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Coupled Mechanical-Electrochemical-Thermal Modeling for Accelerated Design of EV Batteries

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NATIONAL RENEWABLE ENERGY LABORATORY

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NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Introduction

I. The physical phenomena occurring in a battery are many and complex and, in different scales (particle, electrodes, cell, pack)
   1. Electrochemical (e.g., node-cathode interactions)
   2. Electrical (e.g., electron moving in the current collectors)
   3. Thermal (e.g., heat release due cell inefficiencies)
   4. Chemical (e.g., electrolyte reactions with electrode surfaces)
   5. Mechanical (e.g., pressure build-up, deformation after a crush)

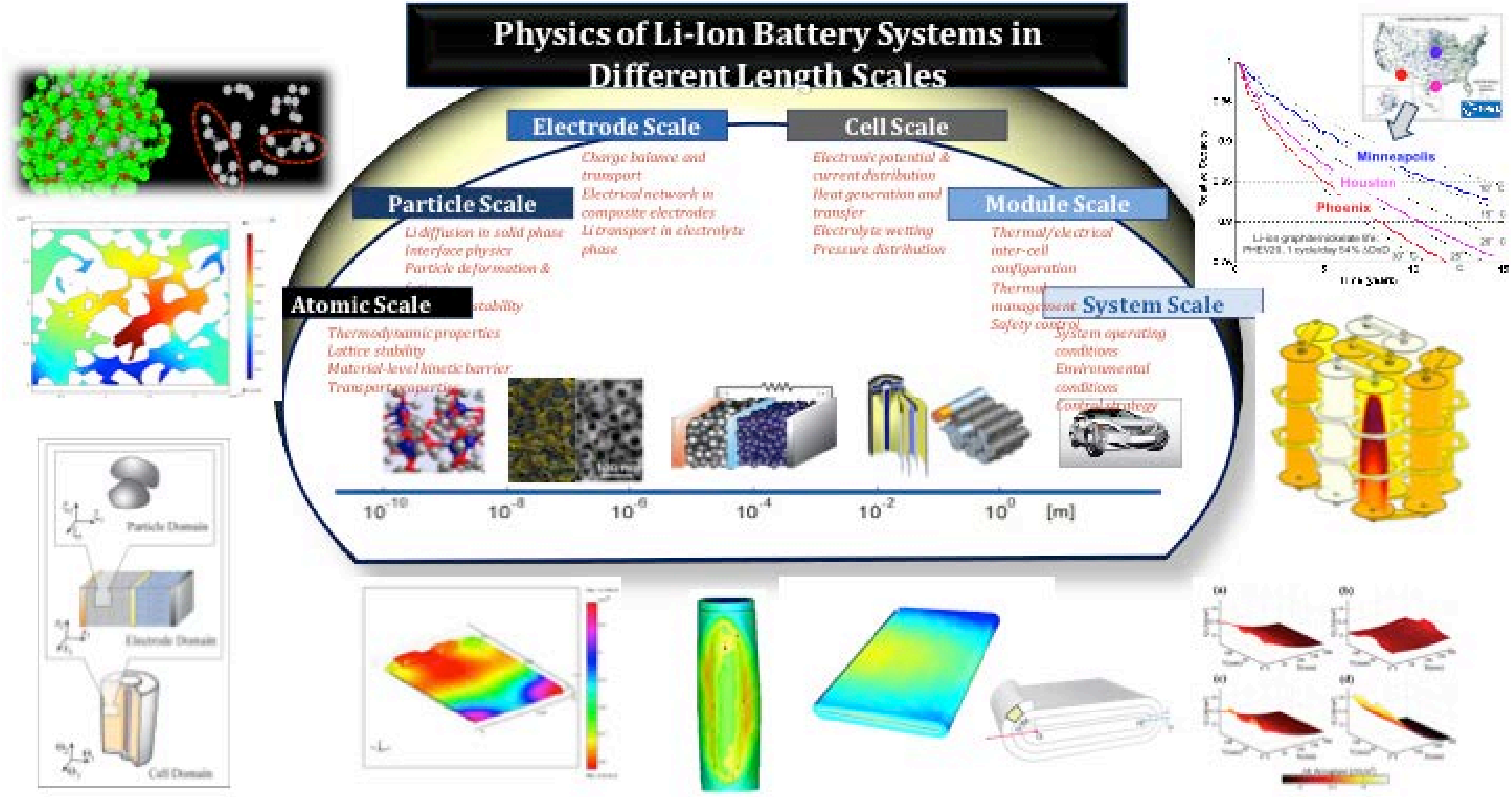
II. Better understanding of interplay between different physics occurring in different scales through *modeling* could provide insight to design improved batteries for electric vehicles

III. Work funded by U.S. DOE has resulted in development of computer-aided engineering (CAE) tools to accelerate electrochemical and thermal design of batteries; mechanical modeling is underway

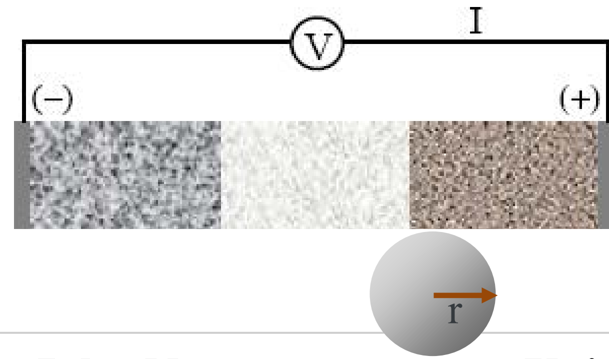
IV. This paper provides an overview of the M-ECT modeling efforts

Battery Modeling at NREL

NREL has developed a unique set of multi-physics, multi-scale modeling tools for simulating performance, life, and safety of lithium-ion batteries



Li-Ion ECT Modeling: Porous Electrode Theory



Charge Transfer Kinetics at Reaction Sites

$$j^{Li} = a_s i_o \left\{ \exp\left[\frac{\alpha_a F}{RT}\eta \right] - \exp\left[-\frac{\alpha_c F}{RT}\eta \right] \right\}$$

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c} \quad \eta = (\phi_s - \phi_e) - U$$

Species Conservation

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_s}{\partial r} \right)$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot \left(D_e^{eff} \nabla c_e \right) + \frac{1 - t_+^o}{F} j^{\mathrm{Li}} - \frac{\mathbf{i}_e \cdot \nabla t_+^o}{F}$$

Charge Conservation

$$\nabla \cdot \left(\sigma^{eff} \nabla \phi_s \right) - j^{\mathrm{Li}} = 0$$

$$\nabla \cdot \left(\kappa^{eff} \nabla \phi_e \right) + \nabla \cdot \left(\kappa_D^{eff} \nabla \ln c_e \right) + j^{\mathrm{Li}} = 0$$

Energy Conservation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

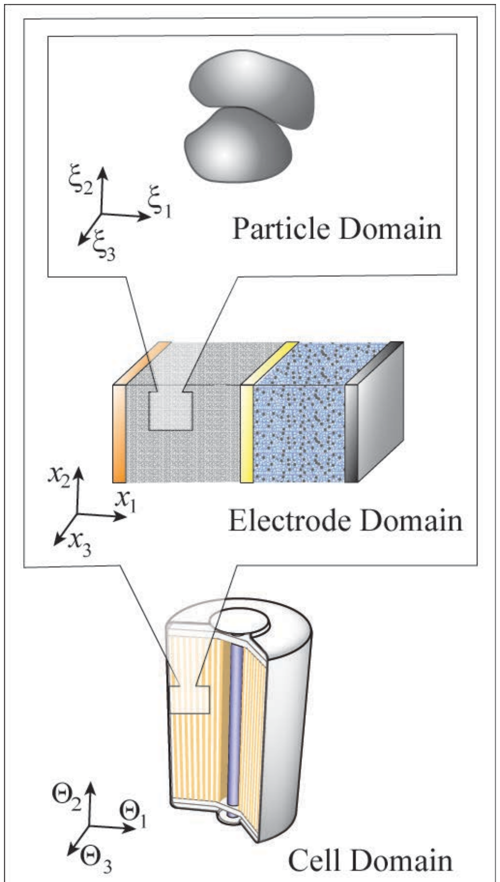
$$q''' = j^{Li}\left(\phi_s - \phi_e - U + T\frac{\partial U}{\partial T} \right) + \sigma^{eff}\nabla\phi_s \cdot \nabla\phi_s + \kappa^{eff}\nabla\phi_e \cdot \nabla\phi_e + \kappa_D^{eff}\nabla \ln c_e \cdot \nabla\phi_e$$

