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How Safe Are Solid-State Batteries? An Exploration of Heat Release

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TMS Conference

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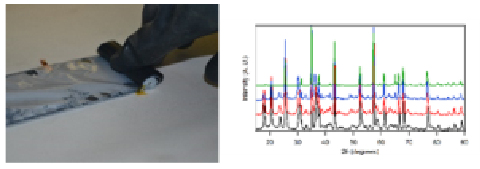
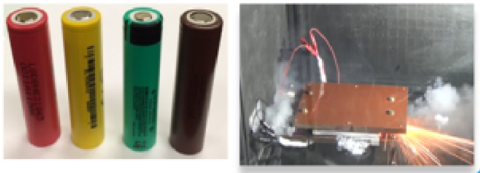
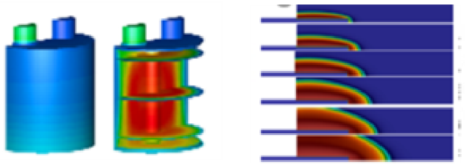
Sandia Addresses all Aspects of Safety & Reliability for Battery Energy Storage



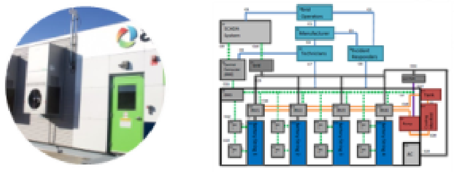
Materials R&D
- Thermal stability and aging impact on battery components
- Vent gas composition
- Solid state battery safety
- Aqueous battery gas evolution



Cell and Module Testing
- High precision cell cycling and degradation
- Electrical, thermal, mechanical abuse testing
- Failure propagation testing on batteries/systems



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



System Level Design and Analysis
- Hazard analysis methods to avoid fire and explosion
- Predictive maintenance
- Improved control using power electronics

Outreach, Codes, and Standards
- Energy storage safety working group
- IEEE battery management system standard
- EPRI energy storage data submission guidelines

Overview

1. Solid-State Battery Introduction
2. Thermodynamic Model
3. Experimental - Differential Scanning Calorimetry

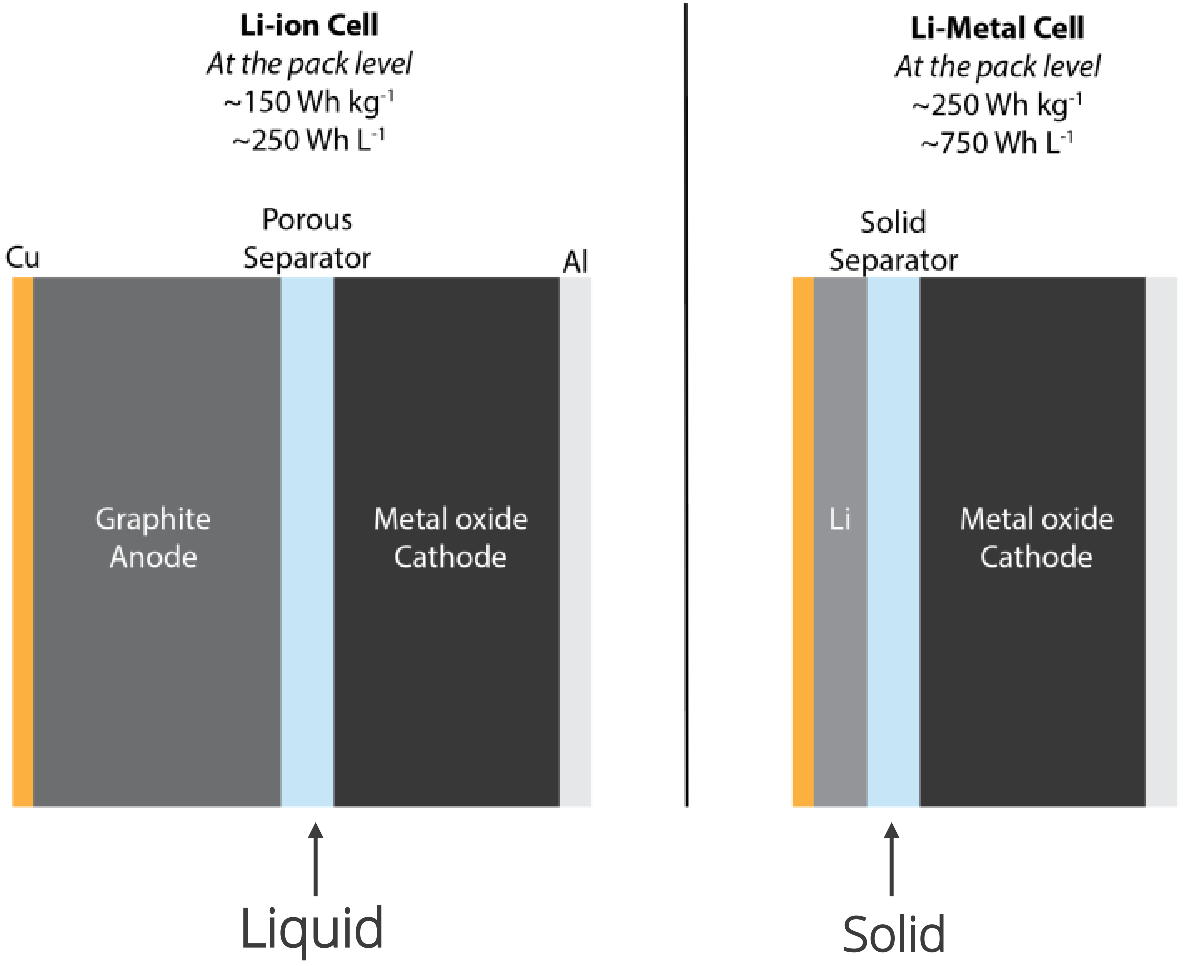
Background: Solid-State Batteries

Liquid Electrolyte (LE)

