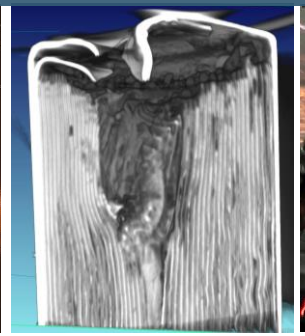
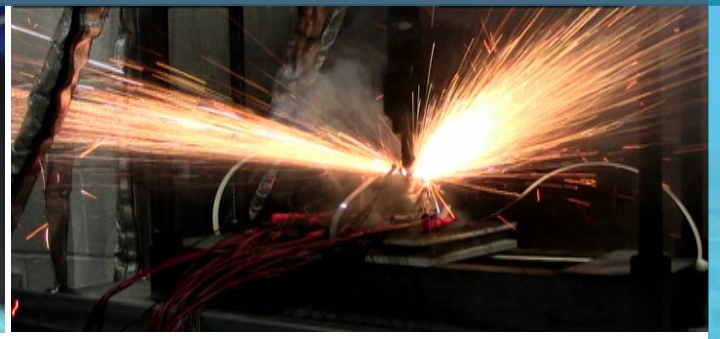
Abuse Test Development: Mechanisms and Materials Impact of Abused Lithium-ion Batteries





PRESENTED BY

Loraine Torres-Castro, Joshua Lamb, June Stanley, Chris Grosso, Lucas Gray and Jill Langendorf

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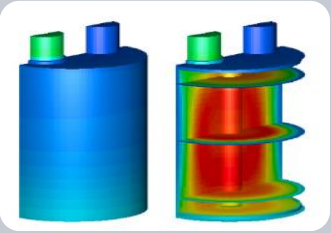
PROJECT OVERVIEW

Science and diagnostics of battery failure

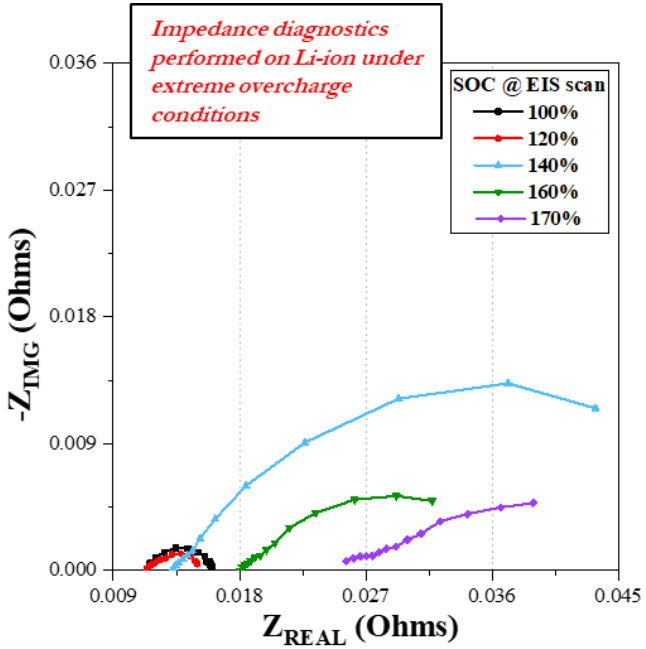
Materials R&D
- Non-flammable electrolytes
- Electrolyte salts
- Coated active materials
- Thermally stable materials
- Battery failure post mortem materials analysis

Testing
- Diagnostics during battery failure (pictured right)
- Gas analysis
- Battery calorimetry
- Electrical, thermal, mechanical abuse testing
- Failure propagation testing on batteries/systems
- Large scale thermal and fire testing (TTC)



Simulations and Modeling
- Multi-scale models for understanding thermal runaway
- Validating failure propagation models
- Fire Simulations to predict the size, scope, and consequences of battery fires

Procedure Development and Stakeholder Interface
- USABC Abuse Testing Manual (SAND 2005 3123)
- OE Energy Storage Safety Roadmap
- R&D programs to inform best practices, policies, and requirements
- Hosted International Battery Safety Workshops and Energy Storage Safety Workshop



- Sandia is uniquely positioned to study the entire life cycle of a technology.
- New technologies present new risks. A high rigor environment at Sandia allows those risks to be adequately managed.
- Diagnostic tests can be performed under extreme failure conditions to understand the *how* and *why* of battery failure.

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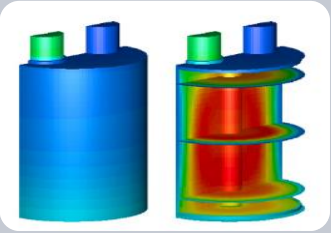

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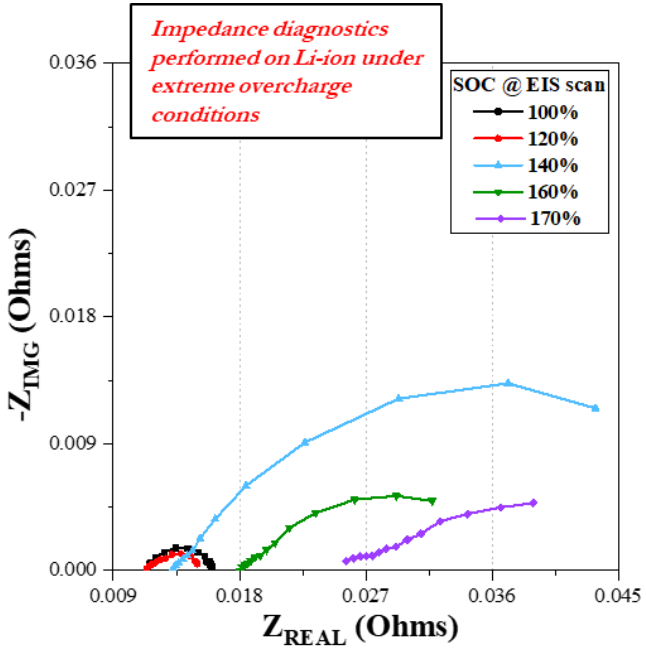

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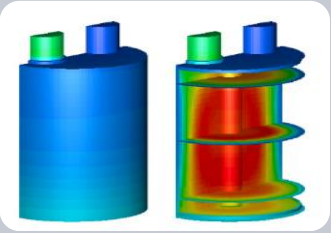

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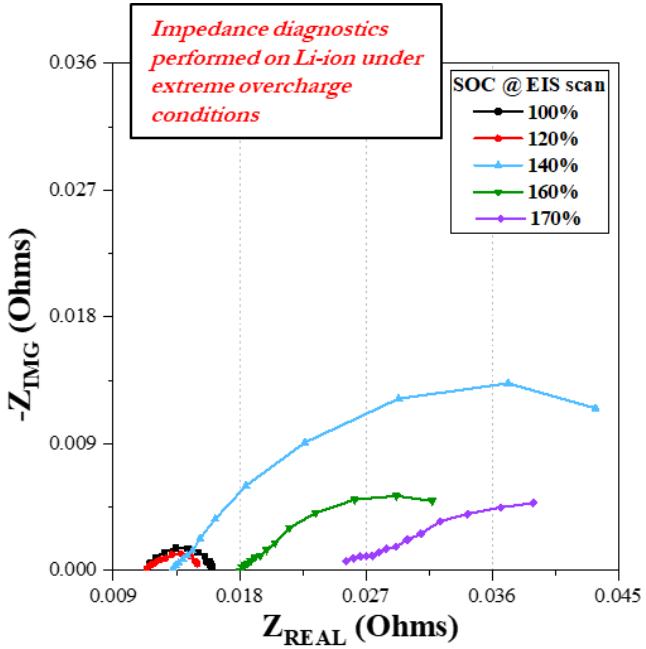