- **Pioneered by John Newman group at University of California–Berkeley (*Doyle, Fuller, and Newman, 1993*)**
- Captures *lithium diffusion dynamics* and *charge transfer kinetics*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

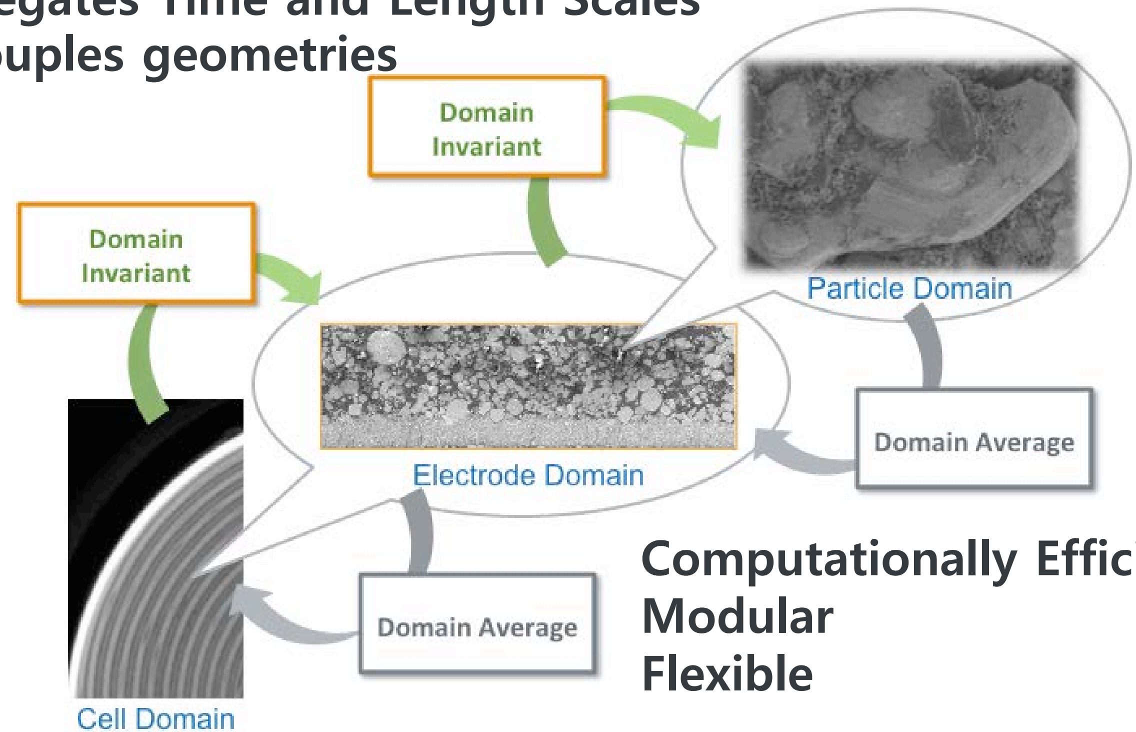
- Difficult to apply in large format batteries where *heat* and *electron current* transport critically affect the battery responses

NREL's MSMD Li-Ion Modeling Framework

Through the multi-year effort supported by U.S. DOE, NREL has developed a modeling framework for predictive computer simulation of Li-ion batteries known as the ***Multi-Scale Multi-Domain*** *(MSMD) model, which addresses the interplay among the physics in varied scales and extends the porous electrode modeling:*



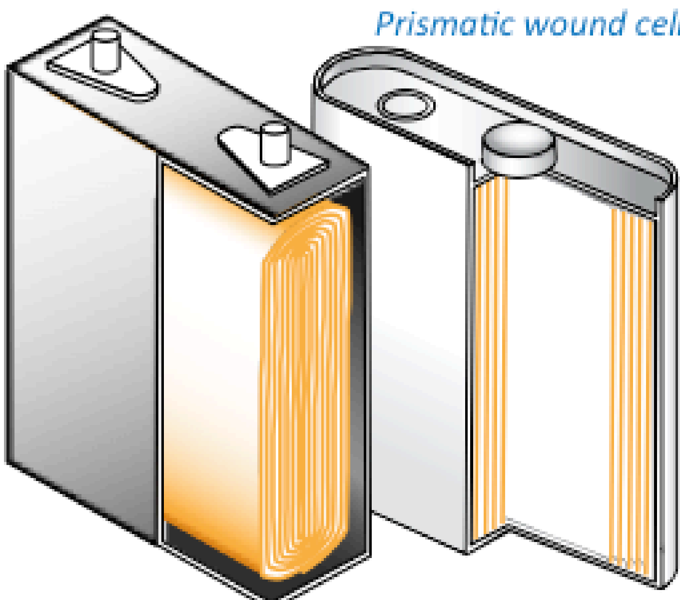
Segregates Time and Length Scales
Decouples geometries

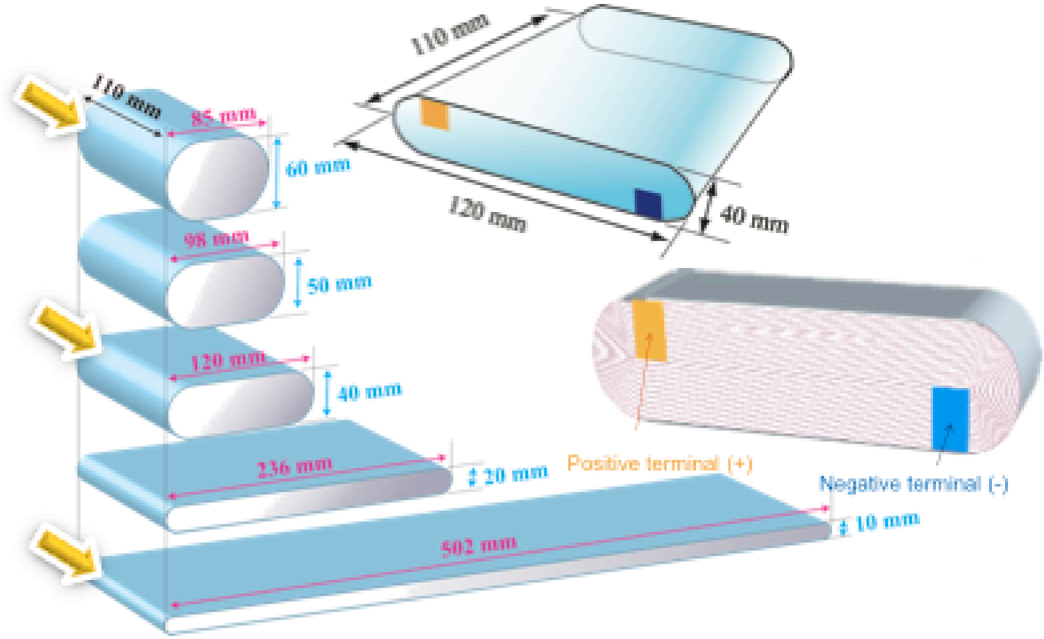


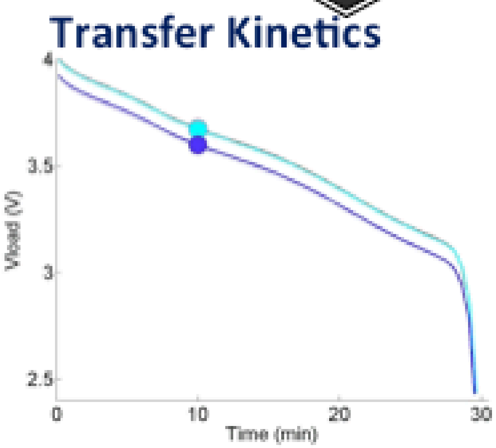
Computationally Efficient
Modular
Flexible