- ✓ High ionic conductivity
- ✓ Fills void spaces
- ✗ Several heat release pathways
- ✗ Flammable solvent

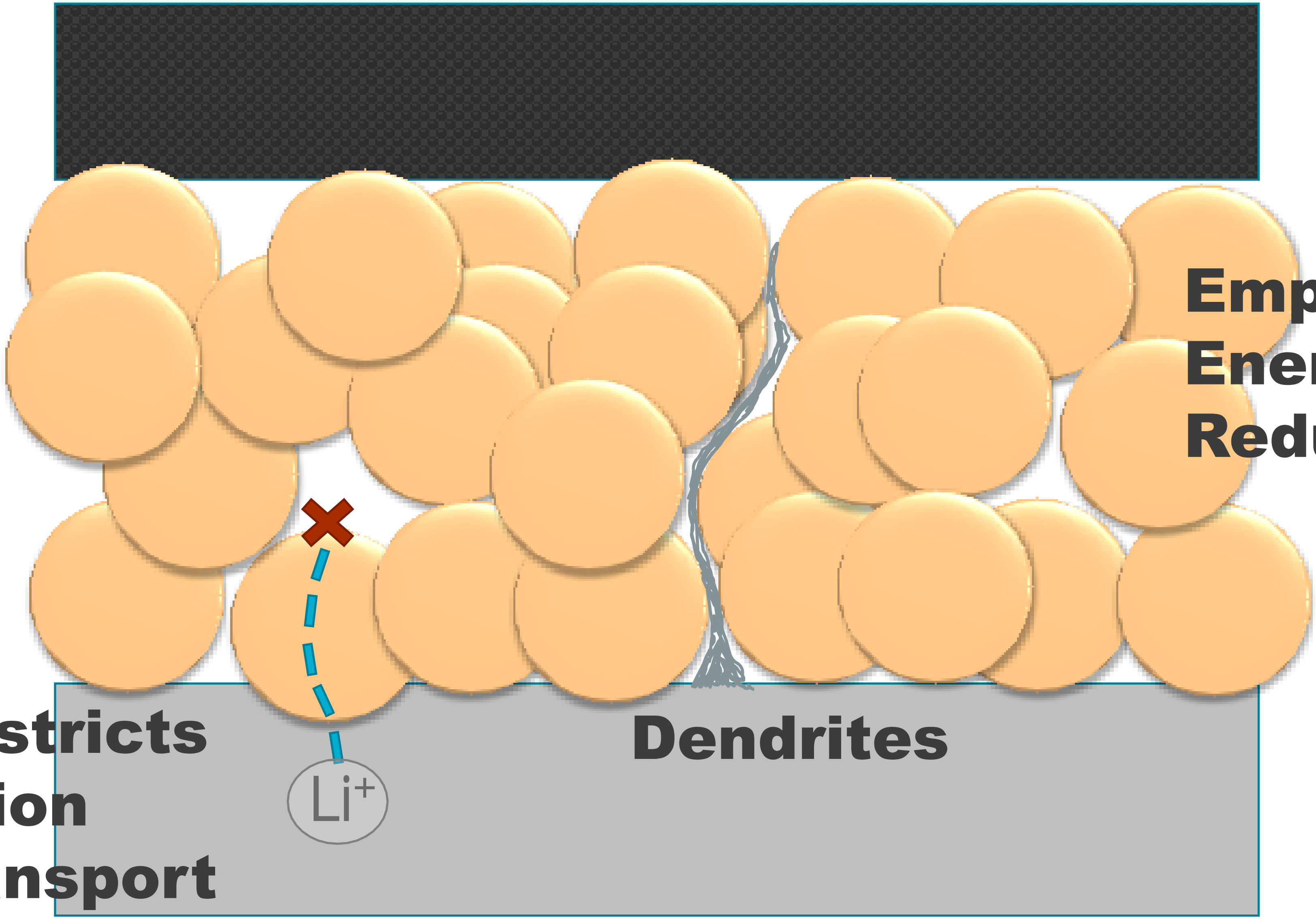
Solid Electrolyte (SE)

- ✓ Sufficient ionic conductivity
  - Highly material dependent
- ✓ Non-flammable
- ✗ Poor interfacial contact



Albertus, P., Babinec, S., Litzelman, S. et al. Status and challenges in enabling the lithium metal electrode for high-energy and low-cost rechargeable batteries.