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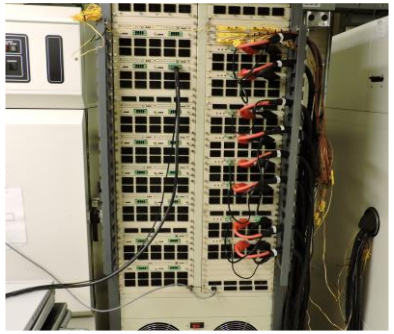
PROJECT TEAM

Sandia Battery Test Facilities



Yuliya Preger
Summer Ferreira
Armando Fresquez
Heather Barkholtz
(former SNL)

Sandia Battery Abuse Testing Laboratory

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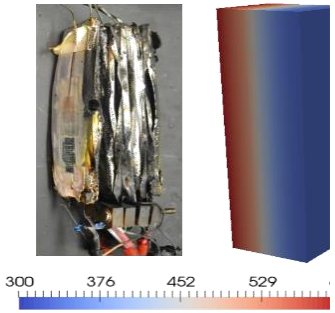
Eric Deichmann

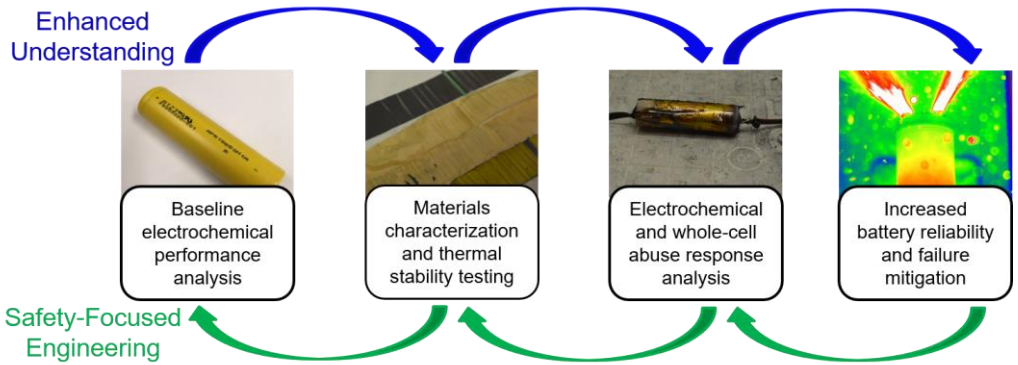
Sandia Fire Sciences



John Hewson
Randy Shurtz
Andrew Kurzawski

Center for Integrated Nanotechnologies

Sergei Ivanov



PROJECT TEAM

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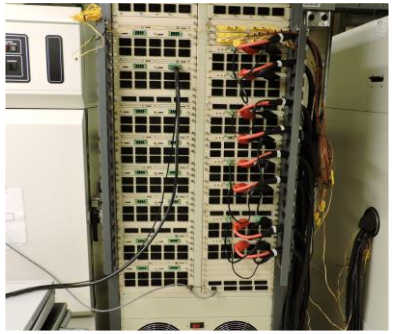

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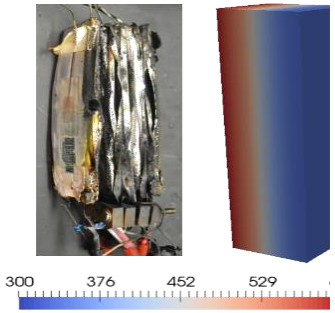

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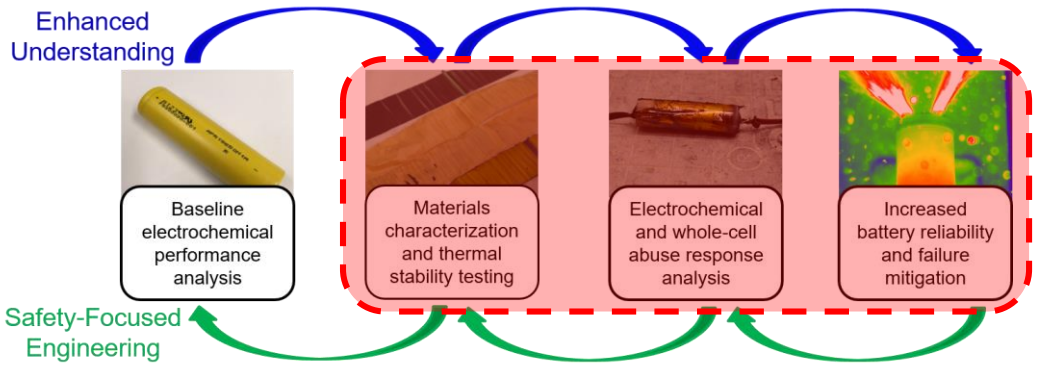


PROJECT OBJECTIVES

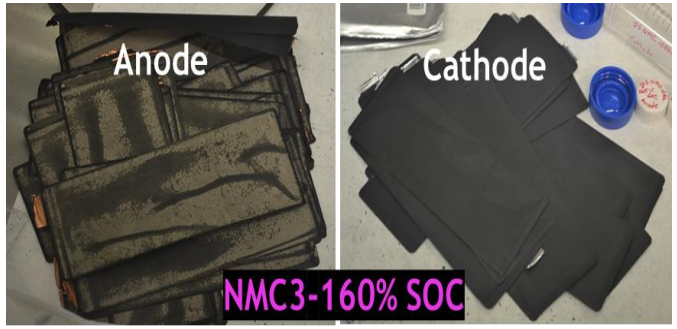
Failure mechanisms of abused cells from a materials and electrochemical perspective

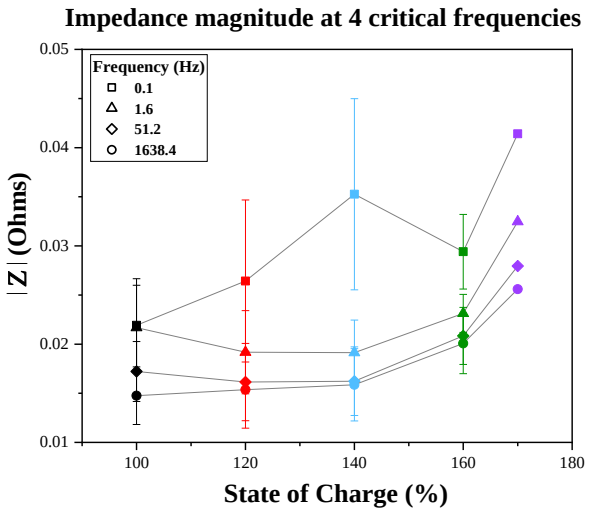
Objective 1

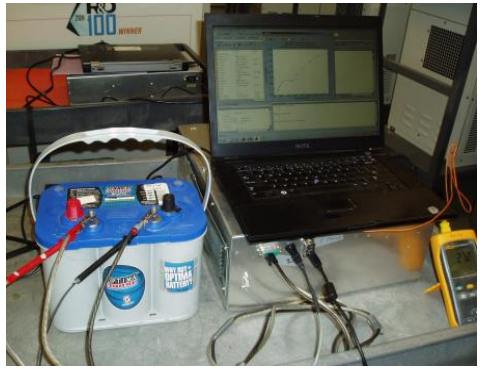
Provide insight into the development of an in-operando diagnostic technique to detect faulty cells within a pack.