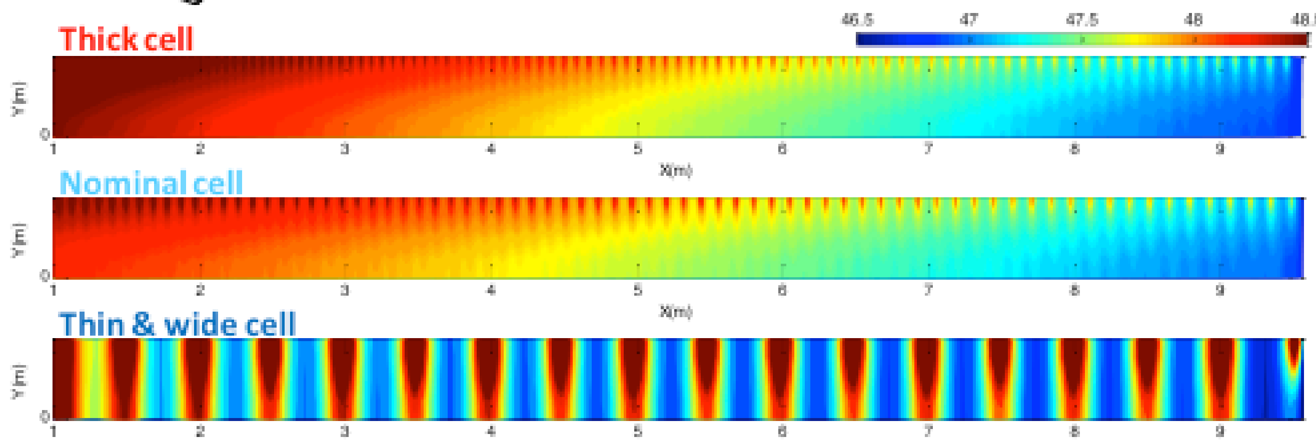
Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemistry*, 2011, Vol. 158, No. 8, pp. A955–A969.

Evaluating Impact of Aspect Ratio



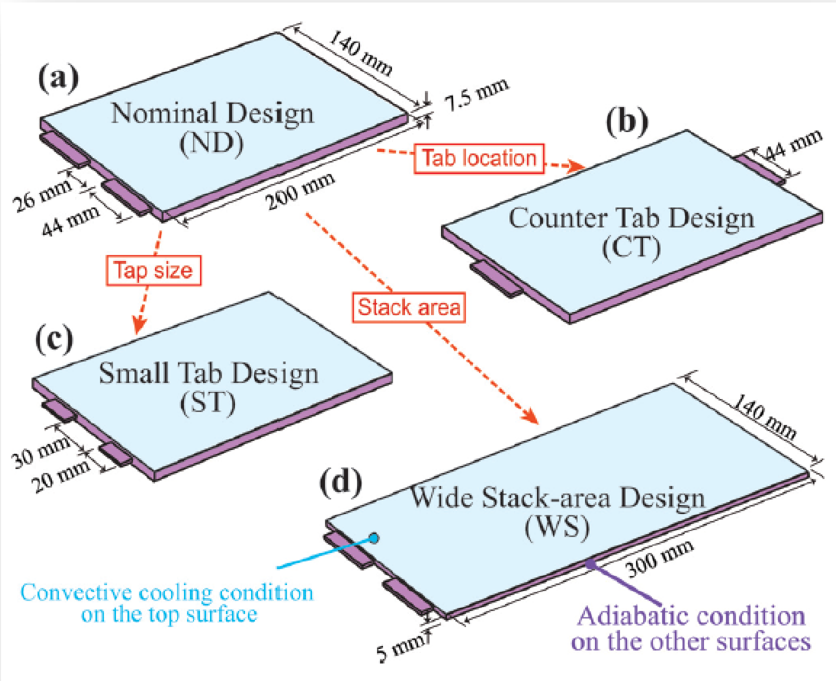




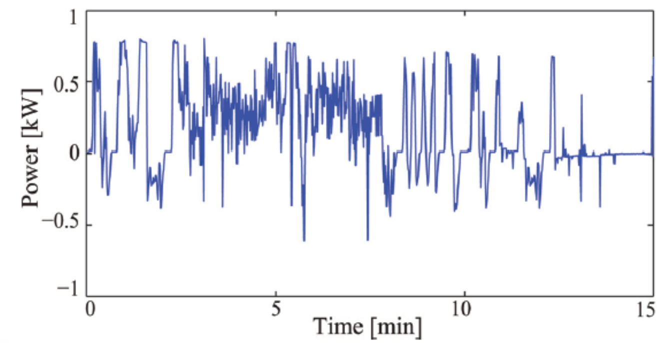


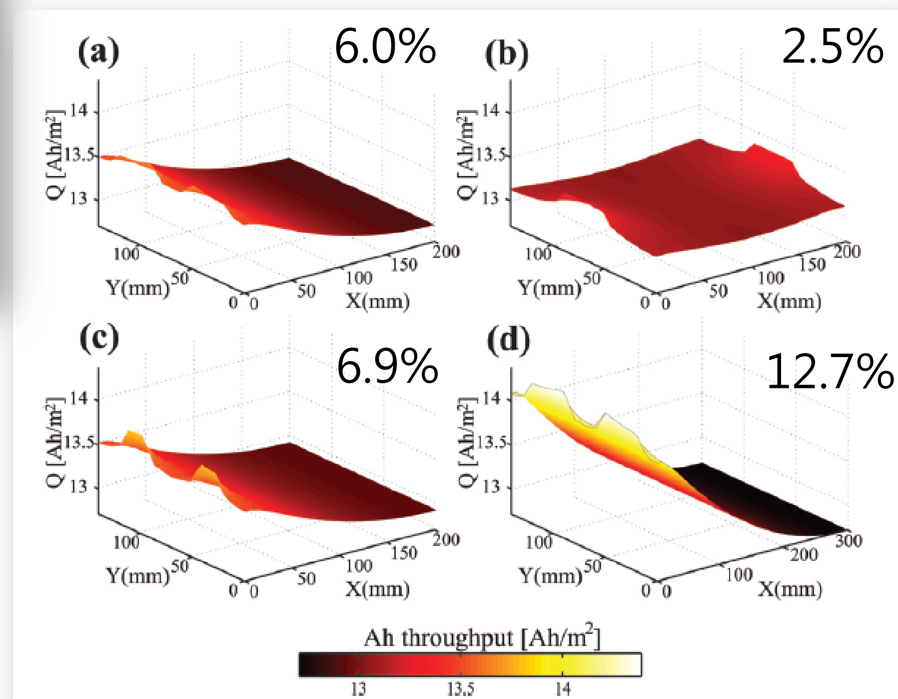
The model quantifies the impacts of the electrical/thermal pathway design on uneven charge-discharge kinetics in large format wound prismatic cells.