Removing Liquid Electrolyte Introduces Challenges by Causing Voids



Empty Space = Energy Density Reduction

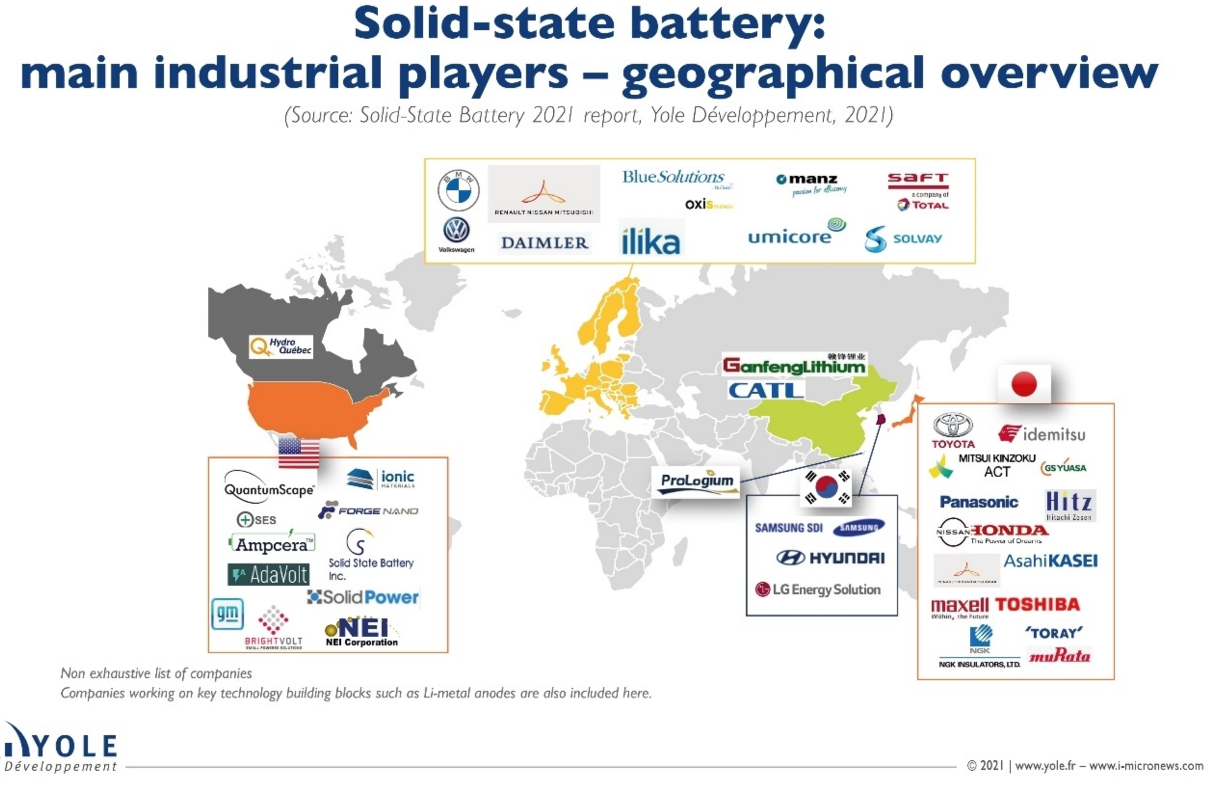
Restricts Li-ion transport

Dendrites

Solid-State Batteries, Why the Excitement?

Two Primary Advantages

- Energy density
  - Li-metal anode
- Safety
  - Removal of flammable liquid electrolyte



Miller T. 247 News Bulletin. 2022 April 30, 2022.

Are Solid-State Batteries Inherently Safe?

Motivation for Thermal Modeling Study

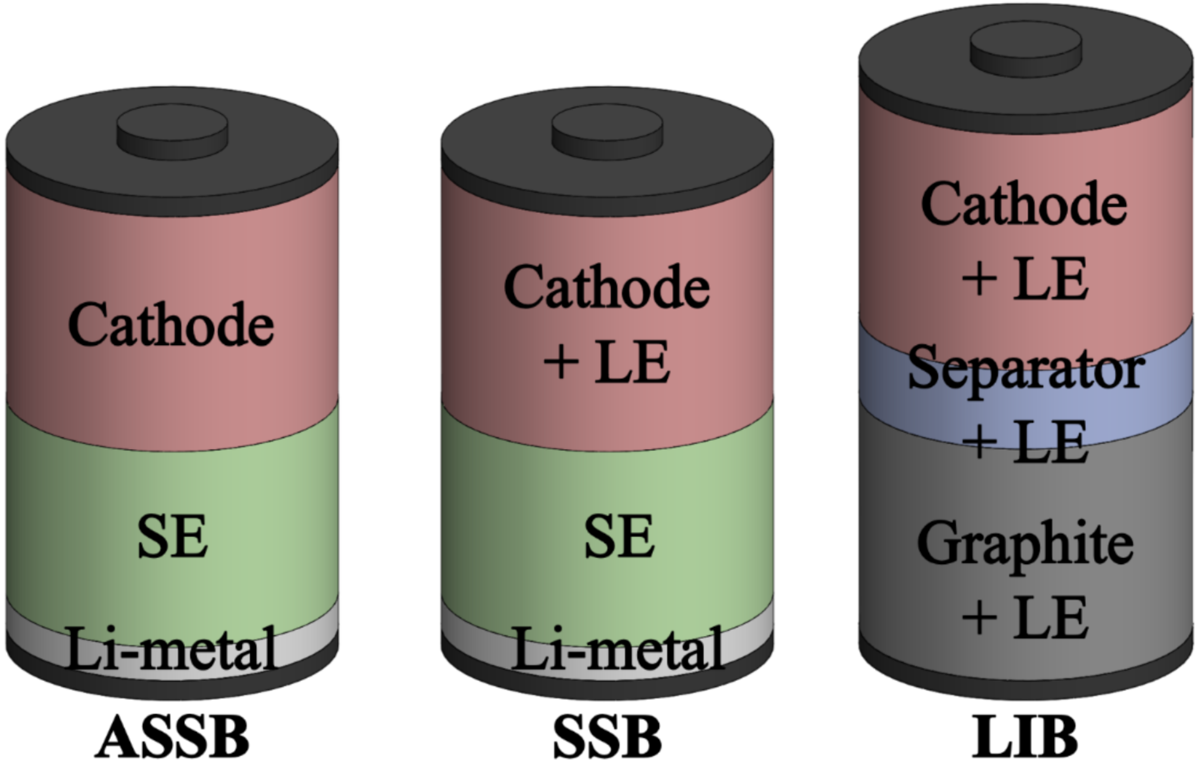
1. Probe the assumption of inherent safety in All-Solid-State Batteries (ASSB)
2. Quantify the safety impact of liquid electrolyte in Solid-State Batteries (SSBs)