Objective 2

Understand battery failure mechanisms during strenuous conditions to lead the design of more resilient and reliable energy storage systems that are inherently safe.







PROJECT METRICS AND MILESTONES

Failure mechanisms of abused cells from a materials and electrochemical perspective

	Milestones	Current Status
#1	Identify the failure mechanisms of NMC and LFP pouch cells during strenuous conditions.	The initial study of the NMC chemistry was completed. The manuscript is being prepared for submission.
#2	Determine the consistency of the failure mechanisms across manufacturers and different capacities.	The identification of the failure mechanisms of LFP cells is 80% completed.
#3	Investigate the effect of initial SOH on the identified failure mechanisms.	Preliminary results confirmed consistency of the failure mechanisms across capacities, manufacturers and different initial SOH.

PROJECT CHALLENGES

Failure mechanisms of abused cells from a materials and electrochemical perspective

Challenges

Simple passive monitoring of a cell is often unable to identify the onset of failure until it is too late to intervene.

The prevention of catastrophic failure requires detection of internal faults well before they have developed.

Commercially available EIS equipment provides an insufficient dataset for cells subjected to abusive conditions.

PROJECT CHALLENGES

Failure mechanisms of abused cells from a materials and electrochemical perspective

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Identify an in-operando technique capable of identifying markers of failure during abusive electrical conditions.

PROJECT CHALLENGES

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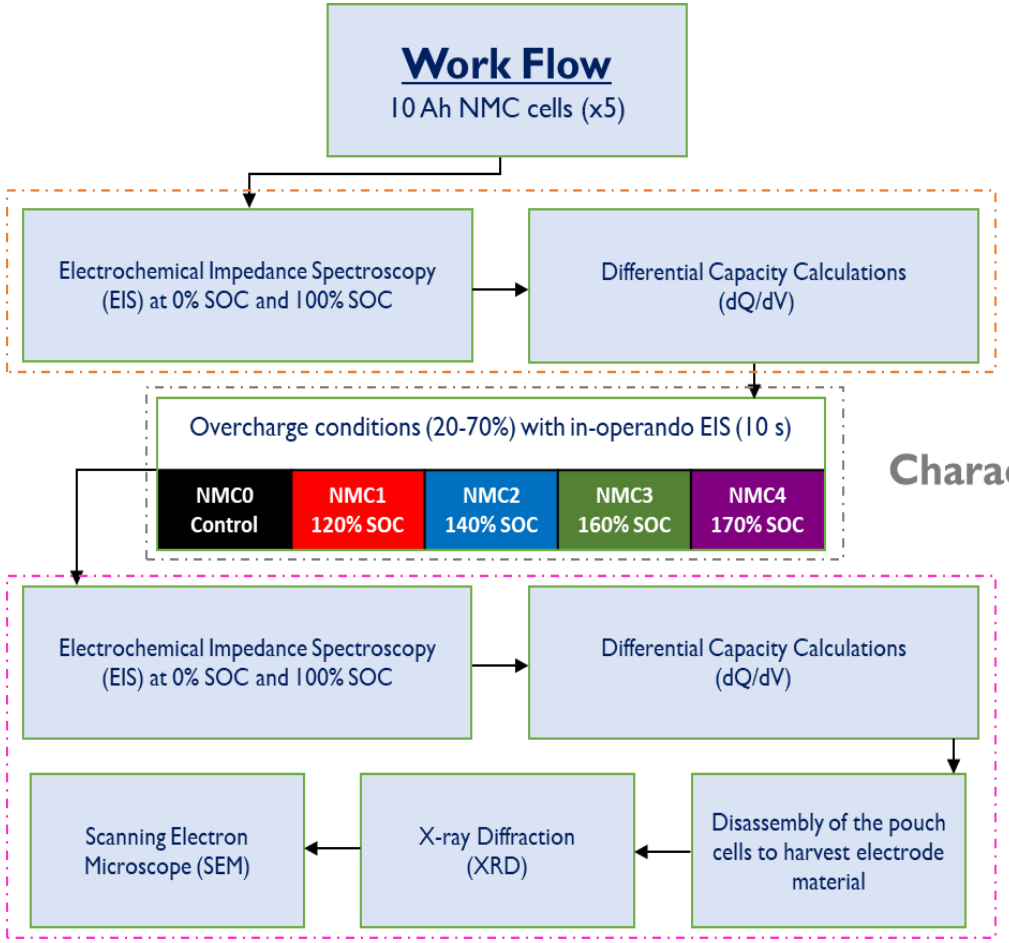
The prevention of catastrophic failure requires detection of internal faults well before they have developed.

Commercially available EIS equipment provides an insufficient dataset for cells subjected to abusive conditions.

Identify an in-operando technique capable of identifying markers of failure during abusive electrical conditions.

Fast EIS equipment developed by INL and Montana Tech provided sufficient information for cells under abusive conditions.

PROJECT RESULTS

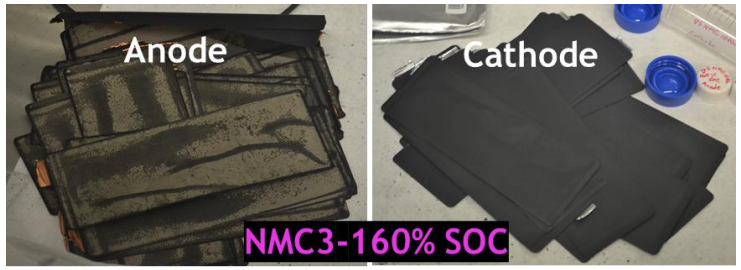


Pre-test characterization

Characterization during test

Post-test characterization

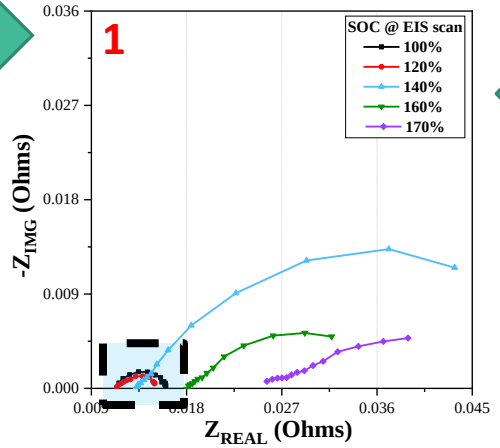
The focus is to understand battery failure mechanisms during strenuous conditions to lead the design of more resilient and reliable energy storage systems that are inherently safe and provide insight into the development of an in-operando diagnostic tool.

