Li-ion Battery Safety Modeling

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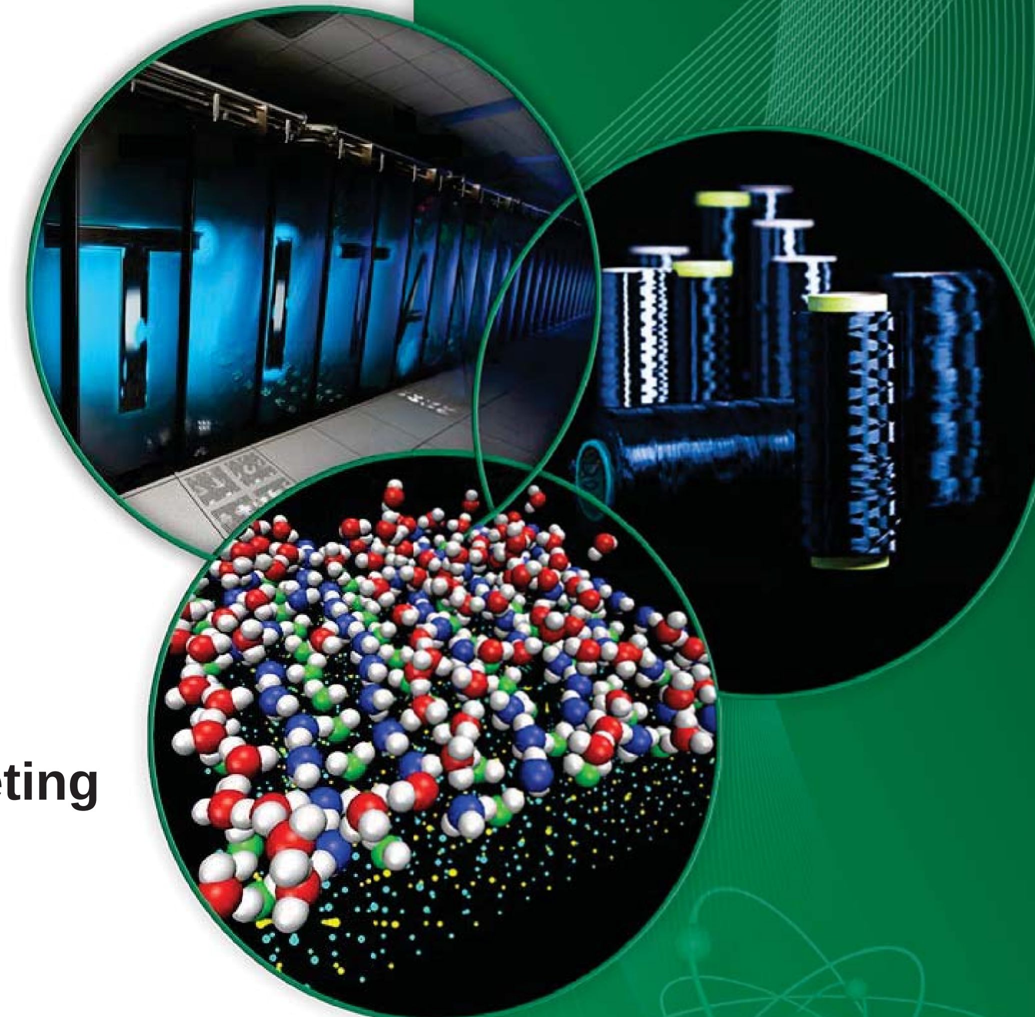

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Goal: Use modeling to design tests that provide leading indicators of failure

Understand deformation
- pinch tests
- pendulum tests

Failure triggers
- rupture of separator
- removal of electrode material

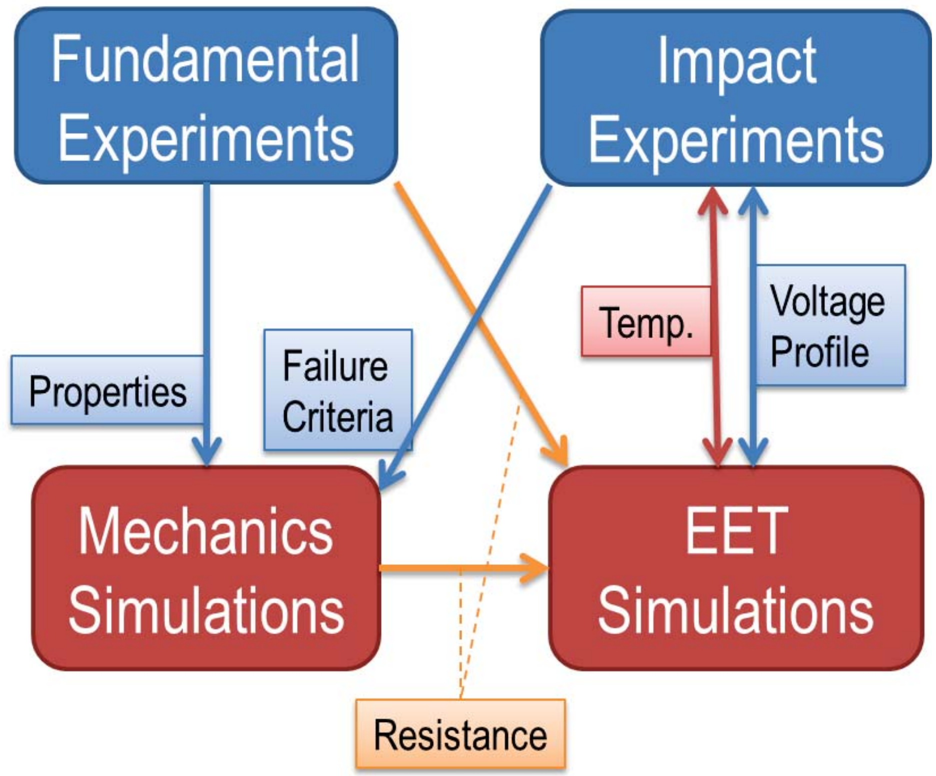
Internal shorts
- anode-Al
- cathode-Cu
- Al-Cu

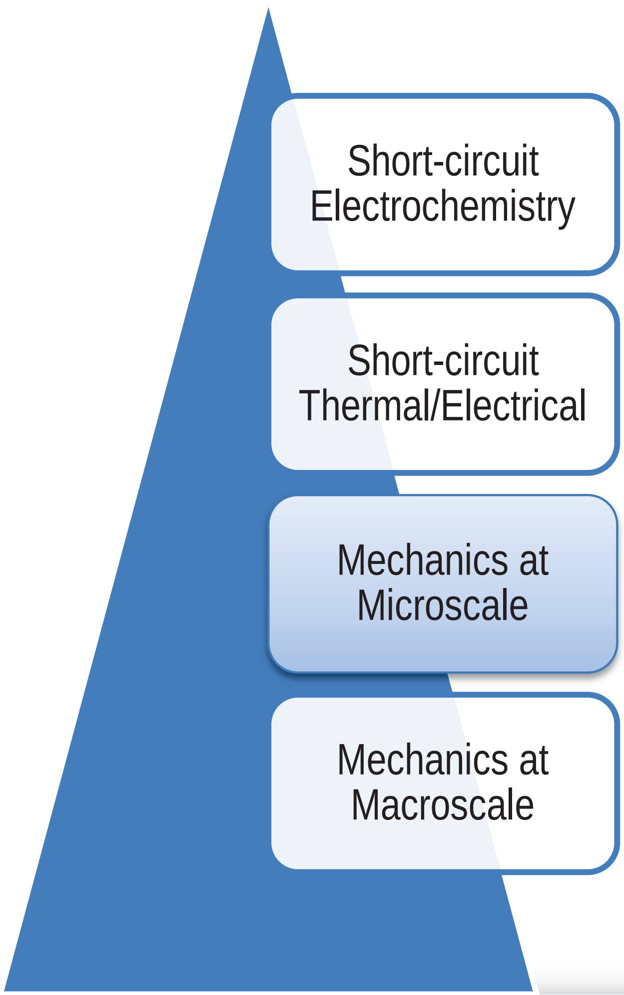
Thermal runaway
- contact area
- contact resistance
- electrochemistry and side reactions

- thermal runaway is key measure of failure
- must understand mechanisms leading to failure in order to predict
- requires predictive pack model
  - hierarchical simulation capability: cell -> cell string -> module -> pack
  - build on current capability, integrate with mechanics, and perform experiments to validate
- simulate a subset of possible modes of battery failure for cell strings or modules
  - mechanics-induced short circuit leading to thermal runaway
    - identify key model parameters
    - identify leading indicators of damage that lead to failure

Tesla explosion in Mexico

Need a complete understanding of shorts in order to design tests for leading indicators of failure.