Scope – 3 Li Battery Configurations

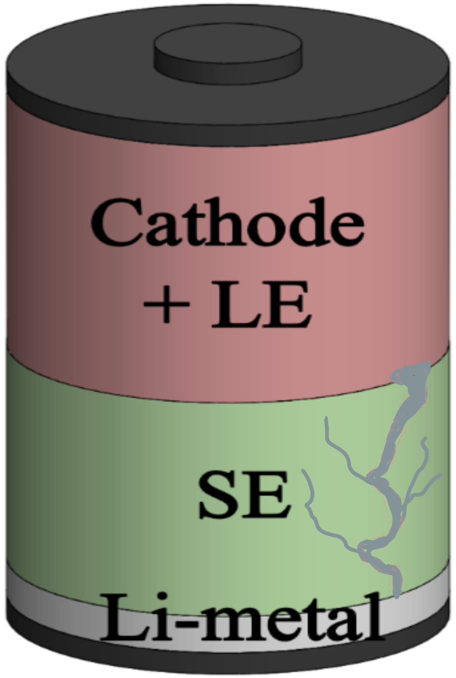
➢ Quantified safety through thermodynamic calculations of heat release

Configurations

- ASSB vs. SSB vs. LIB (Li-ion battery)
  - Cathode – NMC111
  - Solid electrolyte - LLZO
  - Liquid electrolyte – $LiPF_6$ in EMC
  - Anode – Graphite or Li-metal



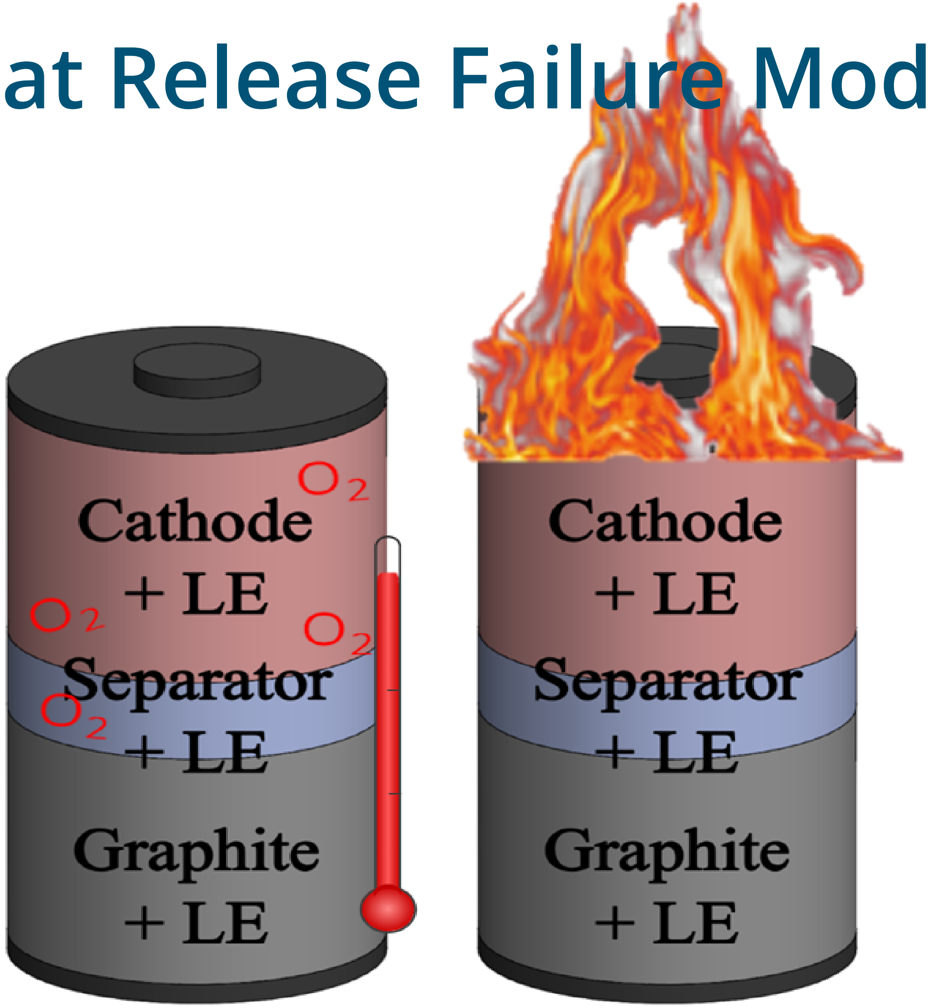
Scope – 3 Heat Release Failure Modes



Short Circuit (ASSB,SSB,LIB)

Dendritic hard short, nail penetration test

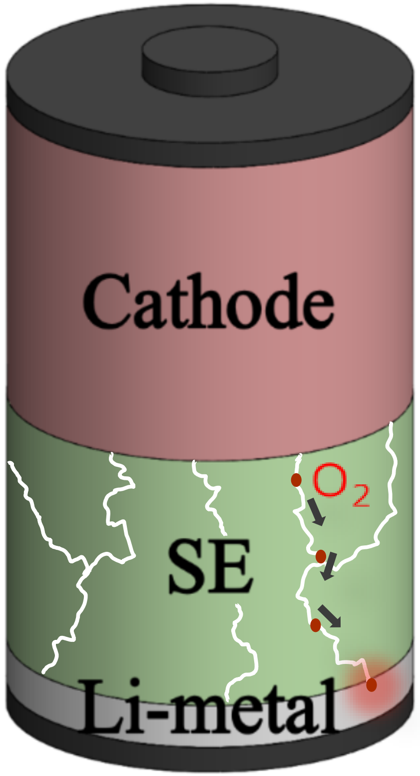
Hard short causes heat release



External Heating (ASSB,SSB,LIB)