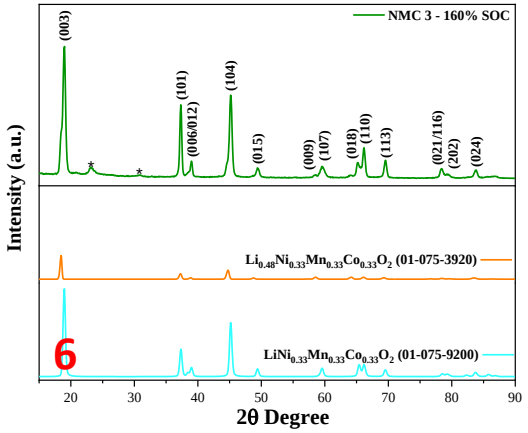


PROJECT RESULTS

Milestone #1 – Identify the failure mechanisms of li-ion batteries during strenuous conditions

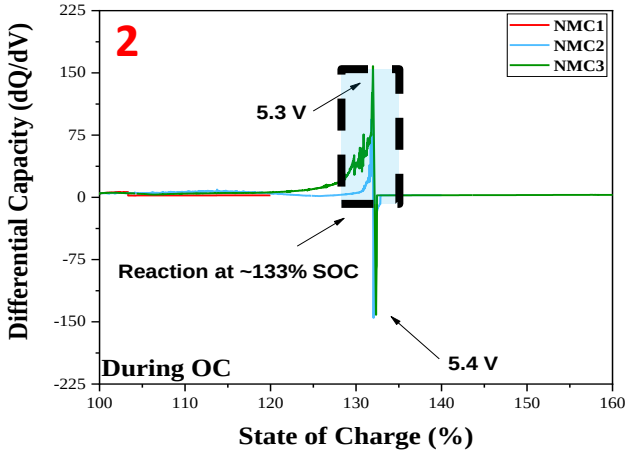
Electrochemical Impedance Spectroscopy during abuse



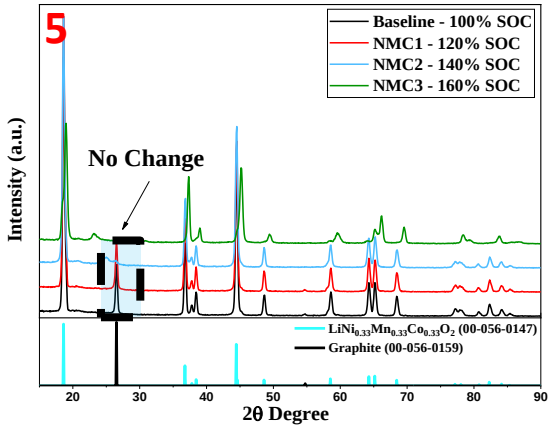


Rietveld Refinement for 160% SOC

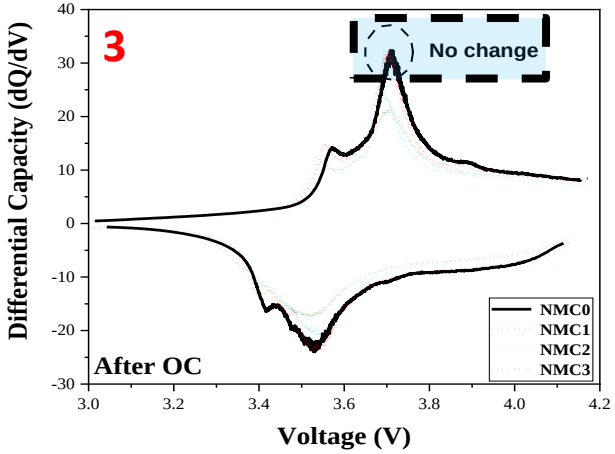
Phase	% (+/- 5%)
Lithiated NMC	86
Delithiated NMC	14



X-ray Diffraction (Cathode)