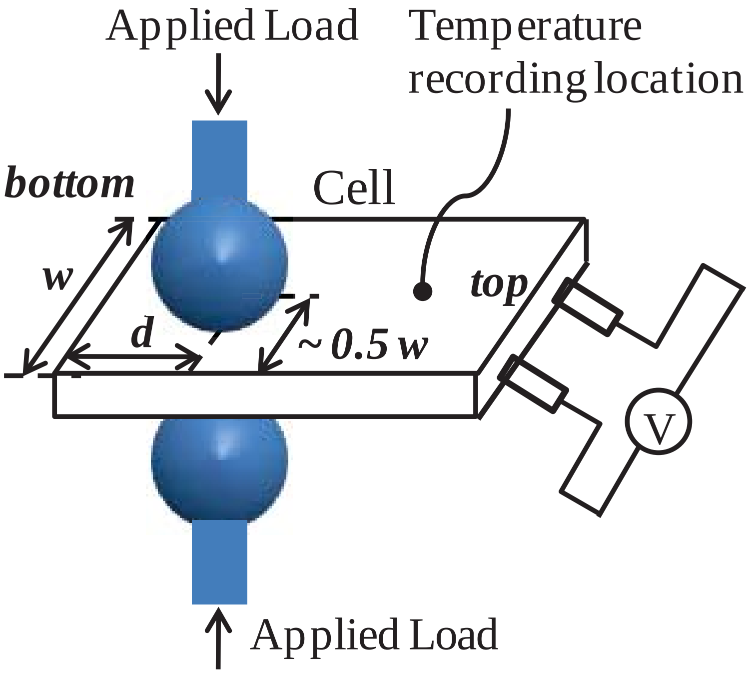


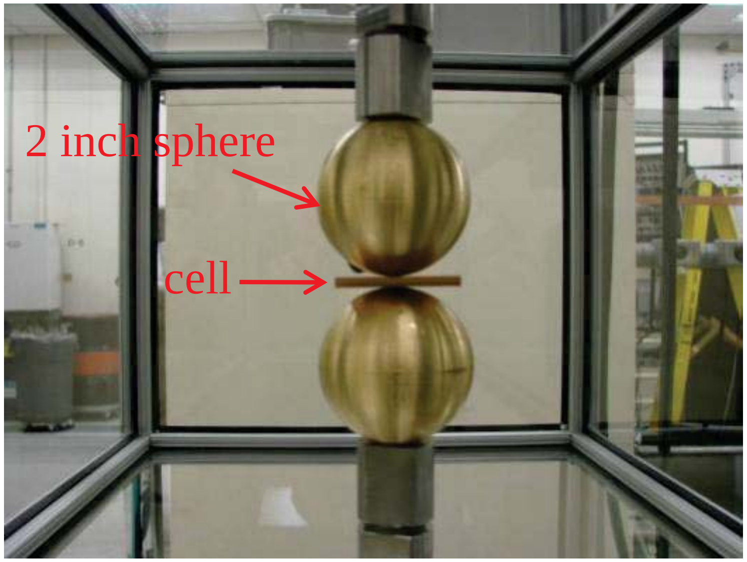


Component	State of understanding
Current collectors	well understood
Electrodes (active material)	not well understood • powder form held together by binders • high degree of porosity • low tensile load capacity
Separator	understood to some extent
Electrolyte	role uncertain
Mechanics of interfaces between components	unknown

Pinch Test rig at ORNL

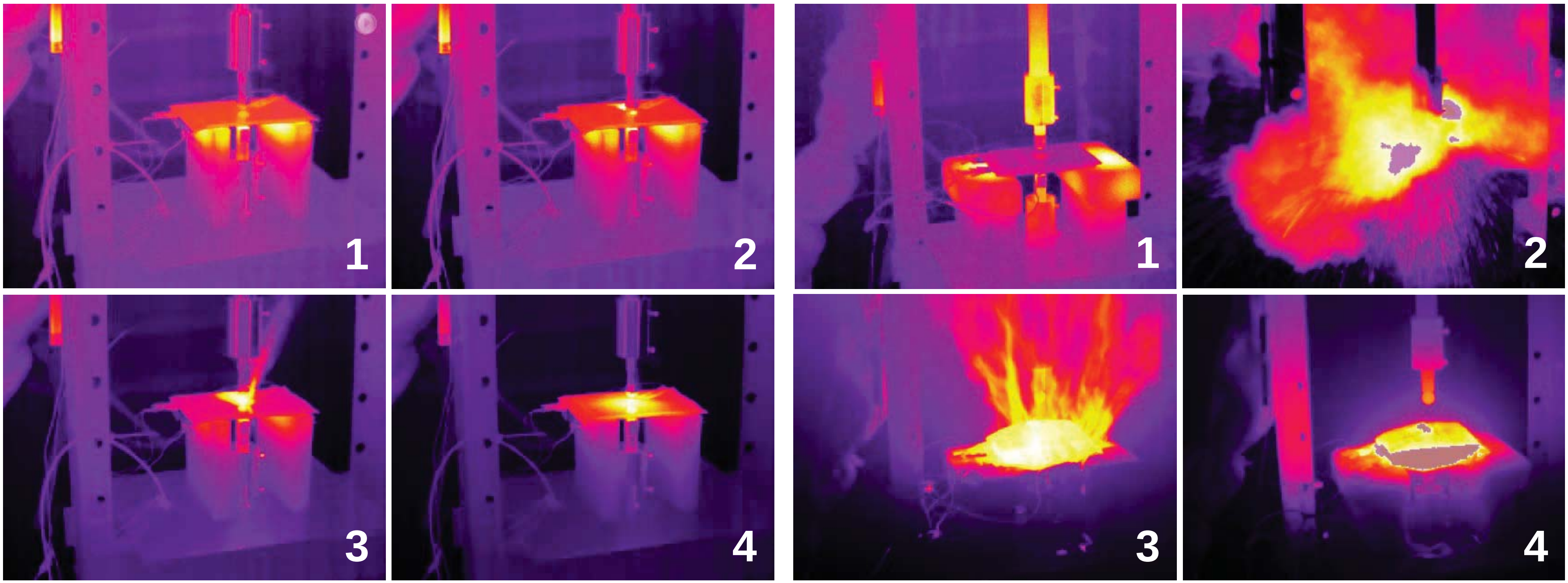
Mechanical Testing System (MTS) Load Frame





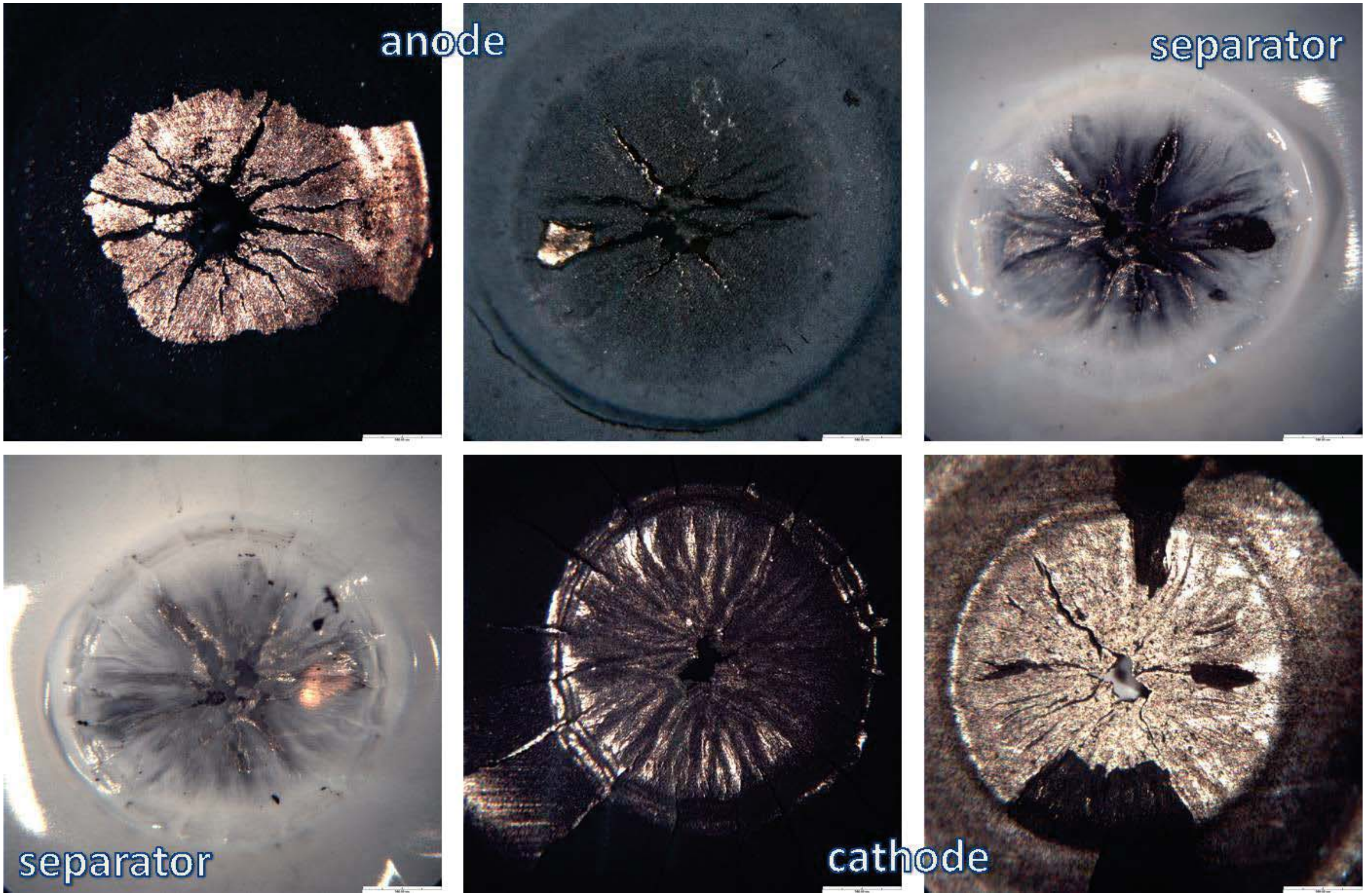
Frames from infrared movies of two pouch-cell batteries subjected to pinch test.

15 Ah | 60 Ah



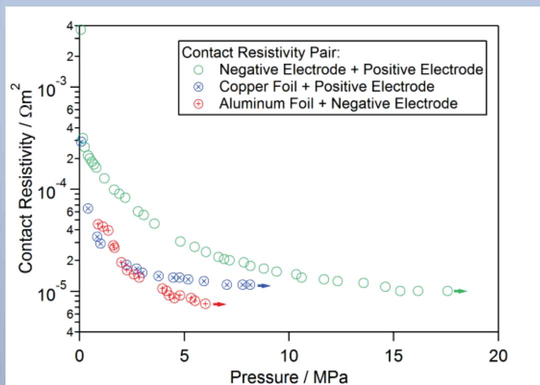
Hsin Wang, ORNL

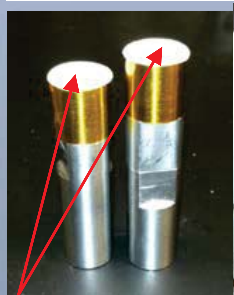
Components exhibit different failure mechanisms – cracking, stretching, tearing.