Thermal Runaway of adjacent battery

Oxygen generated from breakdown of cathode reacts with LE (& anode for LIB)



SE Mechanical Failure (ASSB)

Cracking of SE: ie. Car accident, SE too thin

SE integrity failure allows for oxygen from cathode to mix with Li-metal

Heat Release vs. Liquid Volume Fraction (VF)

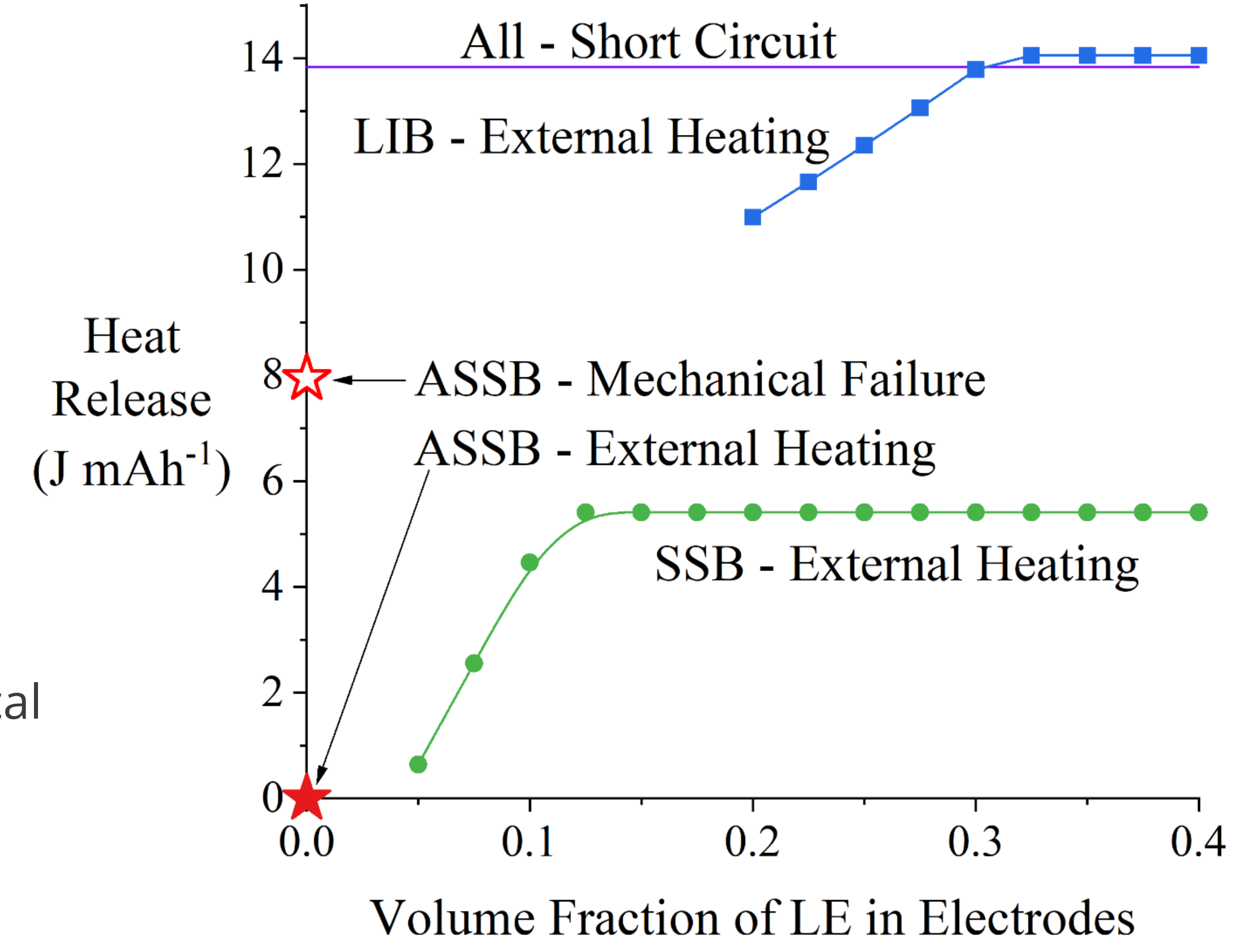
All: short circuit heat release equal among configurations

ASSB: (solid star) no relevant heat release pathways

LIB: heat release dependent on VF (20 to 40%)