Differential capacity of the cell after and during overcharge

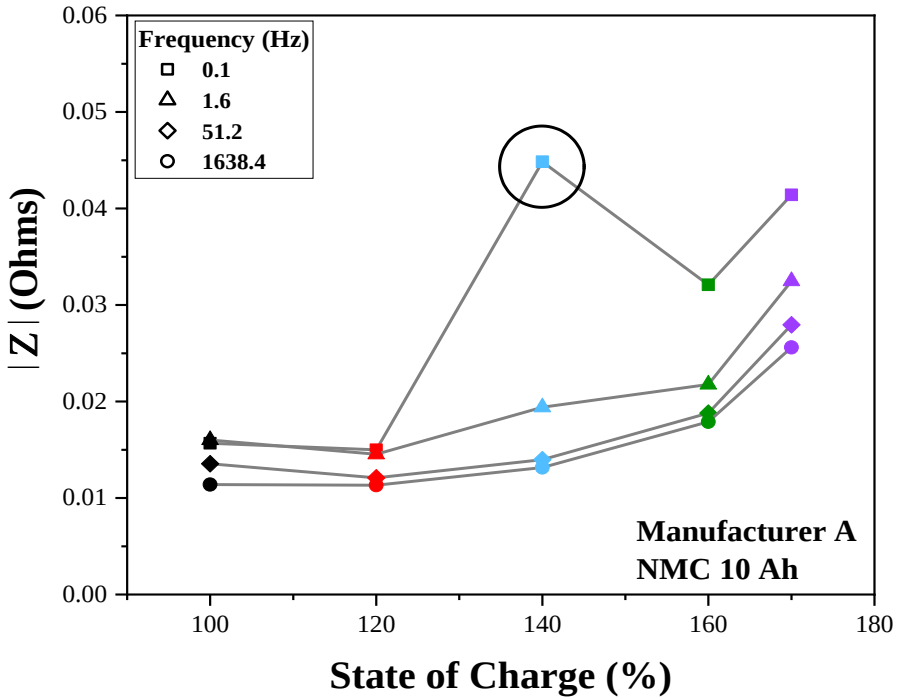


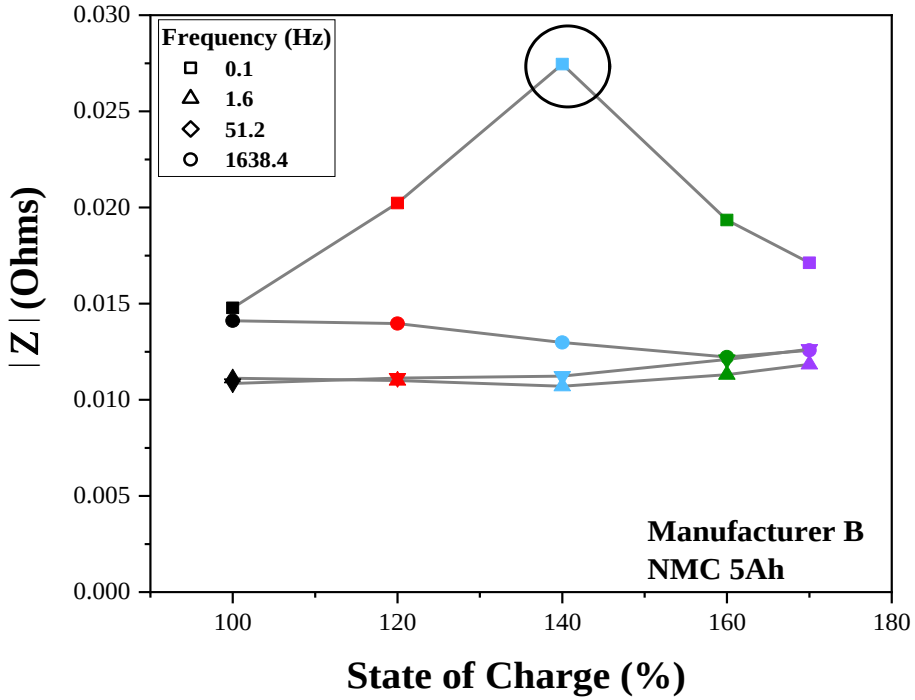
Harvested from NMC3 – 160%SOC

PROJECT RESULTS

Milestone #2 – Determine the consistency of the failure mechanisms across manufacturers and different capacities

Is the marker consistent across manufacturers?





- Representation of the overall amount of resistance in the form of magnitude as a function of the state of charge for two different NMC cells that were subject to strenuous conditions.
- Degradation marker identified for the NMC chemistry during strenuous conditions is independent of manufacturer and capacity.

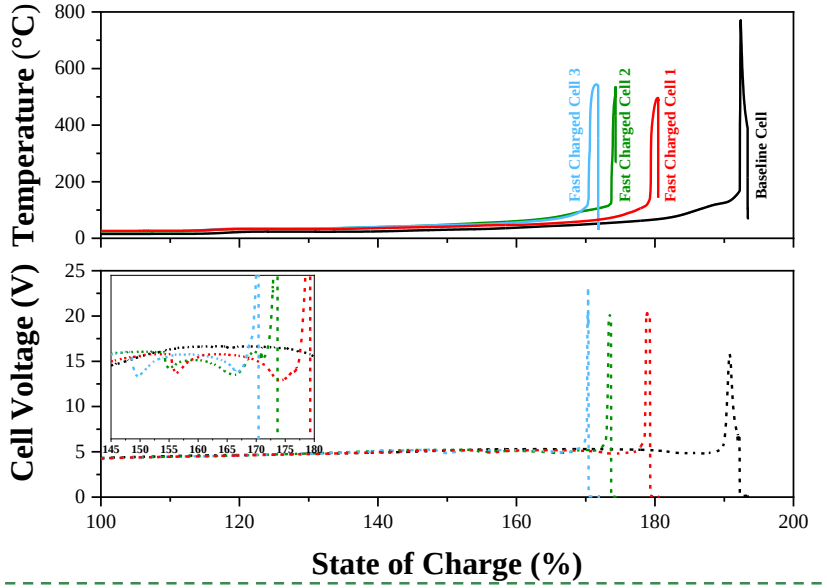
$$|Z| = \sqrt{Z_{REAL}^2 + Z_{IMG}^2}\,.$$

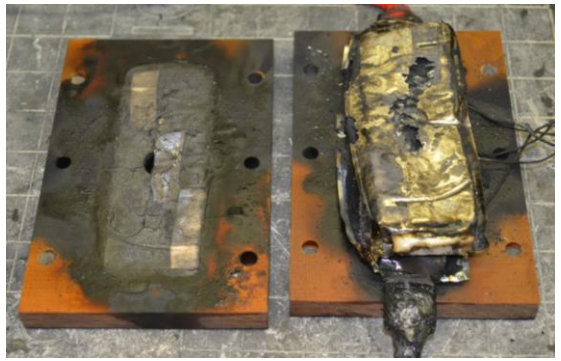
PROJECT RESULTS

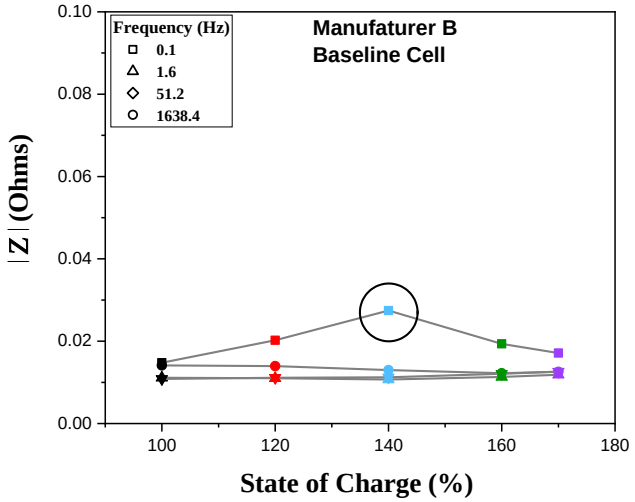
Milestone #3 – Investigate the effect of initial SOH on the identified failure mechanisms.

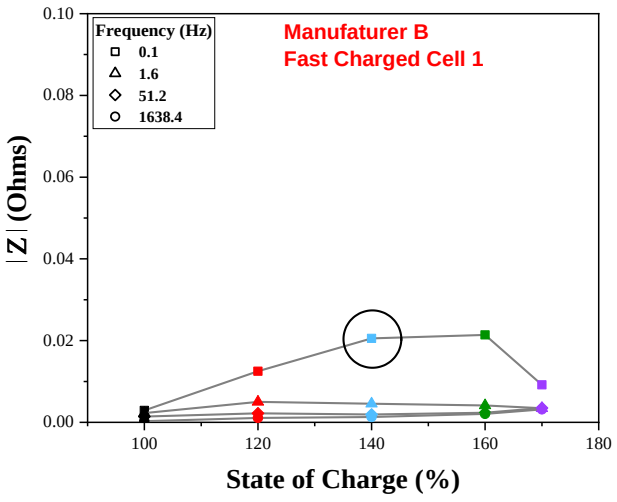
What happens if the initial SOH is compromised?

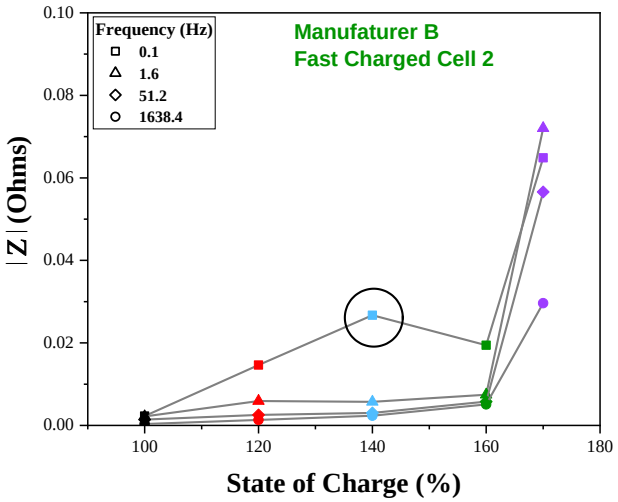
- The initial SOH was manipulated with fast charged protocols, and the abuse response was characterized.
- The onset SOC to thermal runaway decreased as the initial SOH was aggravated.
- The overall resistance in the form of magnitude as a function of the state of charge presented the failure marker at 140% SOC independent of initial SOH.