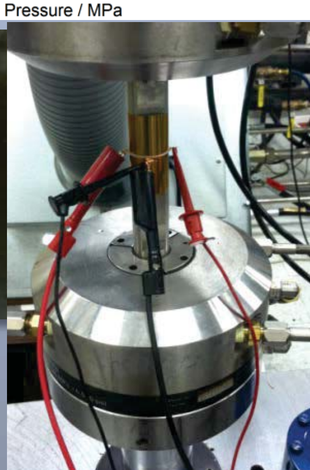
- Circular wrinkles, radial cracks and a hole in center
- Characteristic of tensile failure

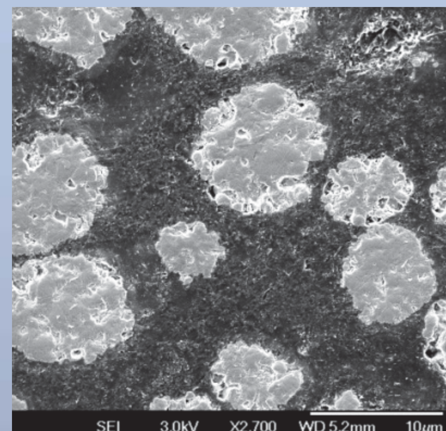
Fundamental Experiments

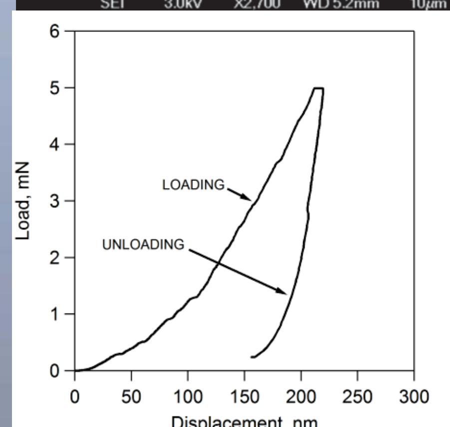


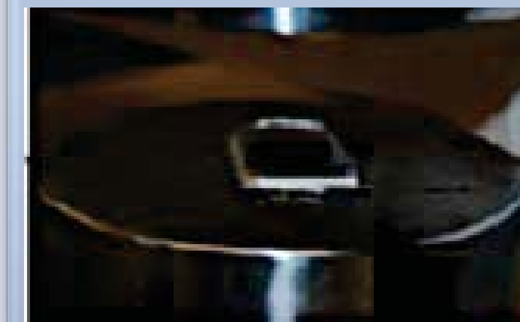


Teflon ®









Sahraei et al J Power Sources 201 (2012), 307-321

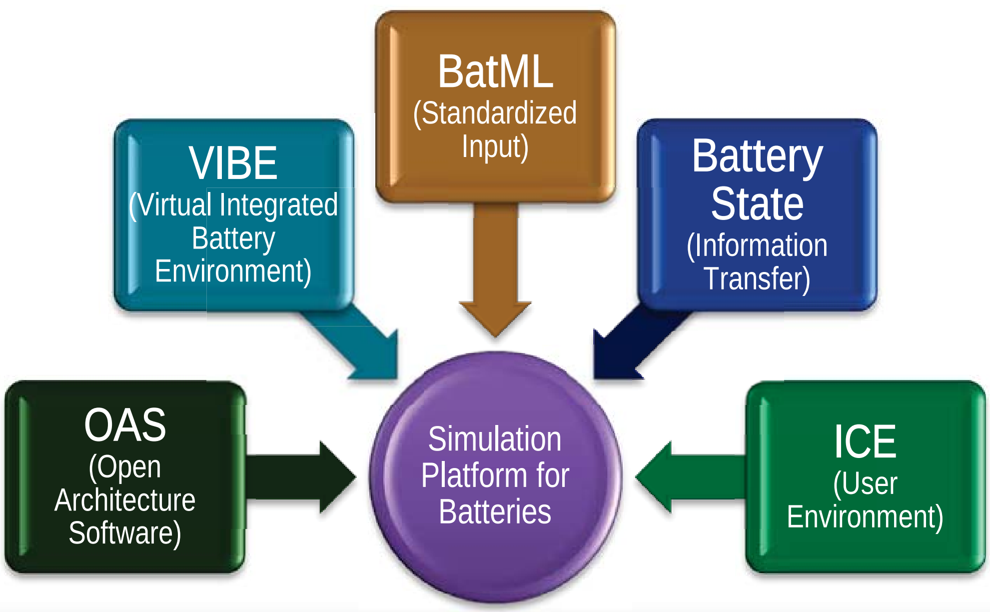
Contact resistance as a function of applied pressure and temperature

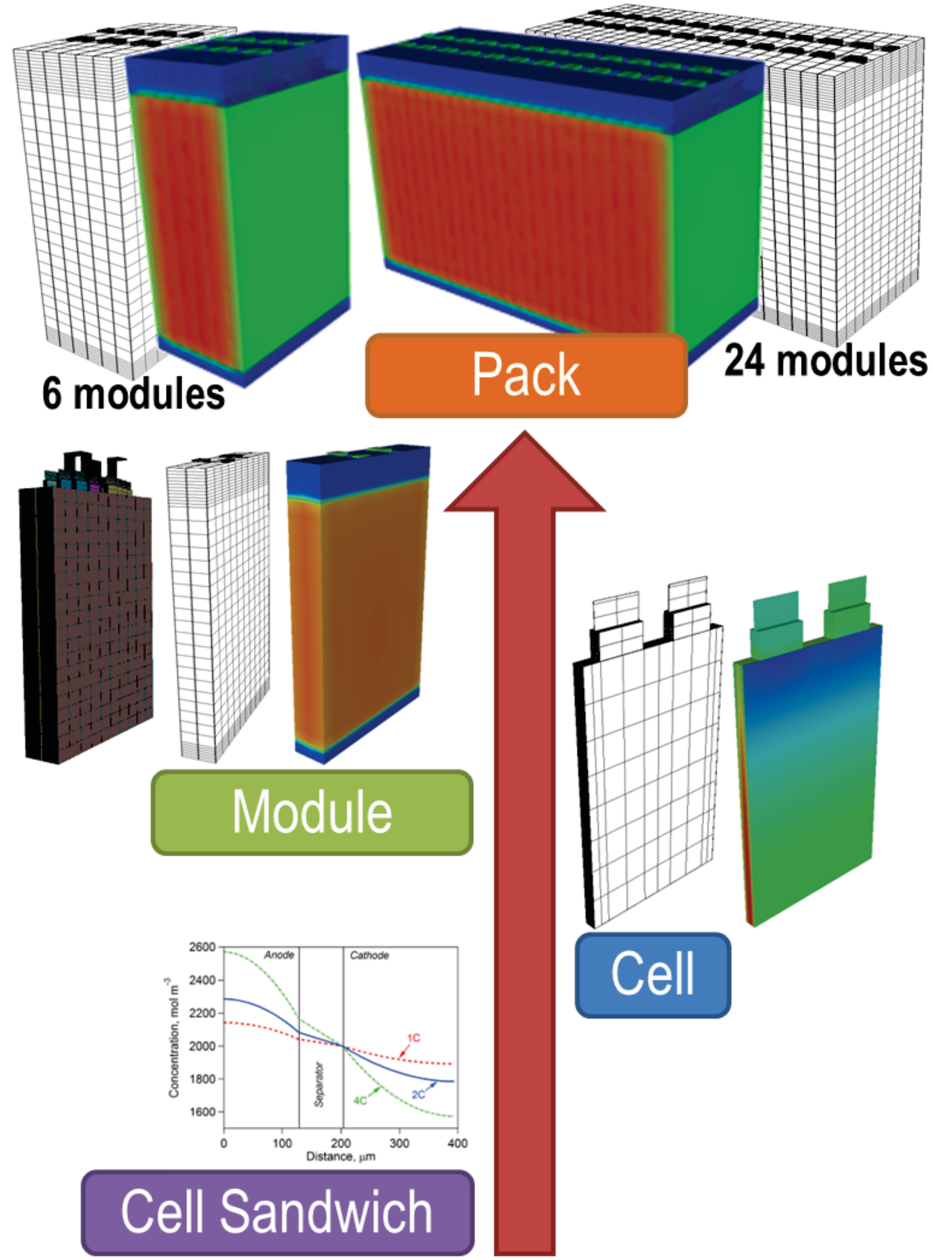
Mechanical properties of electrode materials

Mechanical properties of Li-ion cell layered structure

Computer-Aided Engineering for Batteries (CAEBAT)

- U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE)
  - Vehicle Technologies (VT) Program Office
- Develop and deploy predictive battery design tools for optimizing cost, performance and life
- Partners: NREL, ORNL, INL + three industry teams
  - EC Power / PSU / Ford / JCI
  - GM / ANSYS / Esim
  - CD-adapco / Battery Design / JCI / A123Systems