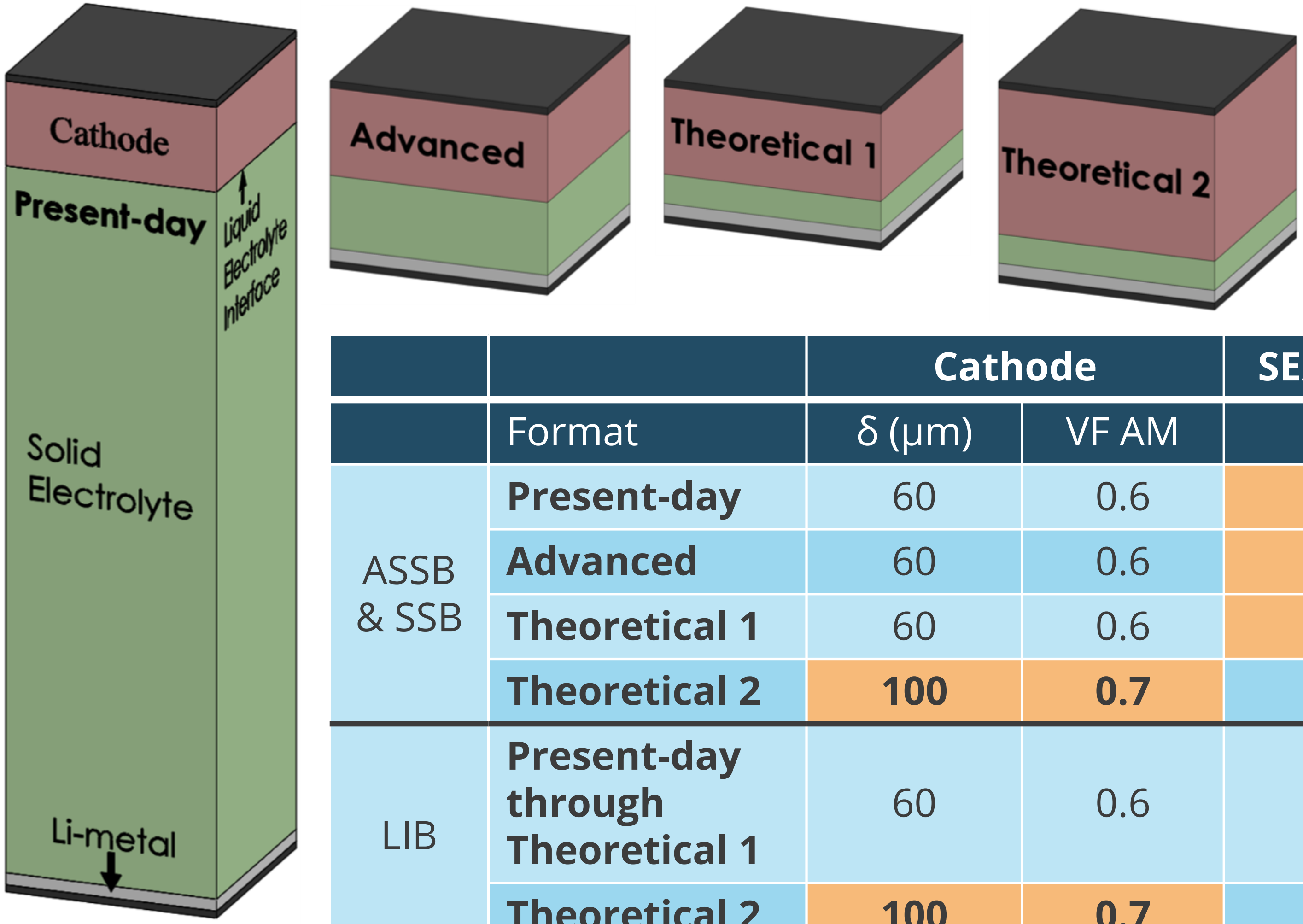
SSB: Heat release reduction <12% VF

ASSB: (open star) large heat release on SE mechanical failure, Li-metal reaction with O_2



Bates AM, Preger Y, Torres-Castro L, Harrison KL, Harris SJ, Hewson J. Are solid-state batteries safer than lithium-ion batteries? Joule. 2022;6(4):742-55.