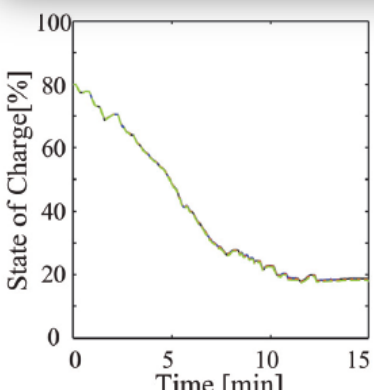
Understanding Non-Uniform Utilization

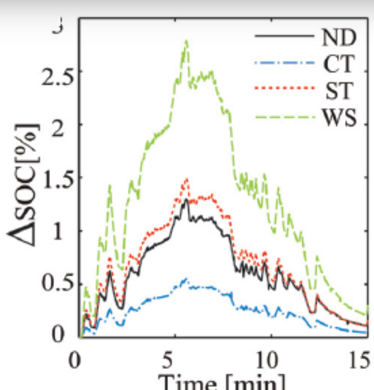


Mid-sized Sedan PHEV10 US06









Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemistry*, 2011, Vol. 158, No. 8, pp. A955–A969

Developing CAE Battery Modeling Tools

I. Realizing the need to develop CAE tools, U.S. DOE initiated the CAEBAT project in 2010

II. Partnerships between national labs, battery developers, software providers, universities, and carmakers were established

III. With technical support from NREL and Oak Ridge National Laboratory, three independent teams developed competitive CAE battery tools

IV. CAEBAT tools are now available for purchase
   1. EC Power's battery design software is called AutoLion™
   2. CD-adapco's battery simulation module is available in STAR-CCM+
   3. ANSYS's battery design tools are an integral part of Fluent 15 and 16

CAEBAT: Computer Aided Engineering for Electric Drive Batteries

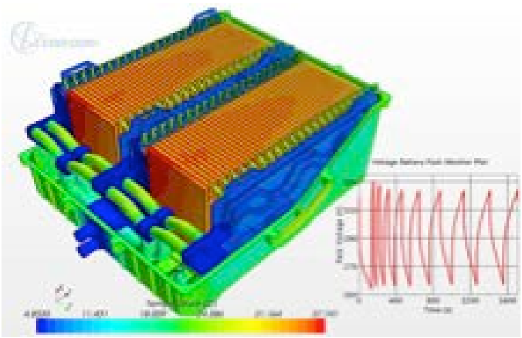
CAEBAT Tools for Battery Design

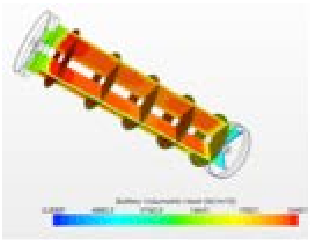
CAEBAT tools could:

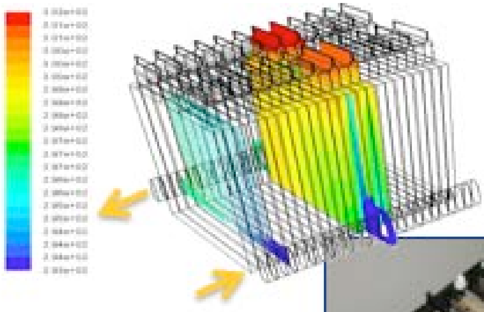
I. Predict electrochemical, electrical, and thermal performance of a cell based on geometry, chemistry, and power load

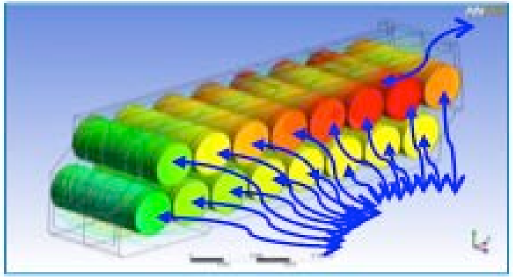
II. Simulate performance of a battery pack with various thermal management designs

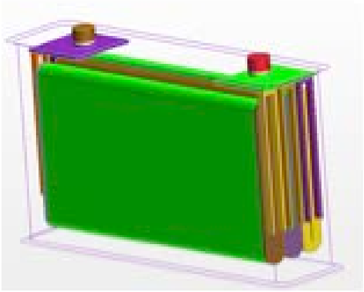
III. Provide insight on the safety and life implications of different loads and designs











Battery Crush and Thermal Runaway

Going beyond today's approach: Battery as a brick

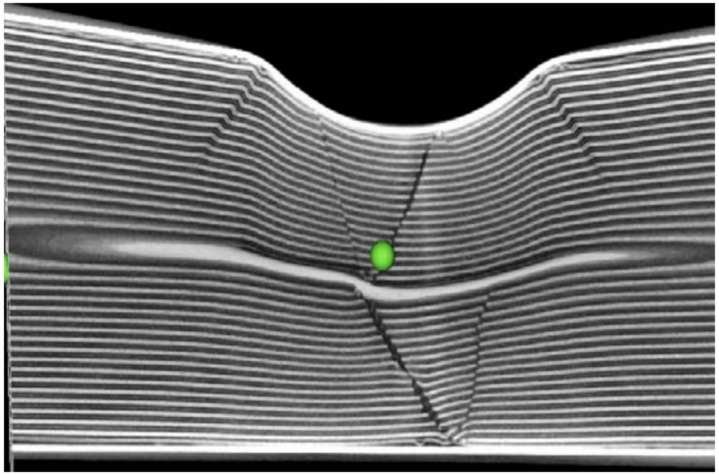
Li battery safety a major concern – need to have CAE tools

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

Modeling Battery Mechanical Crush

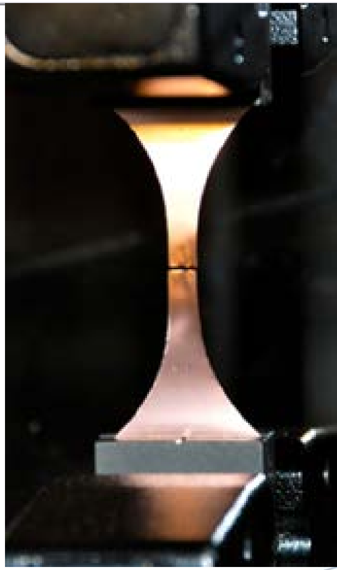
I. Electric vehicles (EVs) must be as safe as other road vehicles, particularly during a crash; need to understand crushed battery's thermal response

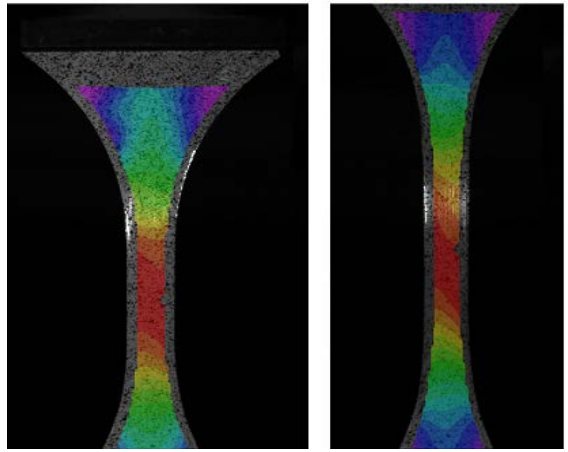
II. In 2014, U.S. DOE initiated the 2^{nd} phase of CAEBAT to include modeling mechanical behavior during EV crash-induced crush

III. NREL initiated collaborating with others to develop coupled mechanical-electrochemical-thermal models to predict the response of cells or modules upon structural failure

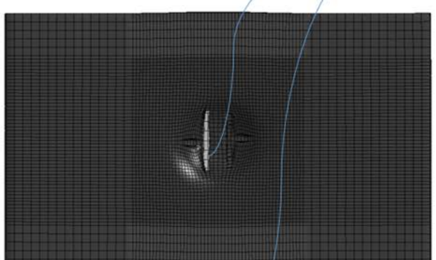
1. Simulating simultaneous mechanical, electrochemical, and thermal response of a cell or module due to crush is very complex and requires modeling simplifications
2. Crush is an event that usually happens in less than $1/10^{th}$ a second while subsequent electrochemical and thermal responses take much longer
3. Our approach is to model structural behavior first; capture the characteristics of damaged zone and use it for electrochemical and thermal modeling to see if thermal runaway could occur
4. This allows us to link the mechanical aspect with the thermal aspect in a sequential, one-way fashion