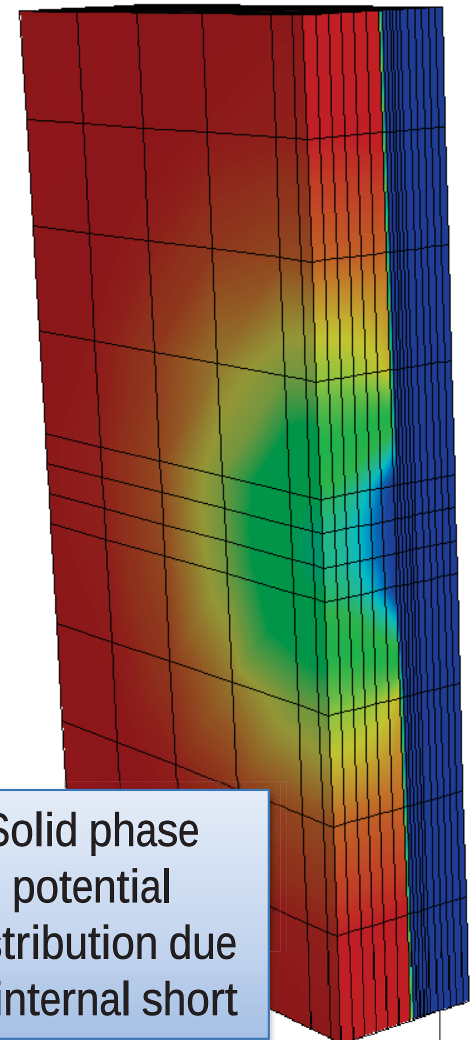


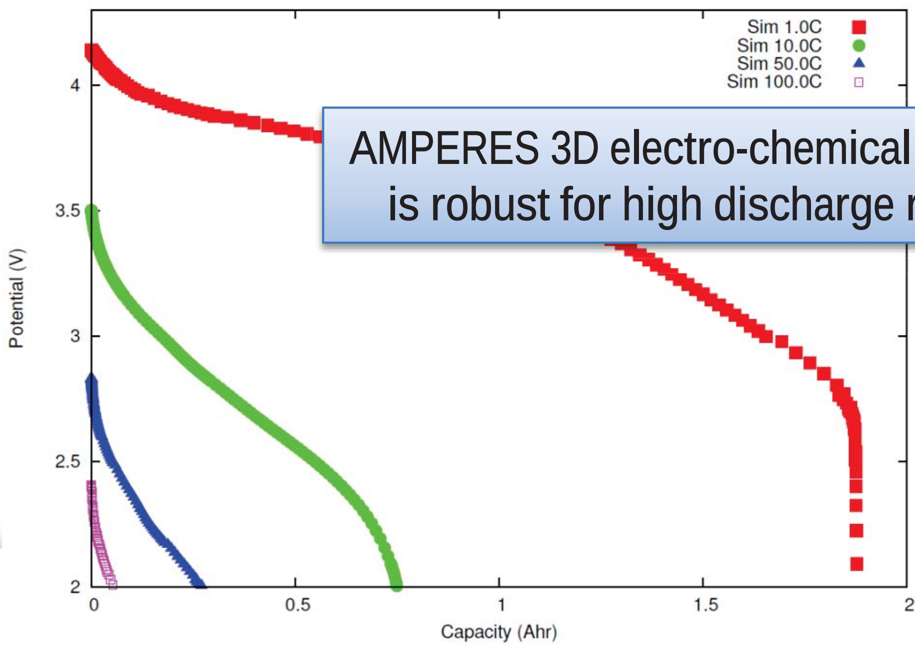


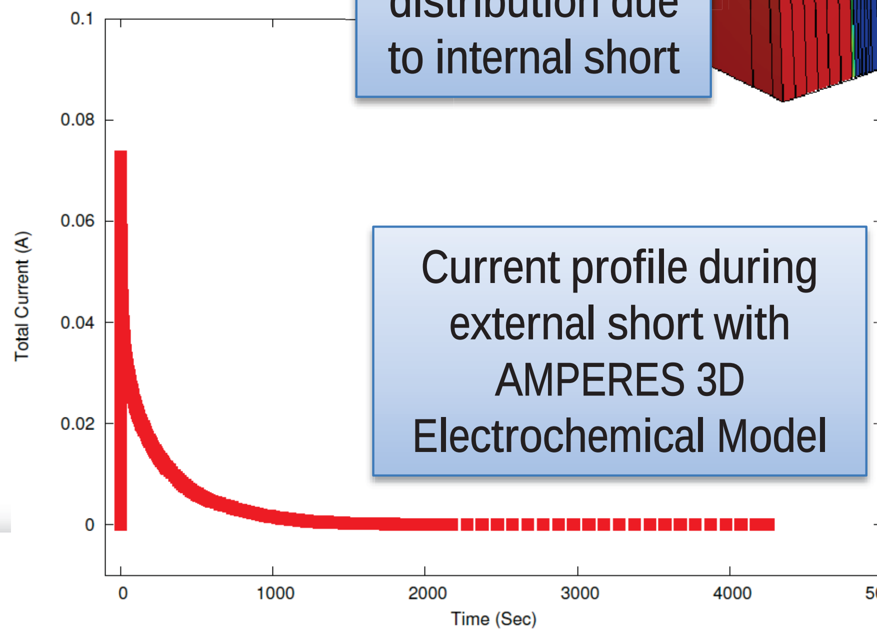
http://batterysim.org/

AMPERES is now robust enough to handle high discharge rates needed for short simulations

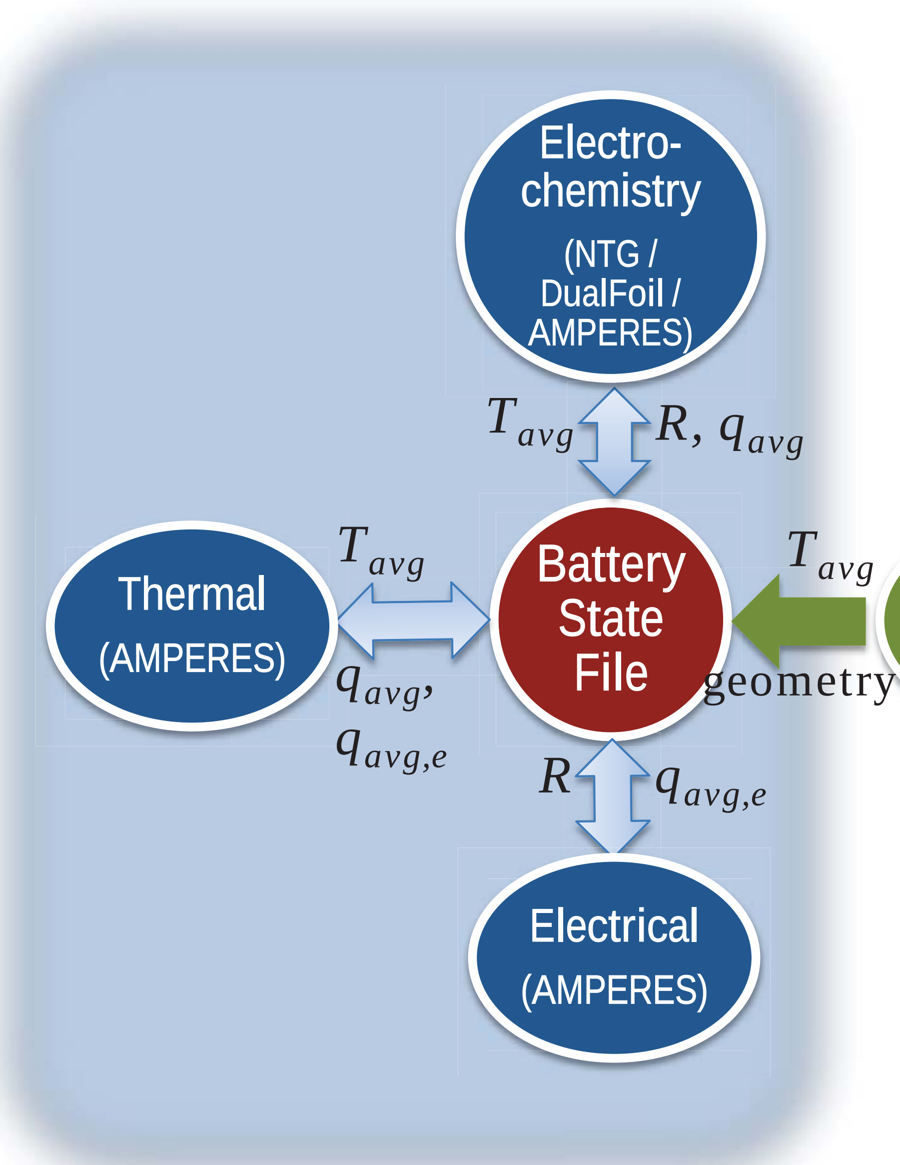
- External short is similar to internal short from an electrochemistry perspective
- Rapidly dropping the potential difference across the terminals in a short time produces exponential rise and decay of current through the battery
  - Now evolving current as part of simulation rather than imposing
- Fully 3D – maps directly to electrical / thermal and mechanical
- Runs in a few minutes