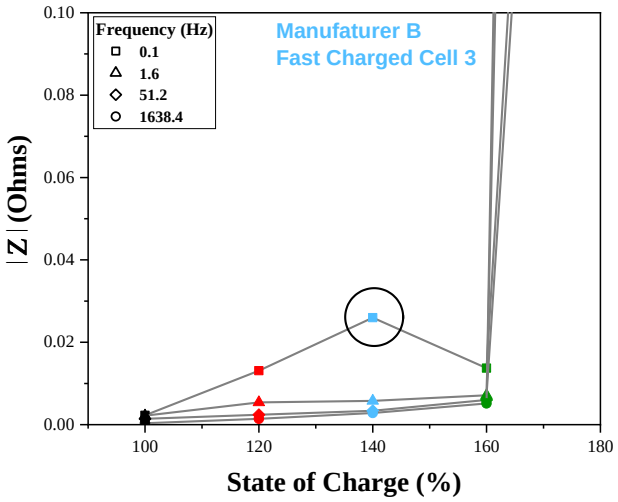












PUBLICATIONS AND PRESENTATIONS

Presentations

- **Evaluating the Impact of Initiation Methods on Propagating Thermal Runaway in Lithium-Ion Batteries**; *Battery Safety 2018*, Arlington, VA; October 30, 31, 2018
- (Invited Talk) **Mechanisms and material impacts of overcharge in lithium ion**; *2018 MRS Fall Meeting*, Boston, Massachusetts; November 25-30, 2018
- (Invited Talk) **Determination of Battery State of Stability Through Advanced Diagnostics**; *IAPG Chemical Working Group Safety Panel Meeting 2019*, Pasadena, California; February 12-14, 2019
- (Invited Talk) **Mechanisms and material impacts of overcharge in lithium ion**; *235th ECS Meeting*, Dallas, Texas; May 26-30, 2019
- (Invited Talk) **The Scalability of Accelerating Rate Calorimetry (ARC) with State of Charge and Capacity**; *235th ECS Meeting*, Dallas, Texas; May 26-30, 2019
- **Failure Propagation Work and Abuse Testing;** *Advanced Automotive Battery Conference*, San Diego, California; June 24-25, 2019

Publications

- H. M. Barkholtz, Y. Preger, S. Ivanov, J. Langendorf, L. Torres-Castro, J. Lamb, B. Chalamala, and S. Ferreira, "**Multi-scale thermal stability study of commercial lithium-ion batteries as a function of cathode chemistry and state-of-charge**," *Journal of Power Sources*, vol. 435, 2019
- R. C. Shurtz, Y. Preger, L. Torres-Castro, J. Lamb, J. C. Hewson and S. Ferreira, "**Perspective—From Calorimetry Measurements to Furthering Mechanistic Understanding and Control of Thermal Abuse in Lithium-Ion Cells,**" *Journal of the Electrochemical Society*, vol.166, p.p. A2498, 2019
- Q. Li, C. Yang, S. Santhanagopalan, K. Smith, J. Lamb, L. A. Steele, L. Torres-Castro, "**Numerical investigation of thermal runaway mitigation through a passive thermal management system**," *Journal of Power Sources*, vol. 429, p.p. 80, 2019
- **Investigations of the Electrochemical and Material Properties of Overcharged Li-ion Batteries** (in preparation)
- **Accelerating Rate Calorimetry: Comparison of Chemistries and Energy** (in preparation)
- **Mitigation of Failure Propagation in Multi-Cell Lithium Ion Batteries** (in preparation)

LOOKING FORWARD

I. Failure mechanisms of lithium-ion batteries subjected to abusive conditions (continuation)

- Harvest battery constituents to understand materials failure mechanisms.

II. Mitigation of failure propagation through active cooling

- Development of a technique to mitigate failure propagation through active cooling.

III. Dendrite formation and lithium plating effect in abuse response of lithium-ion batteries: from single cells to failure propagation

- Produce different levels of lithium plating and dendrite growth by heat exchange and evaluate its safety performance.

PROJECT CONTACTS

- Funded by the U.S. Department of Energy, Office of Electricity, Energy Storage program. Dr. Imre Gyuk, Program Director.
- Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.
- This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Los Alamos National Laboratory (Contract DE-AC52-06NA25396) and Sandia National Laboratories (Contract DE-AC04-94AL85000).
- Fast impedance spectroscopy toolbox was developed by Idaho National Laboratories in collaboration with Montana Tech.

Name of presenter: Loraine Torres-Castro
Corresponding email: ltorre@sandia.gov

For further details on experimental work, see the following posters:

- Abuse Test Development: Mechanisms and Materials Impact of Abused Lithium-ion Batteries
- Mitigation of Failure Propagation in Multi-Cell Lithium Ion Batteries
- Thermal Runaway Testing and Database Development of Large-format Li-ion Cells at ORNL and SNL