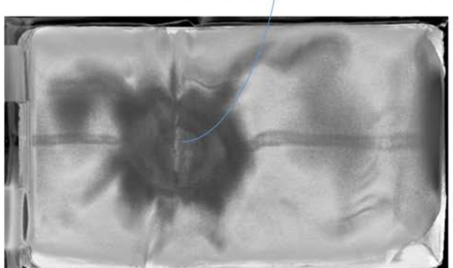
Component Level Characterization at MIT

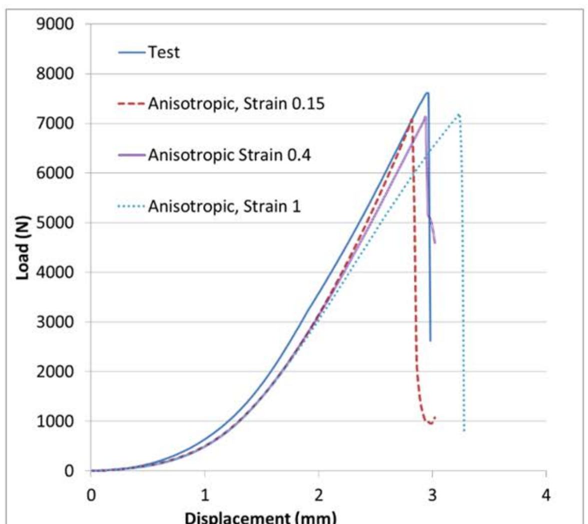




Crack Location and Orientation







I. Crashworthiness lab at MIT performing multi-axial strain measurements
II. Digital Image Correlation used to reduce measurements to material properties for input into LS-DYNA
III. These models are used to predict origin of cracks

Progress to Date: Cell Crush Modeling

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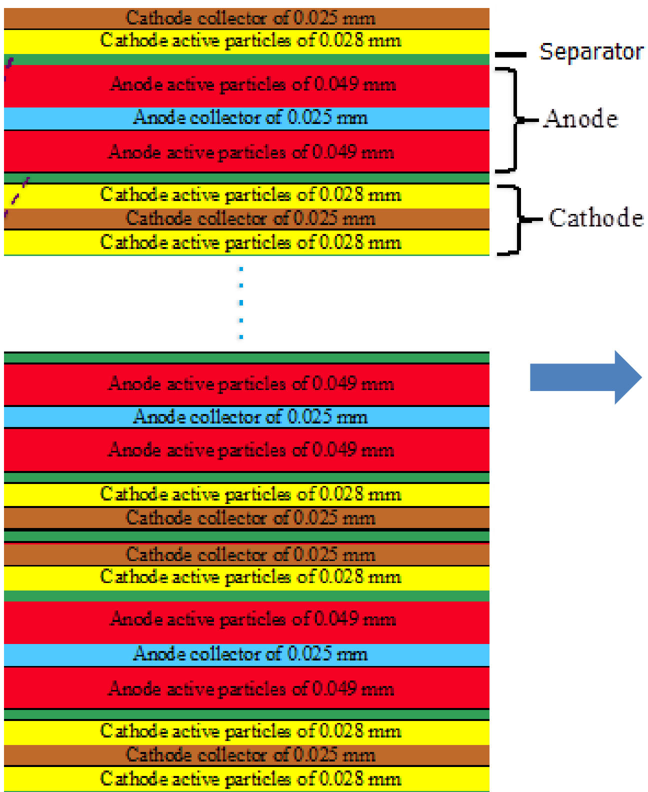
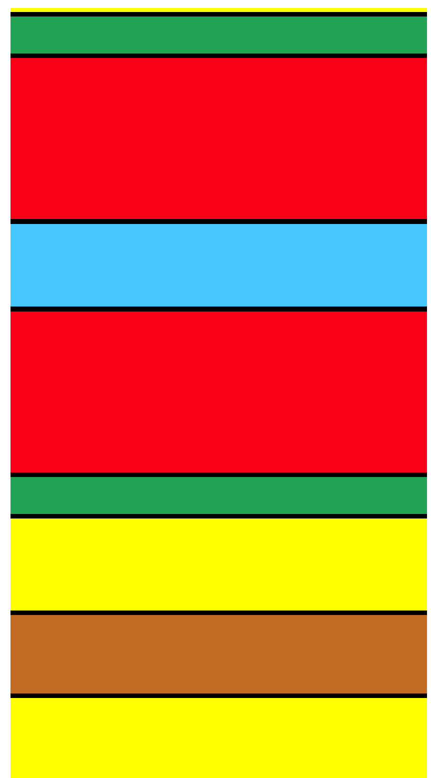
To obtain the structural deformation of layers of cell upon a specified crush and to predict short circuit, we need a refined model to represent each individual layer of current collector, anode, cathode, and separator

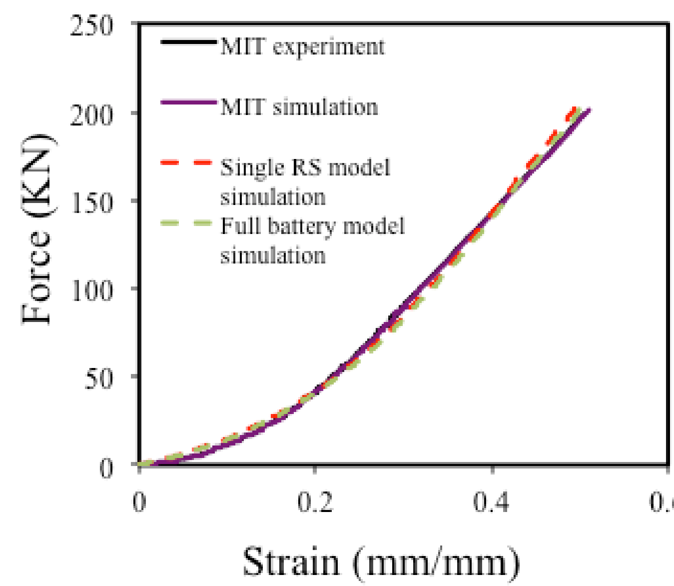


Through-thickness architecture
Multiple layers in a cell



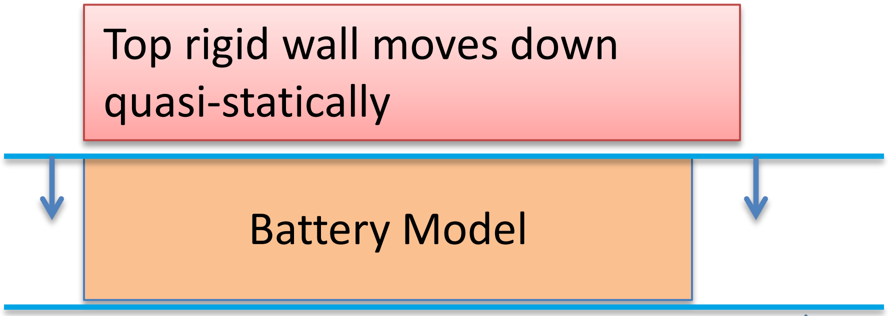
Simplified representative sand
wich (RS) with equivalent mec
hanical properties