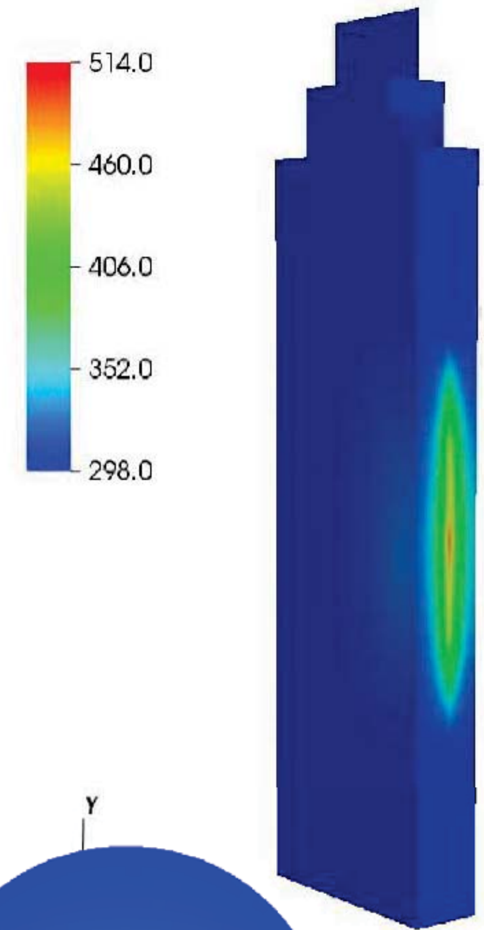


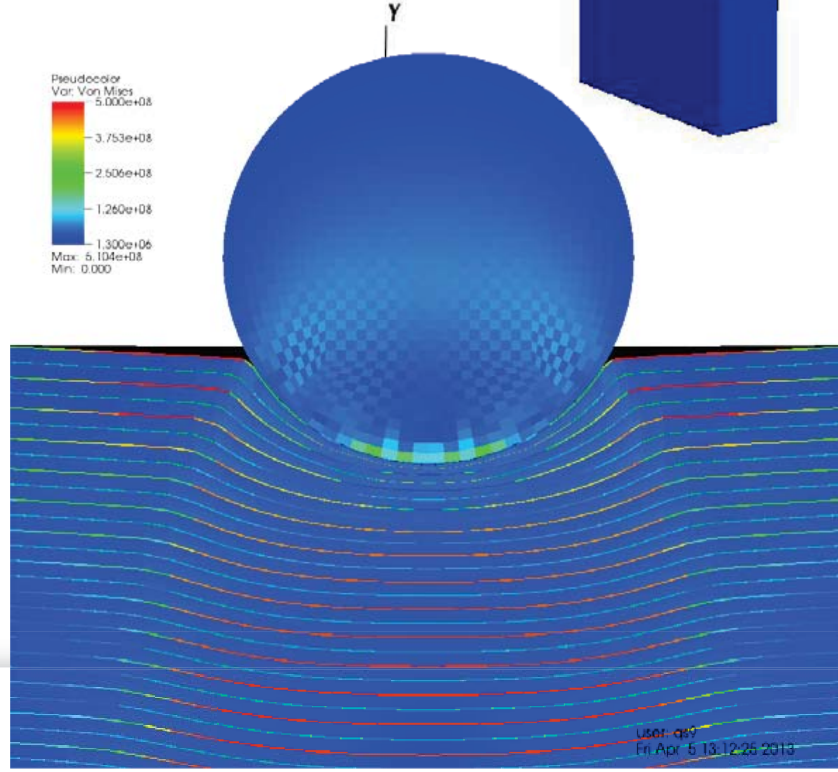




Now coupling VIBE/AMPERES to LS-Dyna for mechanics







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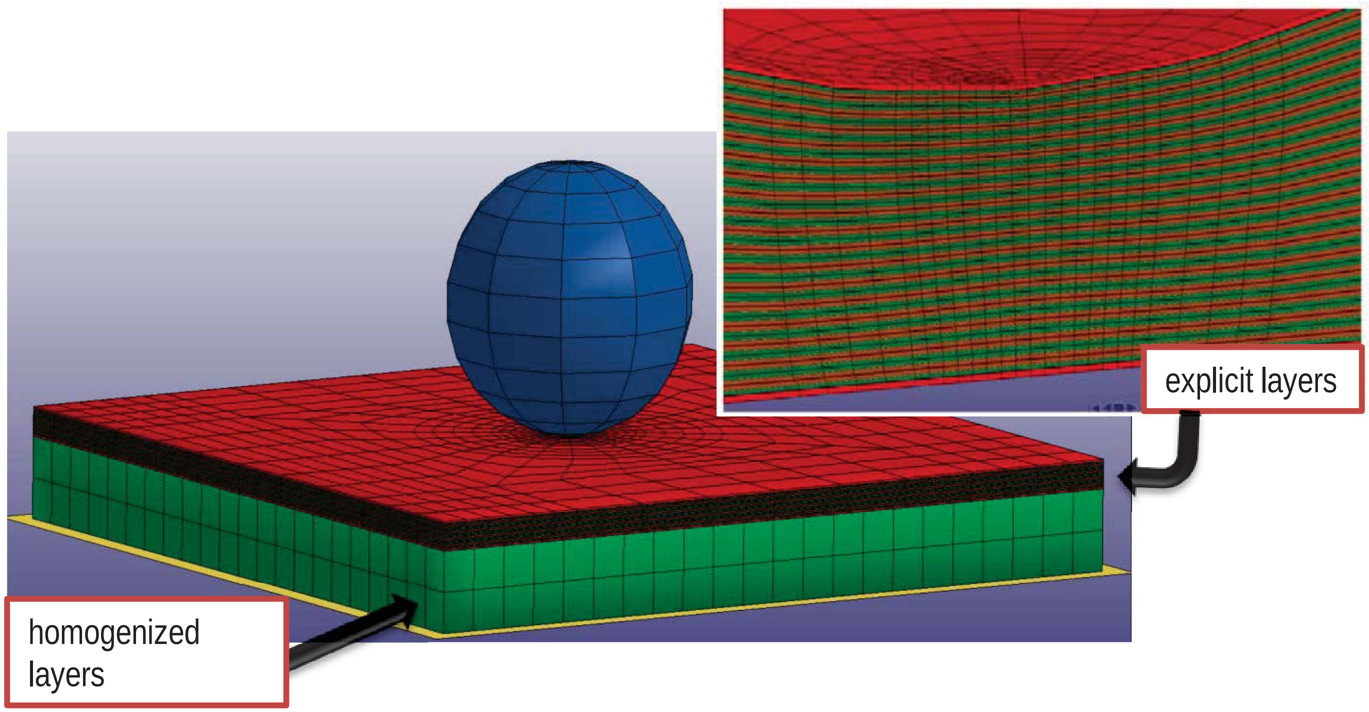
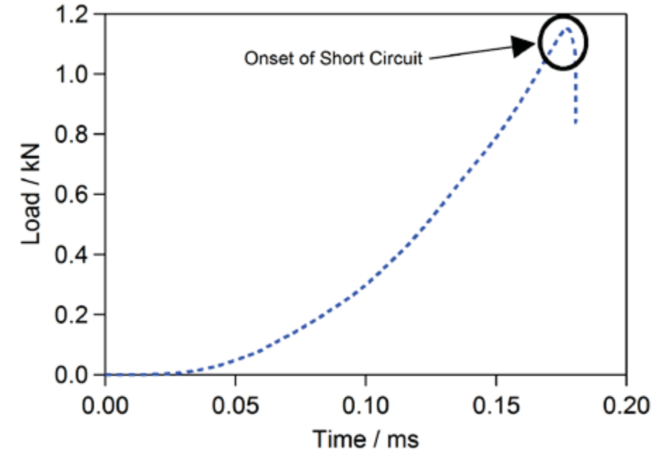
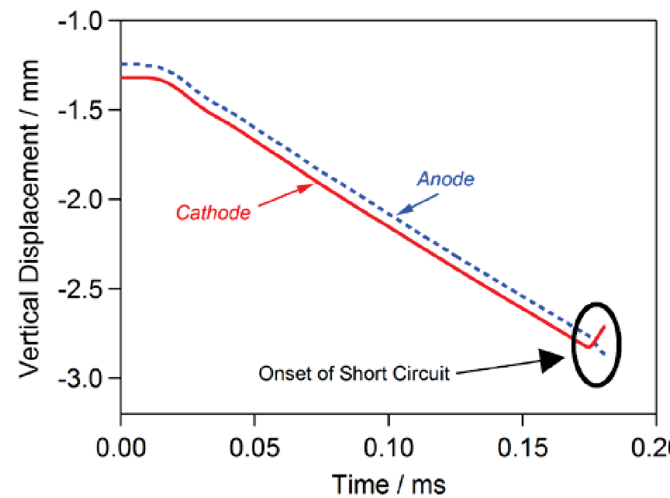
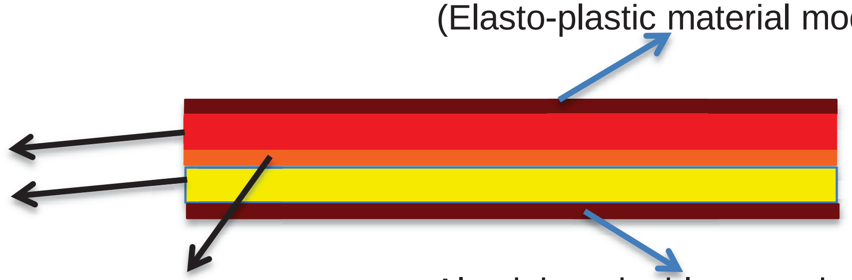
Combining detailed and homogenized representations to efficiently simulate mechanical deformation of pouch cells.





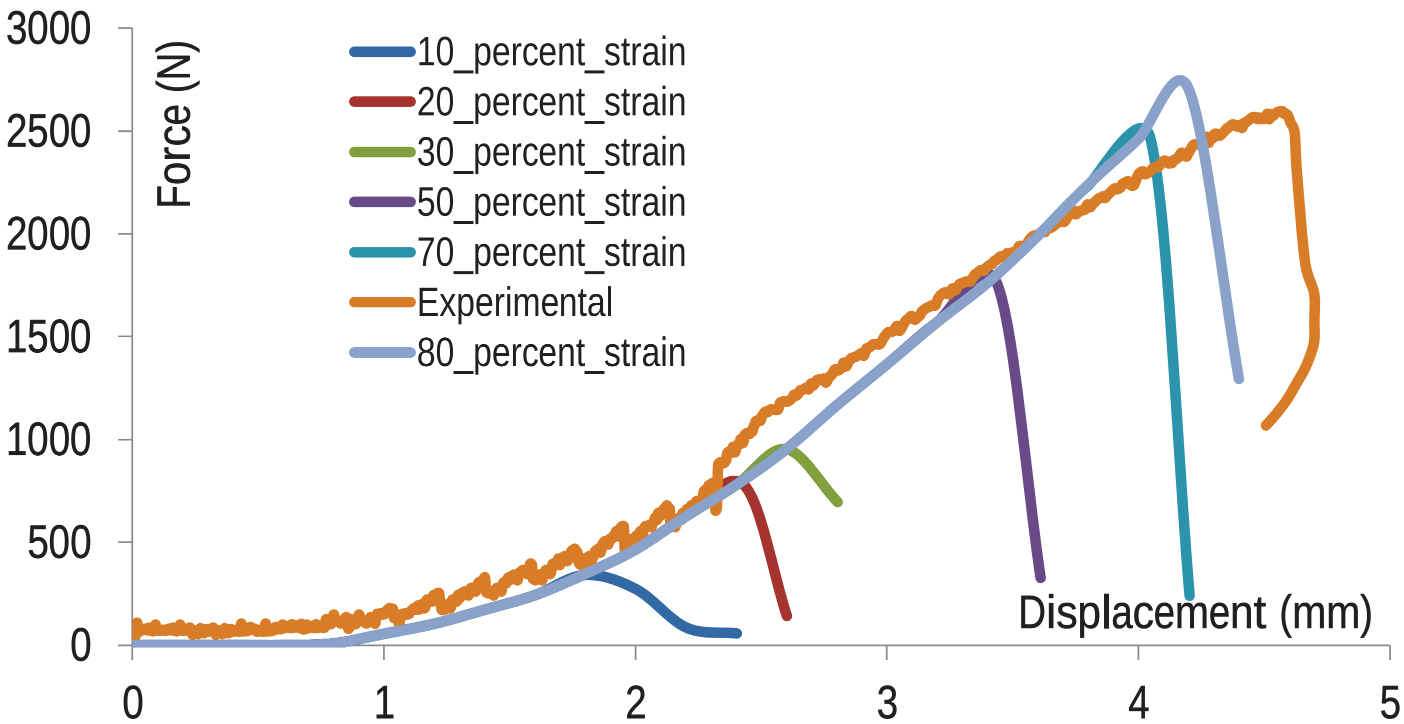




Short occurs when separator fails and cathode and anode come in contact

Failure model for separator is a key parameter in matching observations.