Extra Slides: Failure Propagation Project

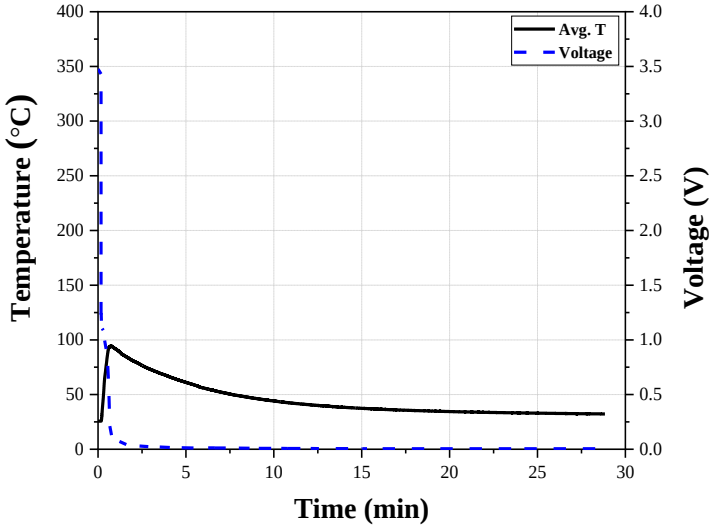
PROJECT OBJECTIVES

Failure propagation

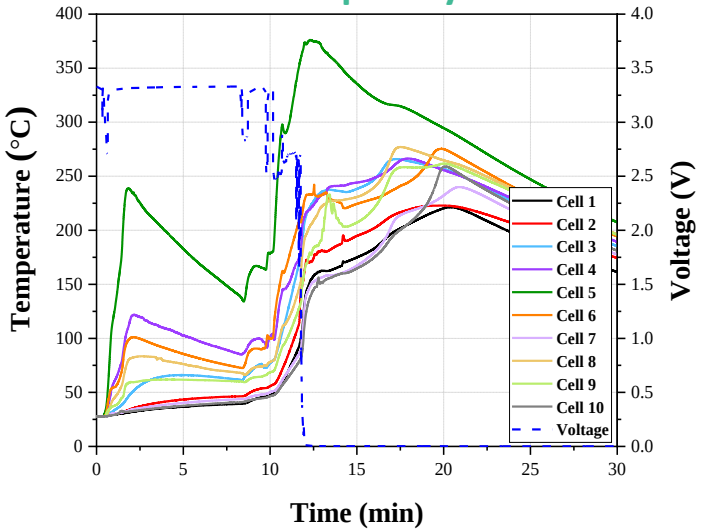
Objective

Understand the extent of propagation with the inclusion of active thermal management in the form of spacers (aluminum and copper) between (i)pouch cells in a 5 cells pack, and (ii) between modules of a 3s3p battery pack.

Single Cell Failure



How do these behaviors impact a larger, more complex system?



Consumer Cells (0.5-5 Ah) → Large Format Cells (10-200 Ah) → Batteries (1-50 kWh) → Vehicle system

PROJECT METRICS AND MILESTONES

Failure mechanisms of abused cells from a materials and electrochemical perspective

Challenges

- Determine a reproducible thermal runaway initiator.
- Evaluate the propagation behavior of (a) single module packs and (b) multi-module packs.
- Identify mitigation strategies for failure propagation.

Current status

- The propagation behavior of both types of packs was successfully studied.
- Thermal management in the form of aluminum and copper spacers were used to mitigate failure propagation.
- Publication related to the failure propagation of single module battery packs was recently published in the Journal of Power Sources in collaboration with NREL.

PROJECT CHALLENGES

Failure propagation

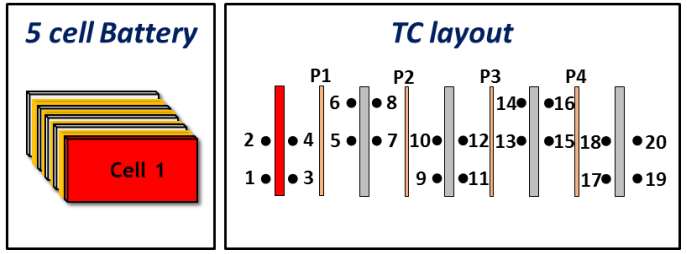
Challenges

Different failure response observed when in a string, module, or pack.	The set of experiments were designed, taking into consideration these variations.
Limiting the SOC to mitigate failure comes at a high cost to total energy storage.	Additional mitigation strategies were identified.
Electrical design plays a crucial role in susceptibility to failure testing.	Different electrical configurations were considered.
Failure testing of large, complex systems is resources intensive.	Collaboration with the modeling team at Sandia facilitated the simulation of failure propagation of large battery packs.

PROJECT RESULTS

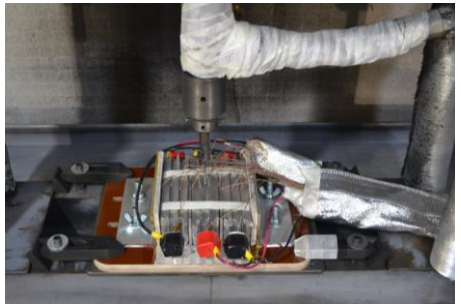
Inclusion of thermal management

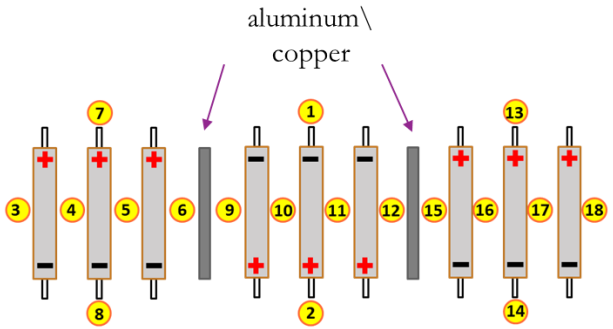
Single module



The focus is to understand the extent of propagation with the inclusion of thermal management in the form of heat sinks between pouch cells in a single module vs. the inclusion between modules in a battery pack.

Multi module pack



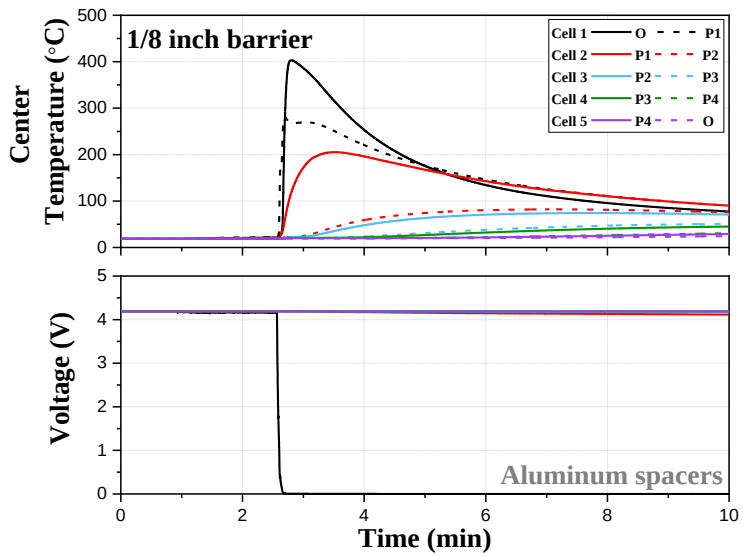


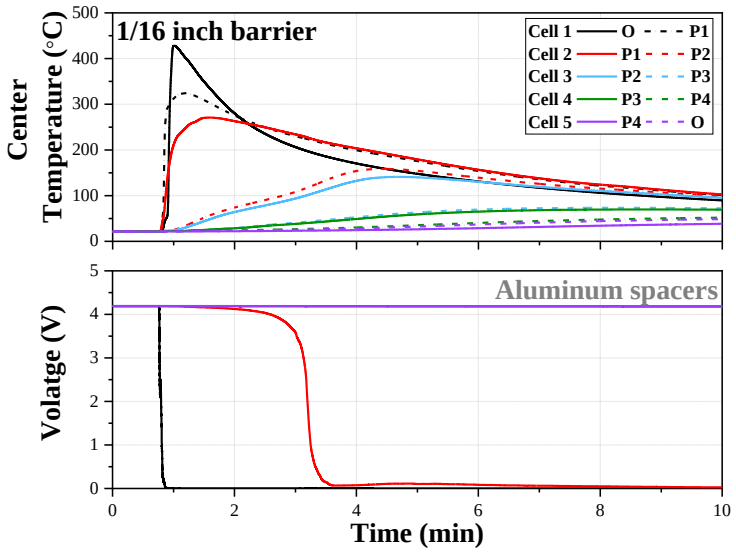
Aluminum plates	Copper plates
1/8 inch	1/8 inch
1/16 inch	1/16 inch
1/32 inch	1/32 inch