Choice of M odel	**Total # of layers**
RS model	8
Full model	166

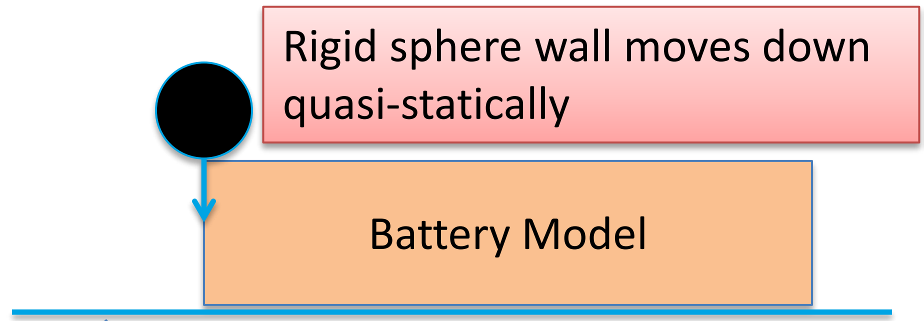


LS-DYNA Mechanical Simulation and Results

❖ Compression



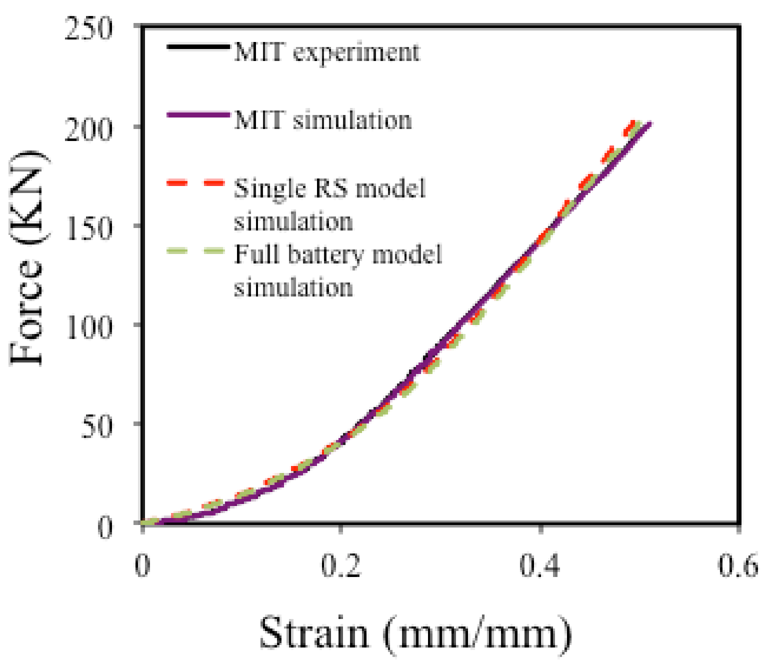
❖ Indentation



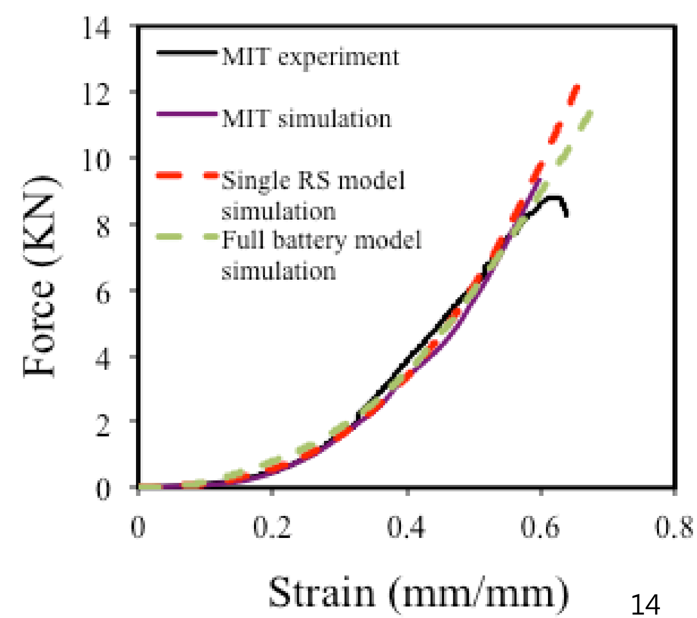
A small friction coefficient (0.01) is defined between the rigid wall and battery to avoid numerical instability.

Bottom rigid walls fixed

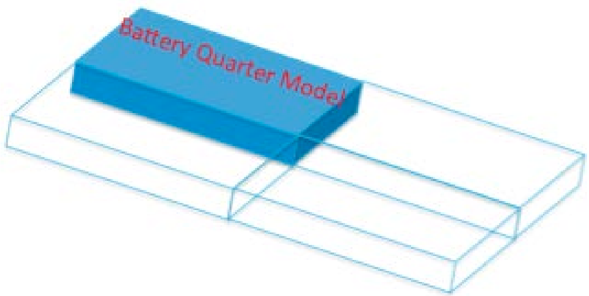
In the present work, fracture (material failure, element deletion) is not considered.



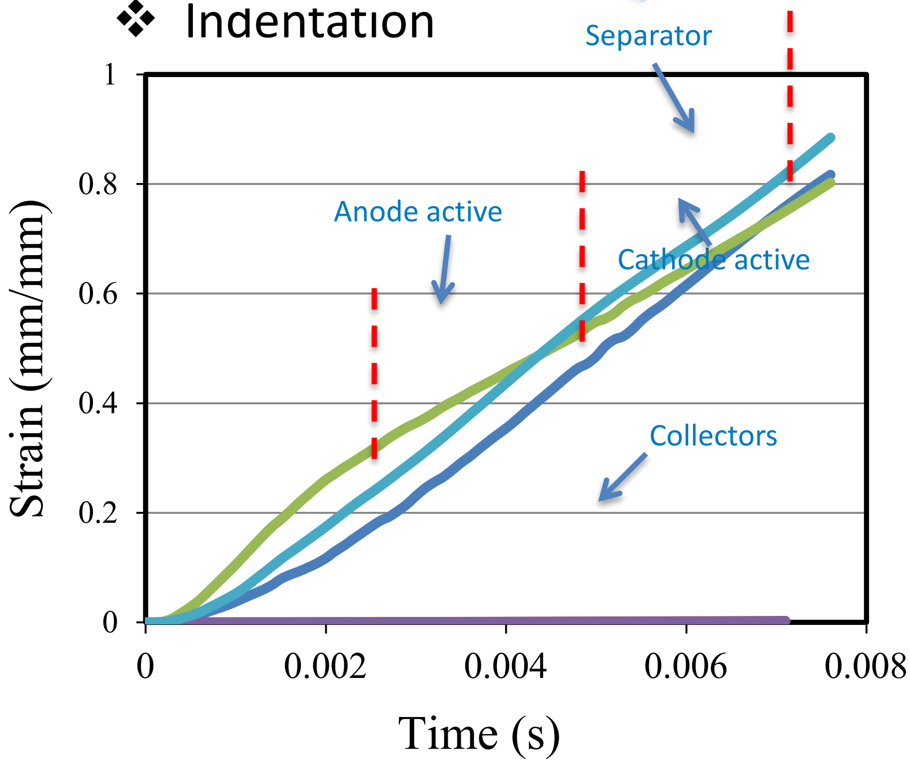
The RS model can correlate with the whole battery model. It can be used to study the individual deformation mechanism and structure-electric-thermal coupled responses.



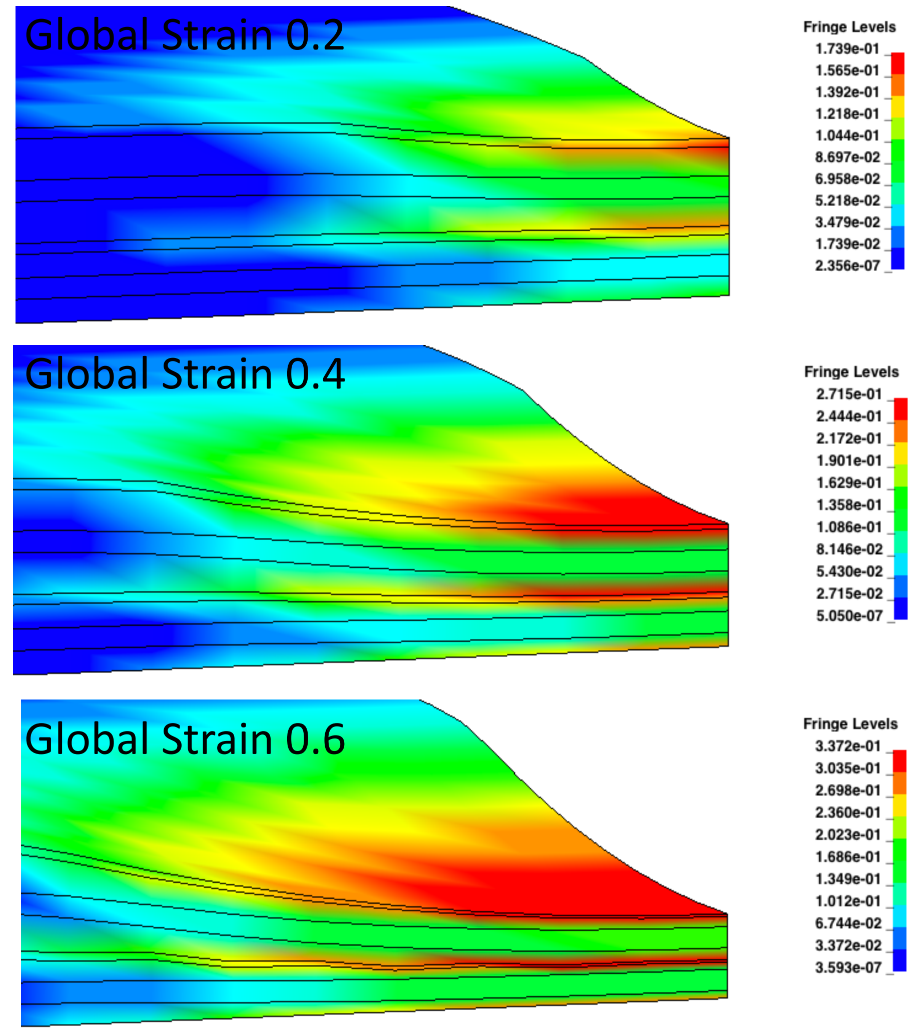
Mechanical Simulation: Individual Deformation