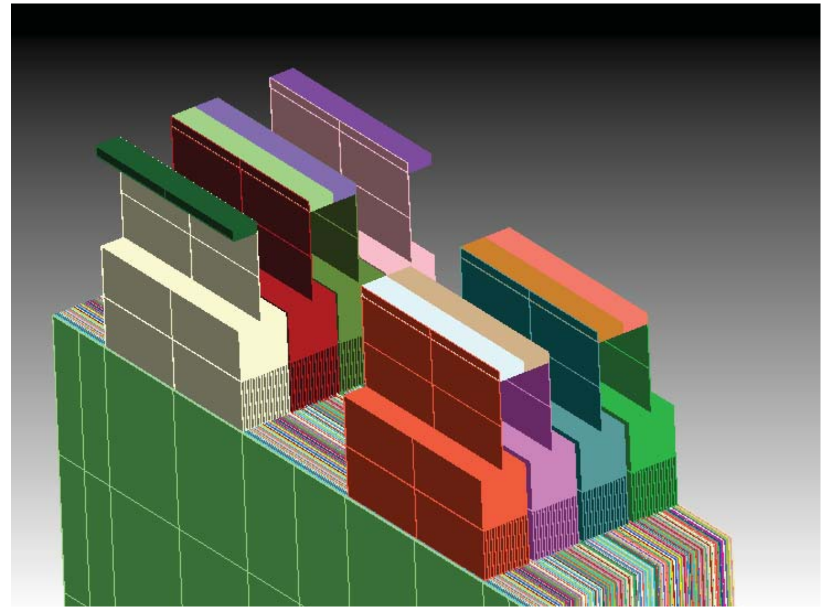
- Failure model -> Effective strain in separator reaches critical value
- Can adjust this parameter to match simulation results to experimental data
- For commercial separator maximum strain before failure can be up to 160 percent [1]



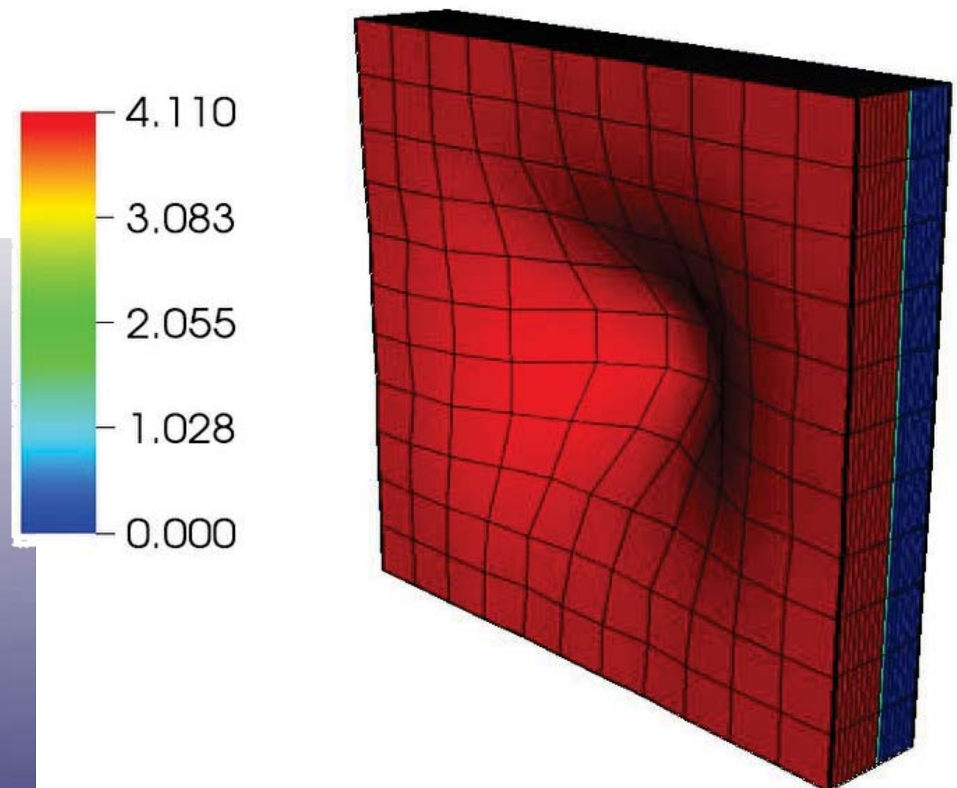
Use this set of properties for other simulations - different punch diameter, speed or stack of cells (a.k.a. string).

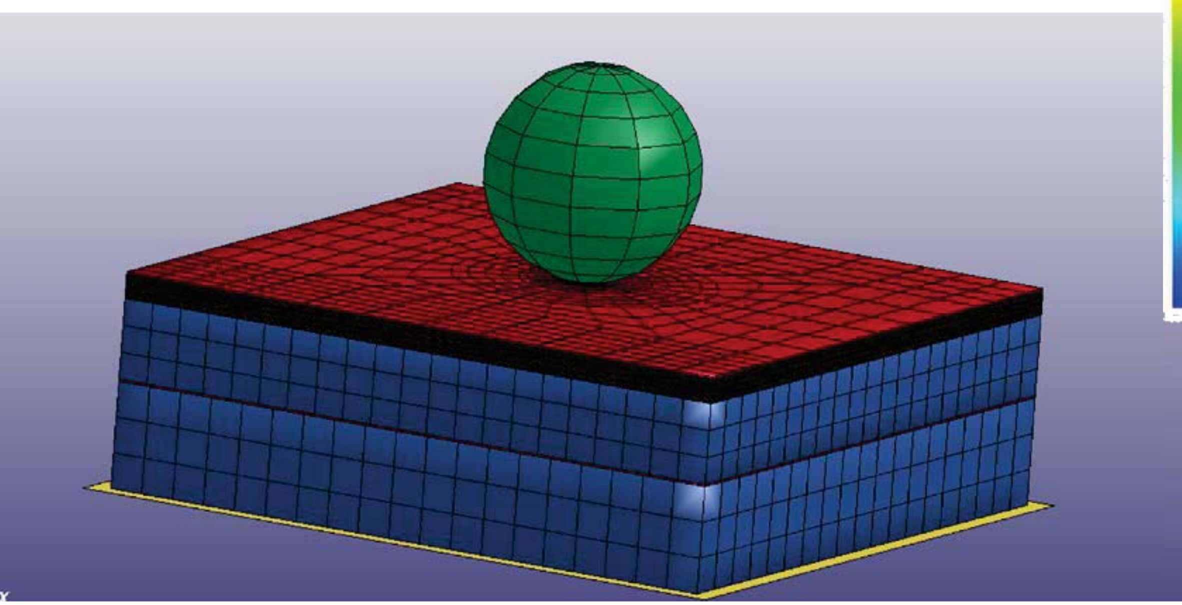
[1] RSC Advances 2014 4 14904

Now scaling to modules and packs.



- Ability to load multiple meshes efficiently
- Important since full 3D EET simulation requires mesh of ~1 million elements
  - Thin current collectors and large aspect ratio
  - Want to minimize mesh size
- Our framework allows use of nonlinear models such as contact resistances at interfaces
- Have developed mapping operators to transfer solution across boundaries





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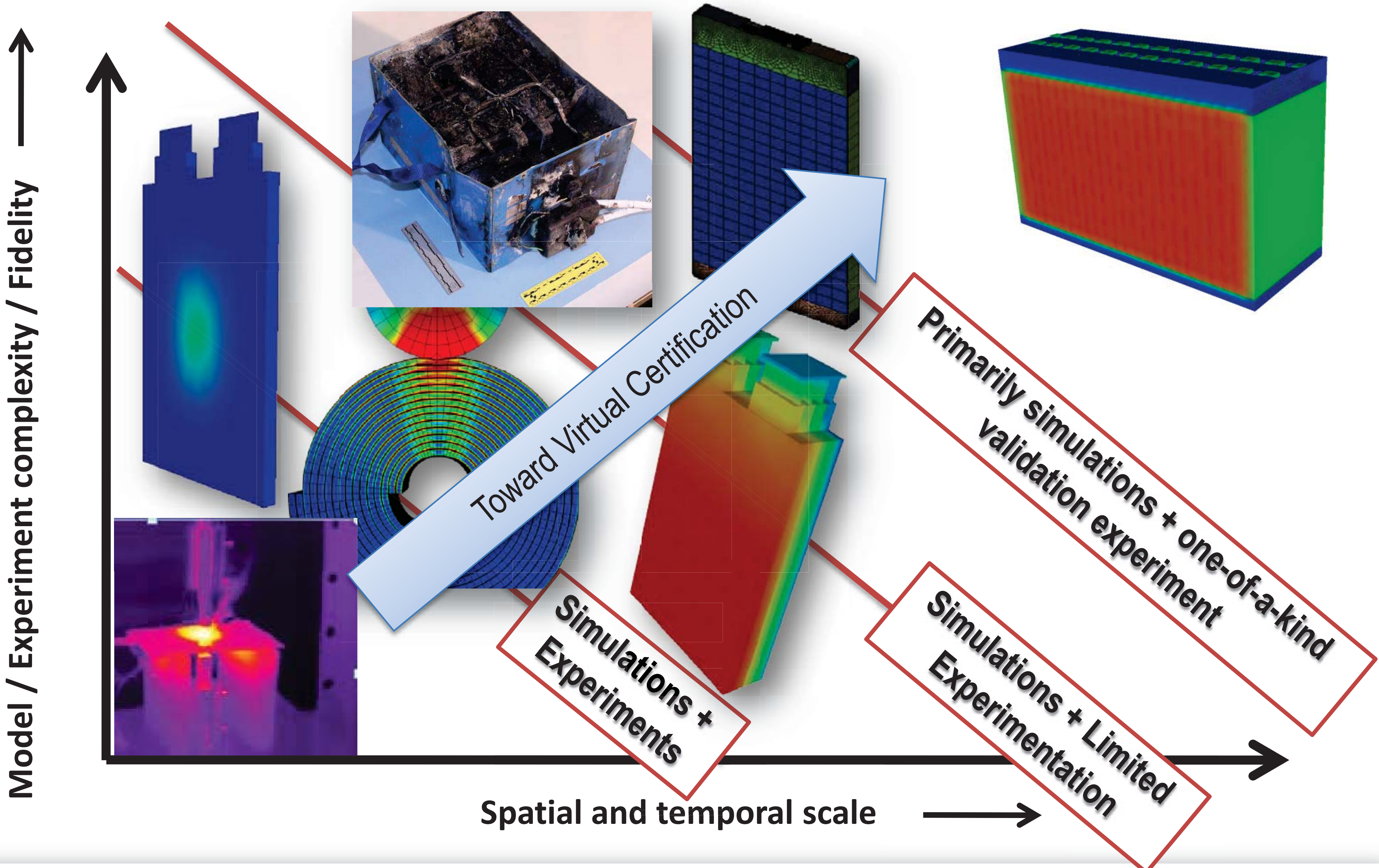
Virtual Certification of Battery Packs
from cell to module to pack