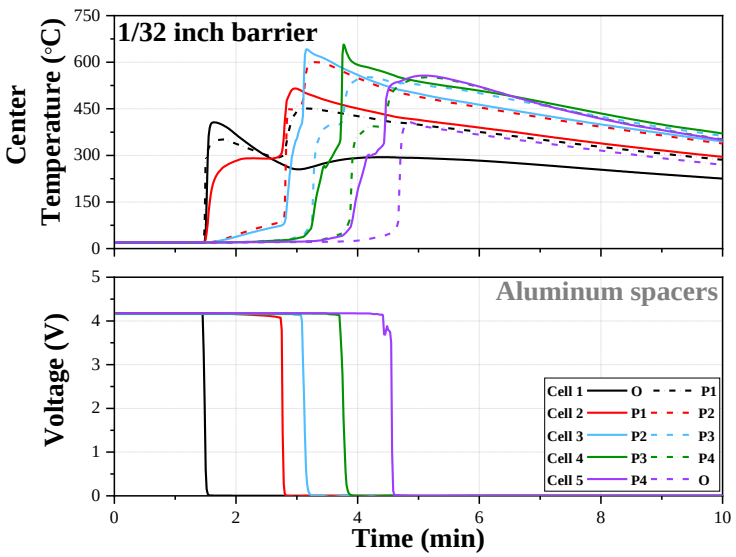
PROJECT RESULTS – SINGLE MODULE PROPAGATION

Thermal Management for single module: 1/8, 1/16, 1/32 inch

Failures initiated by mechanical insult to edge cell of COTS LCO packs (3Ah cells)







1/8 inch

- Peak temperatures reached ~400 ˚C.
- No propagation was realized while using 1/8 inch aluminum or copper spacers.
- Energetic thermal runaway was not observed beyond the initially failed cell.

1/16 inch

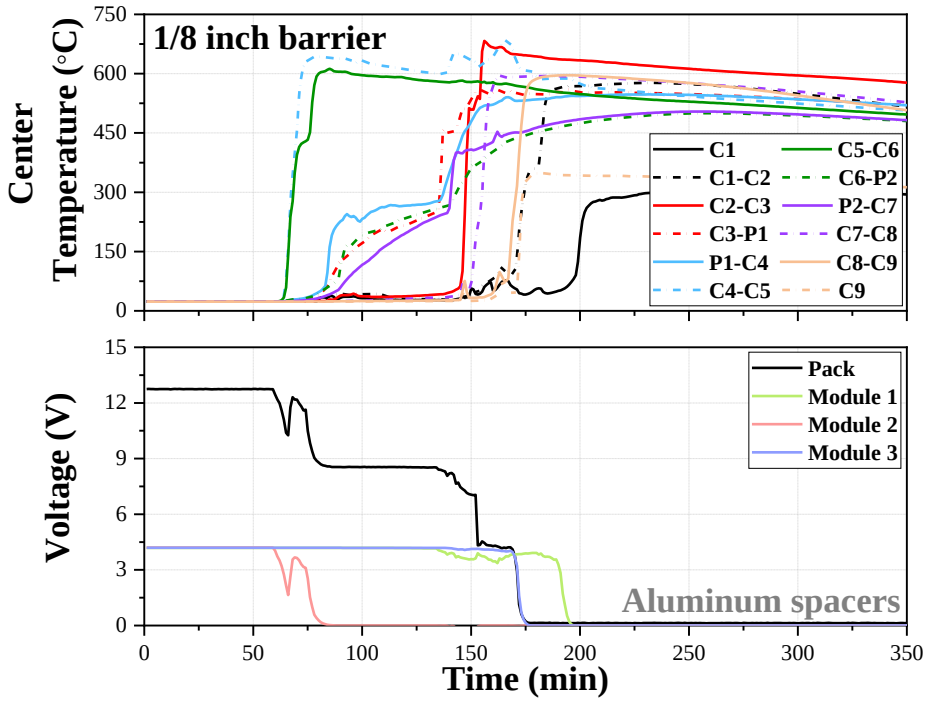
- Limited propagation (from cell 1 to 2).
- For both cases, the second cell was able to reach ~300 °C and eventually lost voltage.

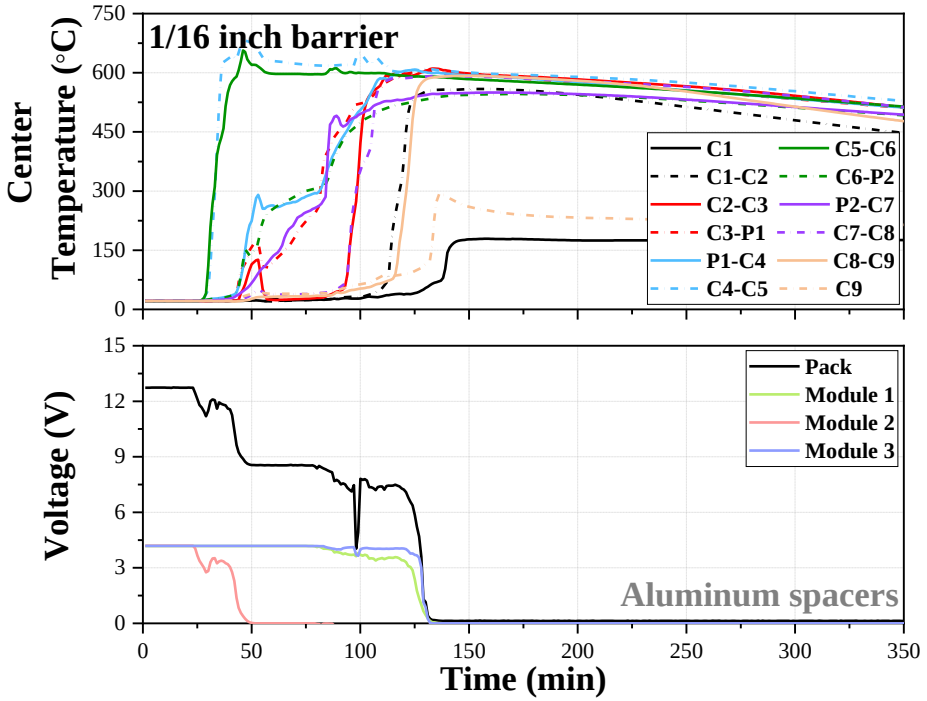
1/32 inch

- Pulsing propagation behavior observed over several minutes.
- Entire pack consumed ~4 minutes after initial failure.

PROJECT RESULTS – MULTI-MODULE PROPAGATION

Thermal Management for multi-modules pack: 1/8, 1/16 barrier





1/8 inch

- Cells within the target 1S3P module were rapidly consumed.
- Outer modules did not initiate thermal runaway until ~120 seconds after initial failure.

1/16 inch

- In both cases, initial failure immediately consumes cells within the central 1S3P module.
- Outer modules show signs of failure ~20 seconds after initial initiation.