❖ Indentation



❖ Von Mises strain contours

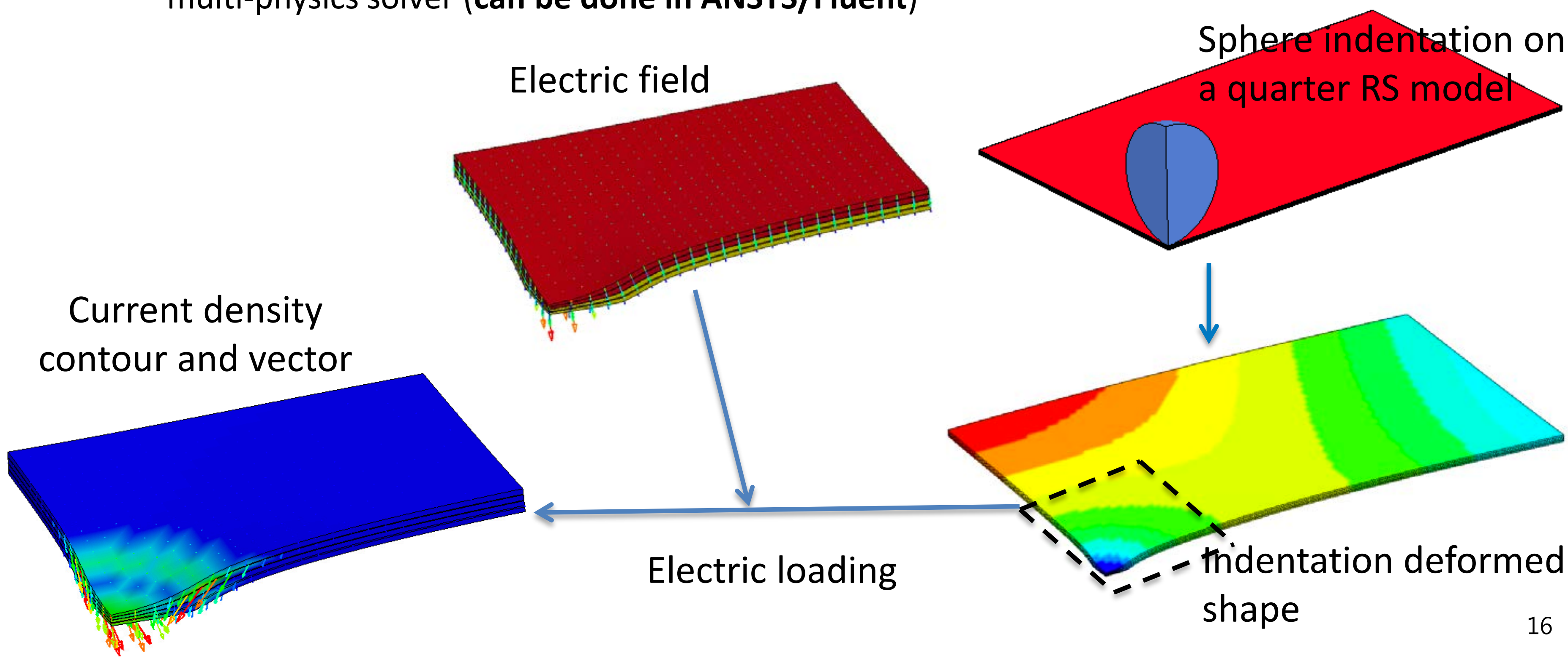


1. Indentation-induced damage is more localized and complicated
2. Separator is very likely the first to fail

Mechanical-Thermal-Electric Coupled Simulation: LS-DYNA Multi-physics Solver

Studies on conducted to predict the electro-thermal responses. As preliminary investigation, only the single RS model is studied.

- Sequential mechanical-electric-thermal coupled analysis:
  - The RS model is first analyzed using LS-DYNA Explicit
  - The deformed shape at a certain stage is exported into a independent mesh file
  - Electro-thermal model is then built on the deformed mesh and solved using LS-DYNA multi-physics solver (**can be done in ANSYS/Fluent**)

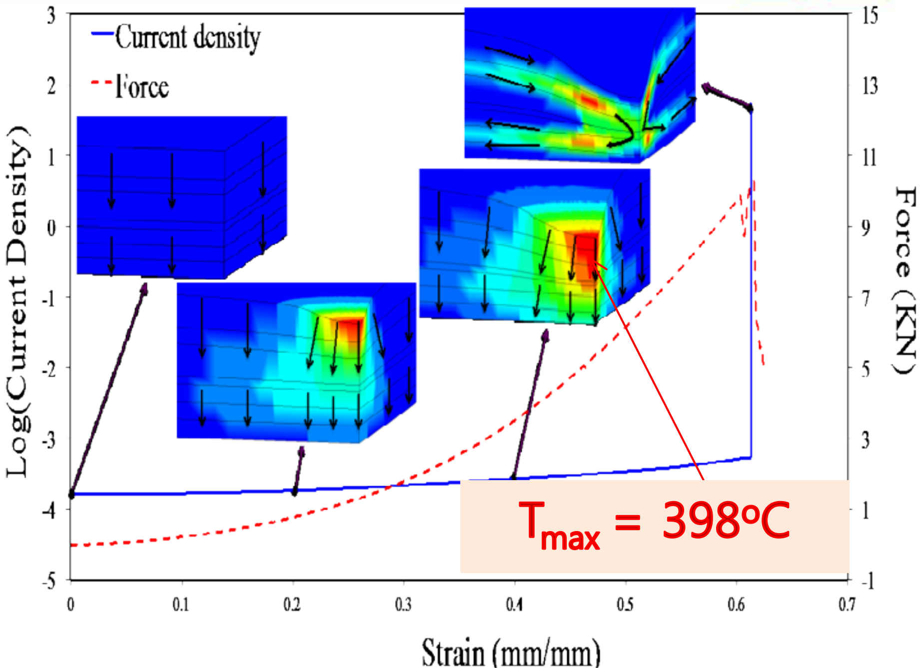


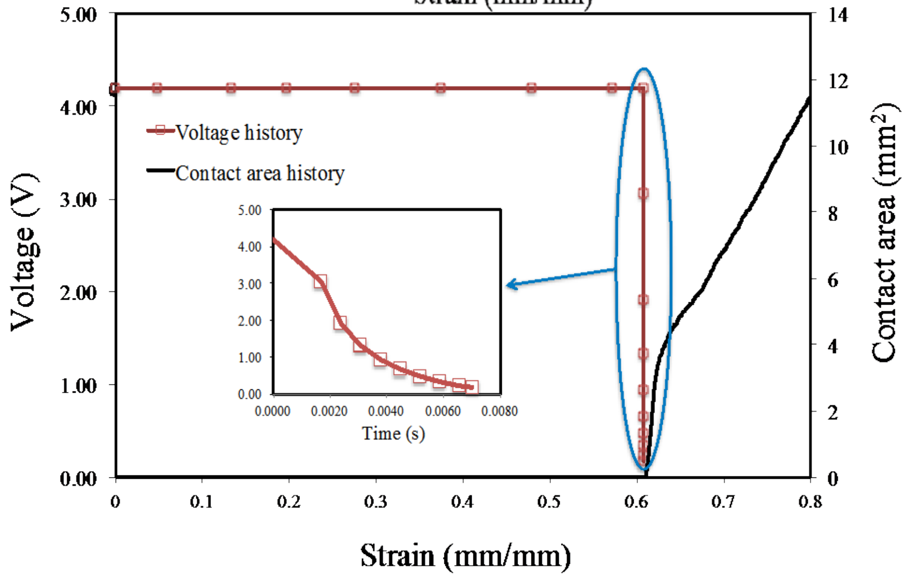
Mechanical-Thermal-Electric Coupled Analysis: Thermal Responses