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Summary

- Integrated experimental-simulation program to understand and develop tests for battery failure due to crush is under way
- AMPERES provides a 3D framework to simulate battery performance under a wide range of conditions
- Through OAS, BatML, and the Battery State file format, VIBE provides a mechanism for linking to other components
- Computational framework and all components presented today are being released as open source
- Open to collaboration opportunities on use of tools we've developed, linking of additional components, validation, …

Our group at ORNL is leveraging multiple projects to develop a system of battery simulation capabilities.

Program	Timeframe	Goals
DOE / EERE / CAEBAT-I	2010-2014	build infrastructure, standards, etc. to leverage existing knowledge and tools
DOE / EERE / CAEBAT-II	2014-2015	develop mechanistic models for thermal runaway (collaboration with SNL)
DOE / ARPA-E / AMPED	2013-2014	develop improved thermal management capabilities
DOE / SC / ASCR	2014-2016	uncertainty quantification, risk estimation, and decision making
DOE / SC / ASCR	2013-2017	multiscale coupled-physics simulations, reduced models, etc.
DOE / ARPA-E / RANGE	2014-2015	(1) shear-thickening electrolyte (2) brittle current collectors
DOT / NHTSA	2014-2015	mechanical abuse of batteries

http://batterysim.org/

Thanks and Acknowledgements

- Sponsors: ORNL LDRD, DOT/NHTSA and DOE/EERE/VT
  - Uzmaa Balbale, Phil Gorney, Steve Summers
  - David Howell, Brian Cunningham
- ORNL program office
  - Ron Graves, Claus Daniel, and Kate Stusrud
- Ford Motor Company
  - Collaboration on DOT/NHTSA project

Questions?

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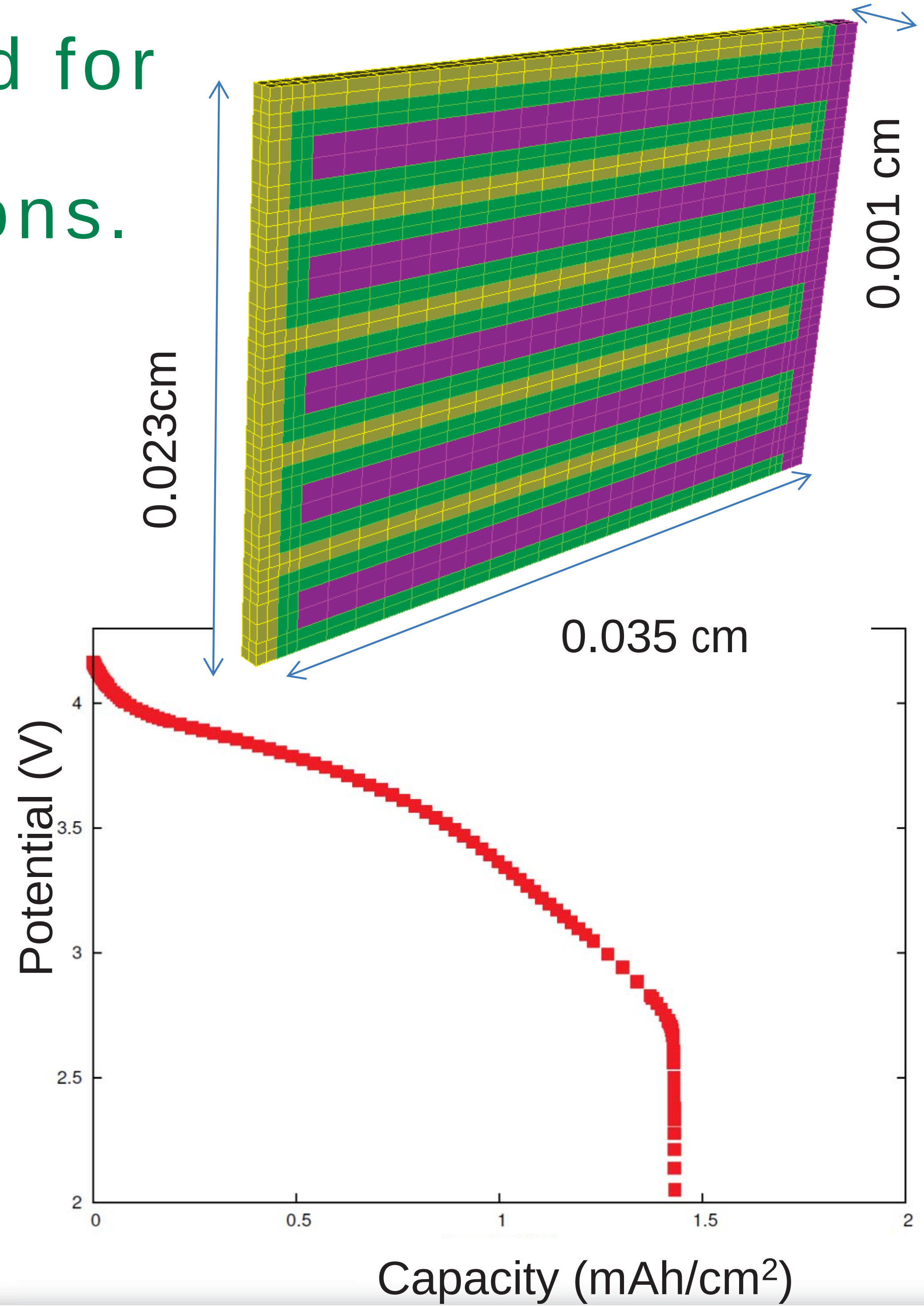
Beyond Li-ion 8 Conference

June 2-4, 2015

OAK RIDGE National Laboratory

AMPERES can be used for more complex cell sandwich configurations.

- Approximately matched thickness
  - Less active material since separator occupies larger volume
  - Match anode / cathode ratio
- Same code was used to compute discharge profile at 1.75 mA/cm^2
  - 10,000 elements
  - ~5 min. compute time
  - Slightly lower capacity, as expected

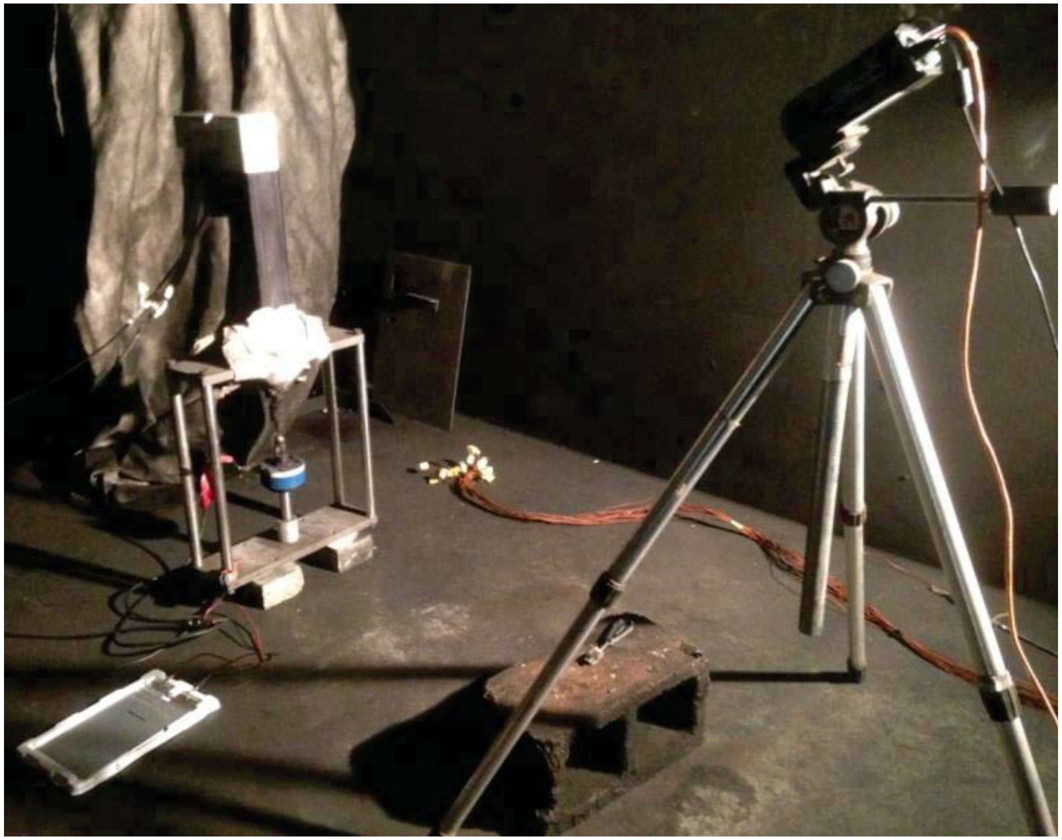


- There is no other battery simulation tool that combines charge / mass transport with electrochemical kinetics with such generality
- Can easily extend to include electrical, thermal, and linear mechanics