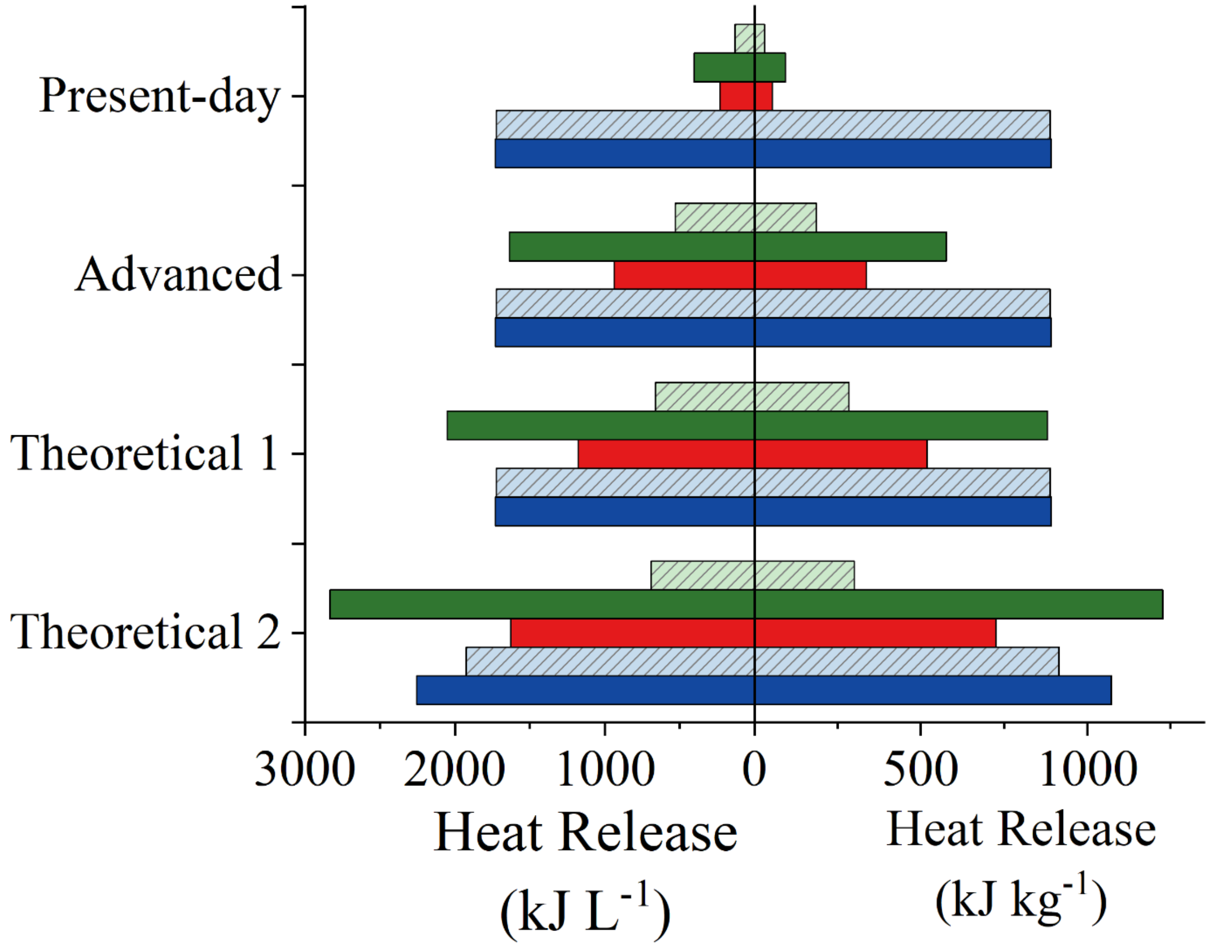
Thermal Modeling Cell Formats



		Cathode		SE/Separator
	Format	δ (μm)	VF AM	δ (μm)
ASSB & SSB	**Present-day**	60	0.6	**500**
	Advanced	60	0.6	**50**
	Theoretical 1	60	0.6	**20**
	Theoretical 2	**100**	**0.7**	20
LIB	**Present-day through Theoretical 1**	60	0.6	20
	Theoretical 2	**100**	**0.7**	20

Increasing Energy Density

Heat Release Dependence on Cell Format



Present day: SSB heat release similar to ASSB

Advanced: Significant jump in ASSB/SSB heat release
ASSB/SSB short circuit approaching LIB

Theoretical 1: ASSB/SSB short circuit exceeds LIB

Theoretical 2: Jump in ASSB/SSB worse than LIB

SSB – external heating
ASSB/SSB – short circuit
ASSB – mechanical failure
LIB – external heating
LIB – short circuit

Bates AM, Preger Y, Torres-Castro L, Harrison KL, Harris SJ, Hewson J. Are solid-state batteries safer than lithium-ion batteries? Joule. 2022;6(4):742-55.

Temperature as a Measure of Safety

- Heat release is great for comparing cell configurations and formats

- However, safety is a measure of risk to human injury

- For batteries, safety implies preventing single cell thermal runaway
  - If that fails: prevent cascading propagation (adjacent cell thermal runaway)

- Temperature is a measure for the vulnerability of a cell to thermal runaway
  - Temperature also indicates the potential for cascading propagation