An adiabatic (perfectly insulated) thermal boundary condition is used

I. Simplified method to couple mechanical crush with the electrical response of the cell that has computational time of a few minutes.

II. Our approach uses multiple criteria to evaluate short-circuit under deformation:
   - mechanical failure of components
   - drop in electrical resistance across the short-circuit
   - temperature-based failure criterion





Linking Deformed Geometry in a Cell to Electrochemical-Thermal Models in CAEBAT

Proposed Approach for Linking Mechanical to ECT - 1

Initial Geometry

↓

Crush Simulations in LS-DYNA

↓

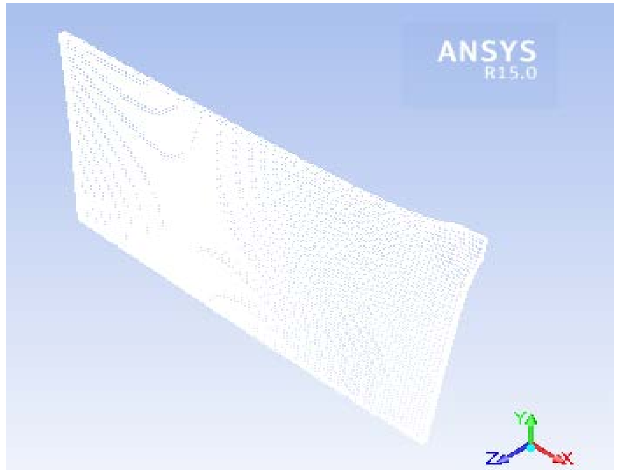
Export Deformed Mesh to ANSYS

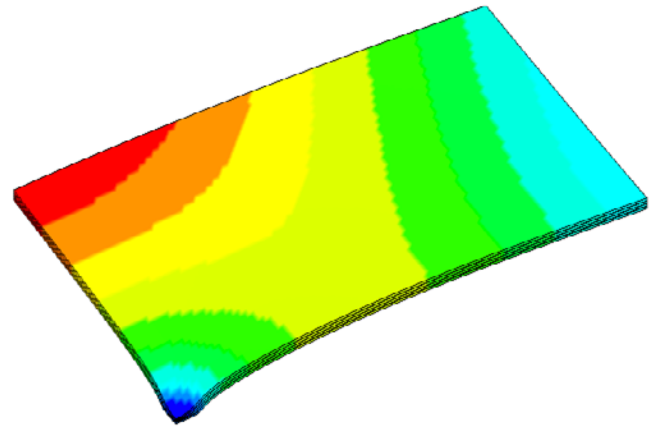
↓

Compute Individual Resistances

↓

Perform ECT Simulations



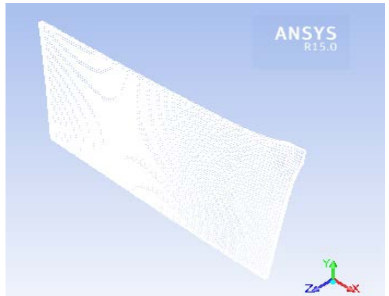


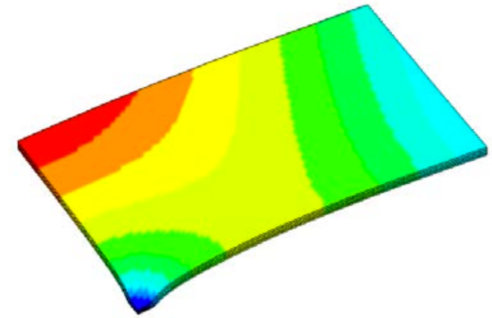
C. Yang et al., 225th ECS Meeting, May 2014, Orlando, FL

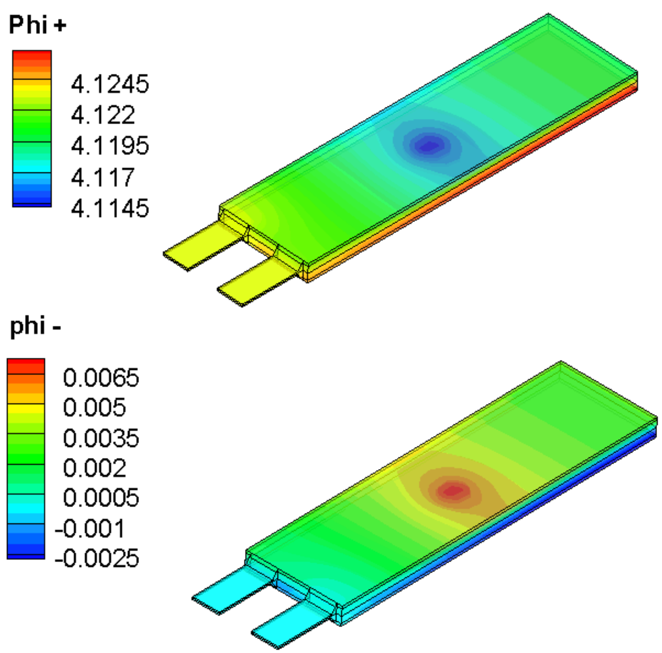
The benefit of using this approach of existing electrochemical-thermal (ETC) in ANSYS/Fluent developed under CAEBAT phase 1

Proposed Approach for Linking Mechanical to ECT - 2

Initial Geometry
↓
Crush Simulations in LS-DYNA
↓
Export Deformed Mesh to ANSYS
↓
Compute Individual Resistances
↓
Perform ECT Simulations







Advantage:

- Better integration of electrical simulations with 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

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Summary

I. Electrochemical-thermal tools under CAEBAT-1
   1. U.S. DOE initiated the development of battery CAE tools for battery design
   2. Three competitive CAE tools are now commercially available

II. Coupling ETC models with mechanical models for simulating cell under indentation and compression (CAEBAT-2)
   1. Incorporating all cell layers, a refined representative sandwich (RS) model is built
   2. The RS model is able to capture the global stress-strain response and predict the local deformation of each component
   3. At the sub-cell level, an anisotropic constitutive model was developed and calibrated against experiments
   4. We also have developed a methodology to capture evolution of contact area during the short circuit
   5. Sequential coupled structure-electric-thermal simulations were conducted using the RS model, which produced reasonable electrical and thermal responses

Future Work – Mechanical ECT Modeling

I. Obtain mechanical properties of various cells and electrodes
II. Further refine the finite element model and apply it to pouch cells with the packaging material
III. Implement fracture in the mechanical simulation
IV. Develop criteria for short circuit using the developed mechanical-electrical-thermal model
V. Sequential analysis using the ANSYS ECT model
VI. Perform simulations of mechanical ECT for a typical crash-induced crush for a cell
VII. Perform experiments on crushing a cell to thermal runaway
VIII. Compare experimental data with the simulation results for refining the model

Acknowledgments

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   - Brian Cunningham
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