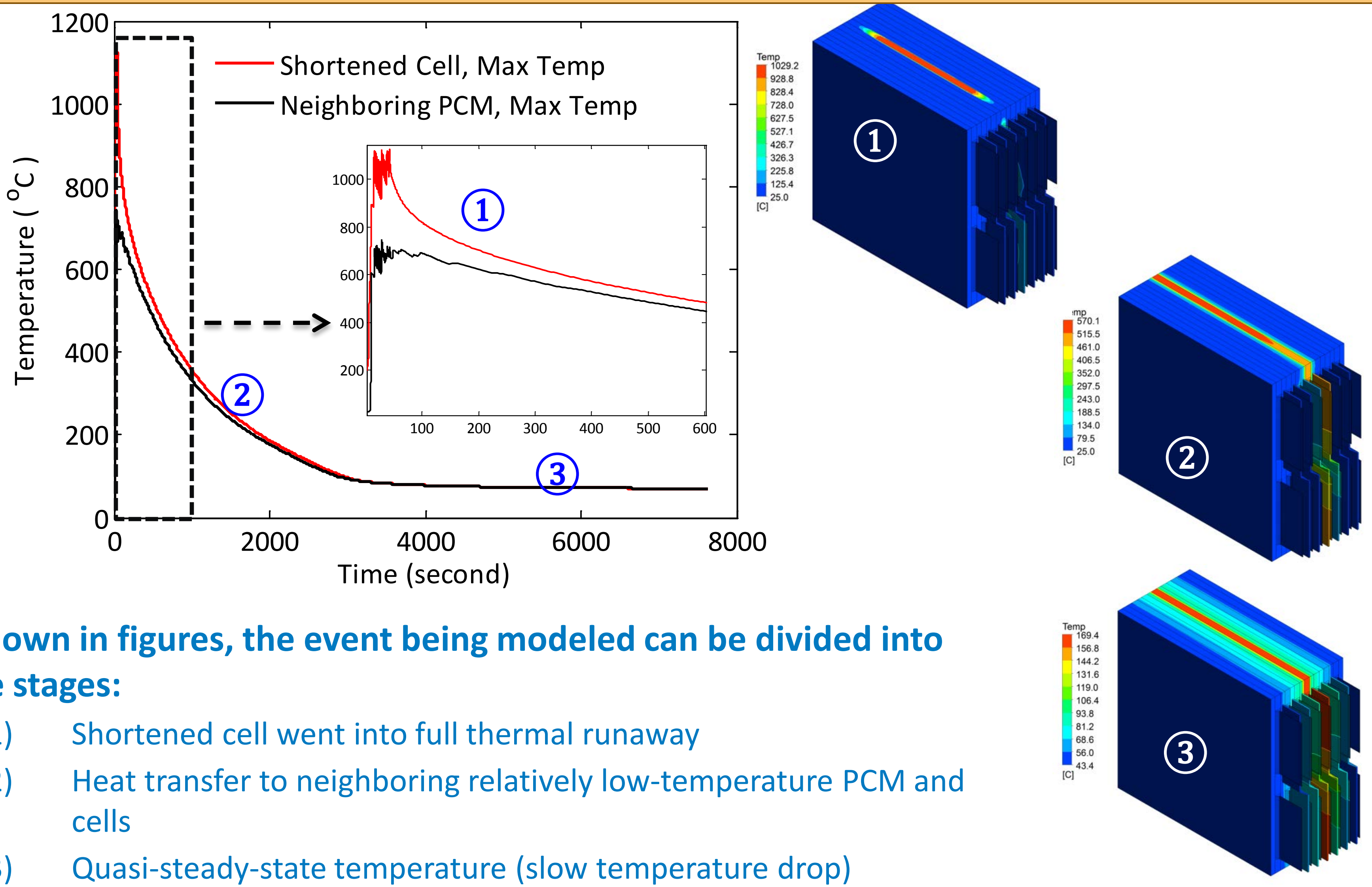
7S1P Pouch Cell Module with Phase Change Material (PCM)



- **Numerically evaluated thermal management design with NREL safety model**
- **Passive cooling technique using PCM was developed to prevent thermal runaway propagation in module**
- **Safety modeling demonstrated design effectiveness and provided design suggestions**

With PCM TR Propagation Prevented

Without Phase Change Material (PCM) Thermal Runaway (TR) Propagated to All Cells



As shown in figures, the event being modeled can be divided into three stages:

1) Shortened cell went into full thermal runaway
2) Heat transfer to neighboring relatively low-temperature PCM and cells
3) Quasi-steady-state temperature (slow temperature drop)

Summary

- Modeling and CAE tools have provided insight to improving electrochemical-thermal performance
- Modeling can also reduce the number of build-test-break cycles and save battery development costs
- NREL has developed a portfolio of battery safety modeling for various abuse conditions
- Abuse reaction kinetics models will be available in ANSYS tools soon
- Variability of nail penetration response of li-ion cells could be explained by our models
- First ever coupled structural-electro-thermal model has been developed for cash-induced crush
- NREL models are available for use by industry

Acknowledgements

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- **Collaborating Partners**

CD-adapco
ANSYS
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Sandia National Laboratories
Oak Ridge National Laboratory