http://batterysim.org/

Zadin *et al.*, SSI, 2001

Pinch Test Setup at Carderock



Test chamber:
- Load frame
- Infrared camera

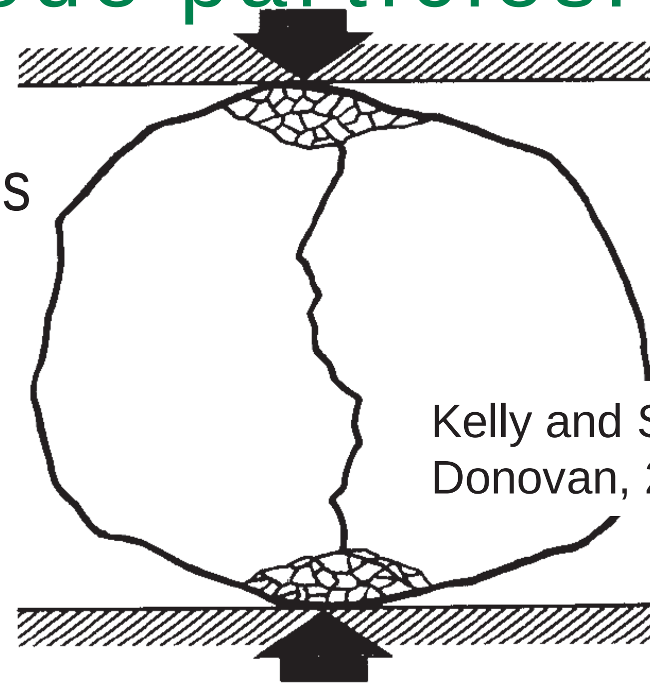
Test Conditions:
- 2 one-inch diameter spheres
- Pinching at fixed speed
- Displacement limit control
- Hold load until short circuit
- Return condition: 0.3V voltage drop

Speed	inch/min	mm/sec
Low	0.25	0.105
Medium	7	2.96333
High	12	5.08

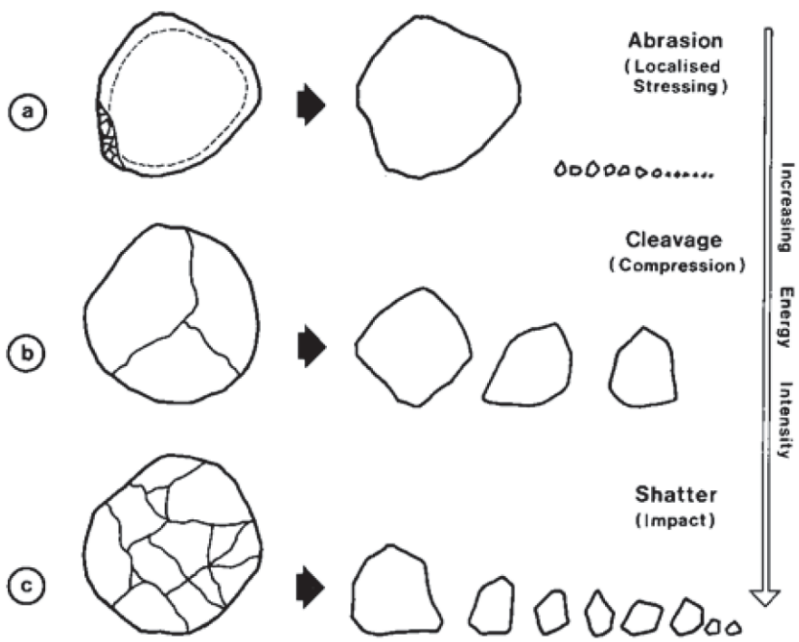
- single cells
- "strings" of 3 cells

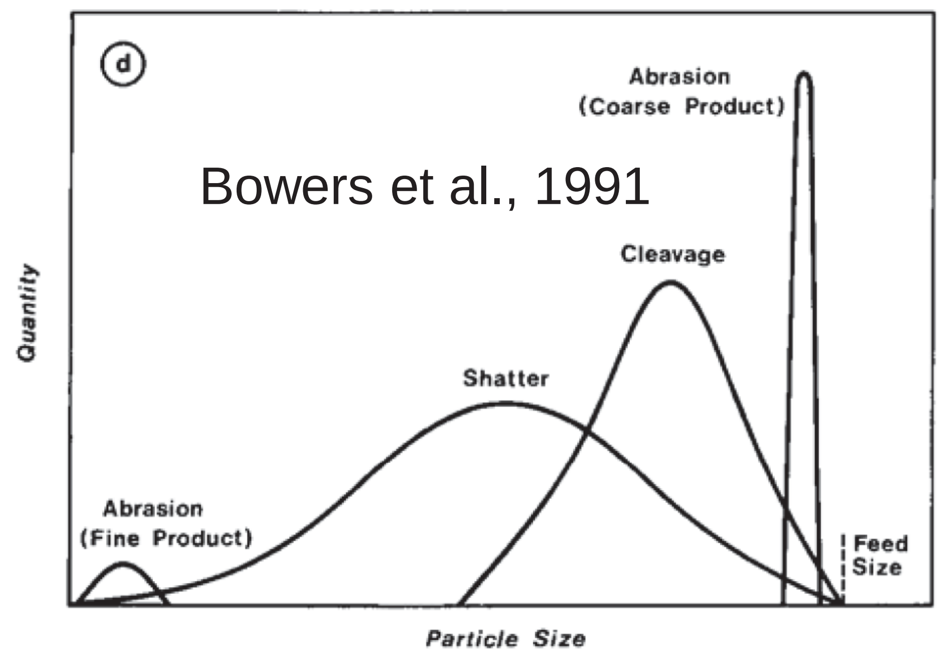
Also need to understand the mechanics of electrode particles.

- Electrode particles rearrange and fracture under externally applied loads
- The relative roles of the deformation mechanisms depend on the material and loading
- Particle interactions with adjacent components, current collectors, separators



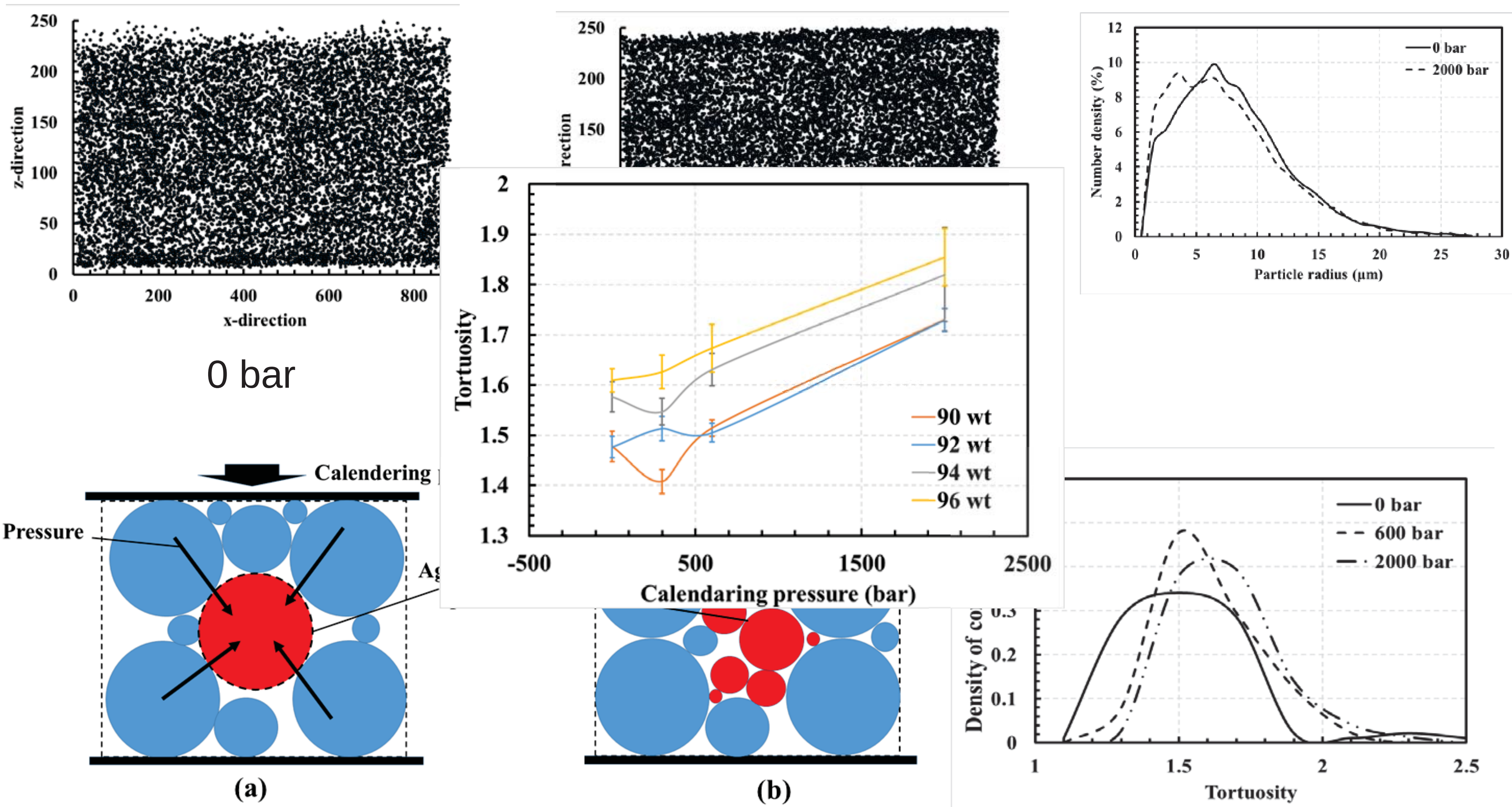
Kelly and Spottiswood, 1982
Donovan, 2003





Bowers et al., 1991

What is the effect on transport properties?



0 bar

2000 bar

http://batterysim.org/

Chien-Fan Chen, Texas A&M