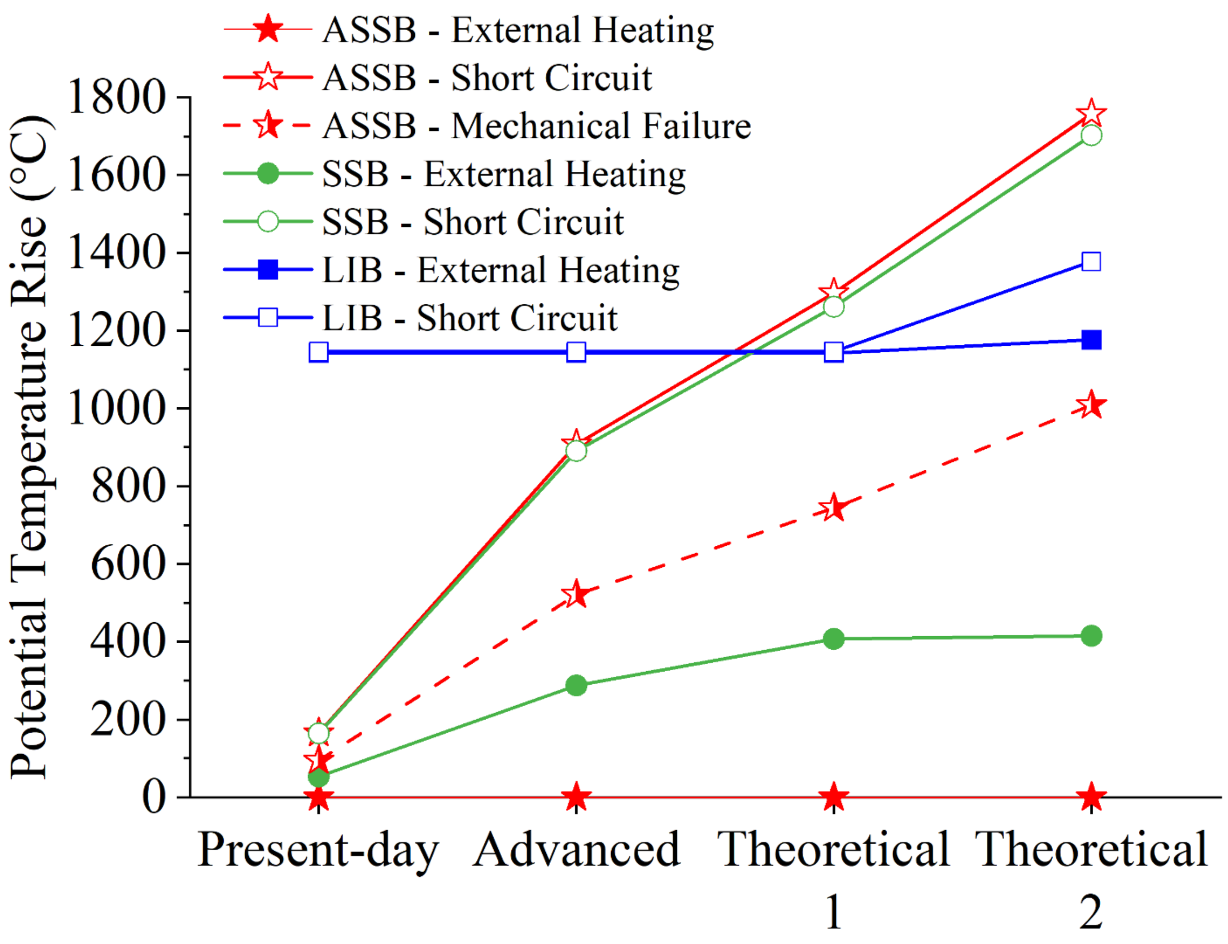
Potential Temperature Rise

External Heating: LIB highest

SSB below typical propagation (400 ºC)

Short Circuit: ASSB/SSB exceeds LIB at Theoretical 1

Mechanical Failure: ASSB approaches LIB



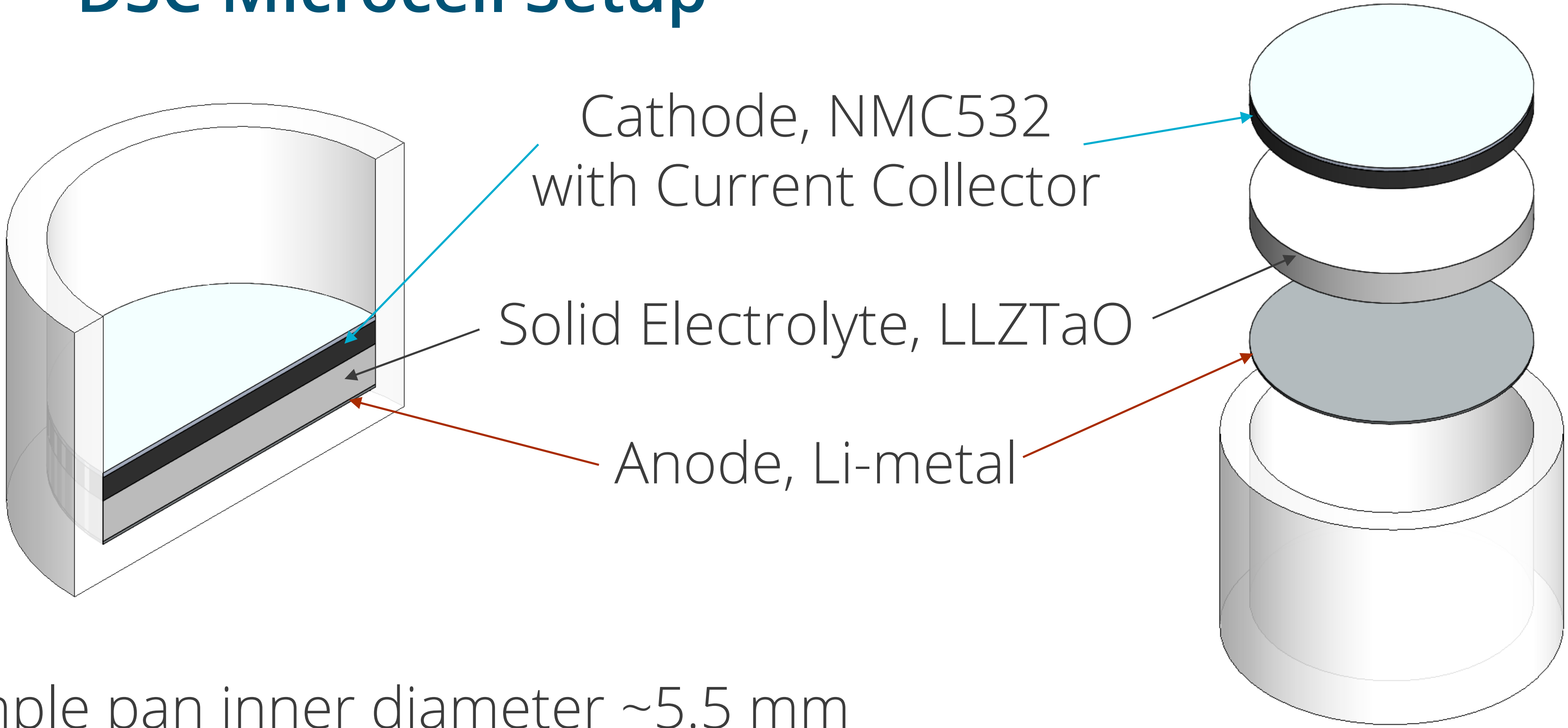
Bates AM, Preger Y, Torres-Castro L, Harrison KL, Harris SJ, Hewson J. Are solid-state batteries safer than lithium-ion batteries? Joule. 2022;6(4):742-55.

Torres-Castro, L., Kurzawski, A., Hewson, J., and Lamb, J. (2020). Passive Mitigation of Cascading Propagation in Multi-Cell Lithium Ion Batteries.

Summary – Thermodynamic Modeling

- We consider potential temperature rise as our safety measure
  - SSBs are not ALWAYS inherently safe
- Potential temperature rise increases significantly with energy density
  - Critical consideration for future ASSBs/SSBs
- High heat release from SE mechanical failure
  - O_2 reaction with Li-metal, potential for large heat release
- SSBs with <10% liquid electrolyte by cathode volume
  - Heat release small enough that cost, manufacturability, and performance enhancements may allow for commercialization

DSC Microcell Setup



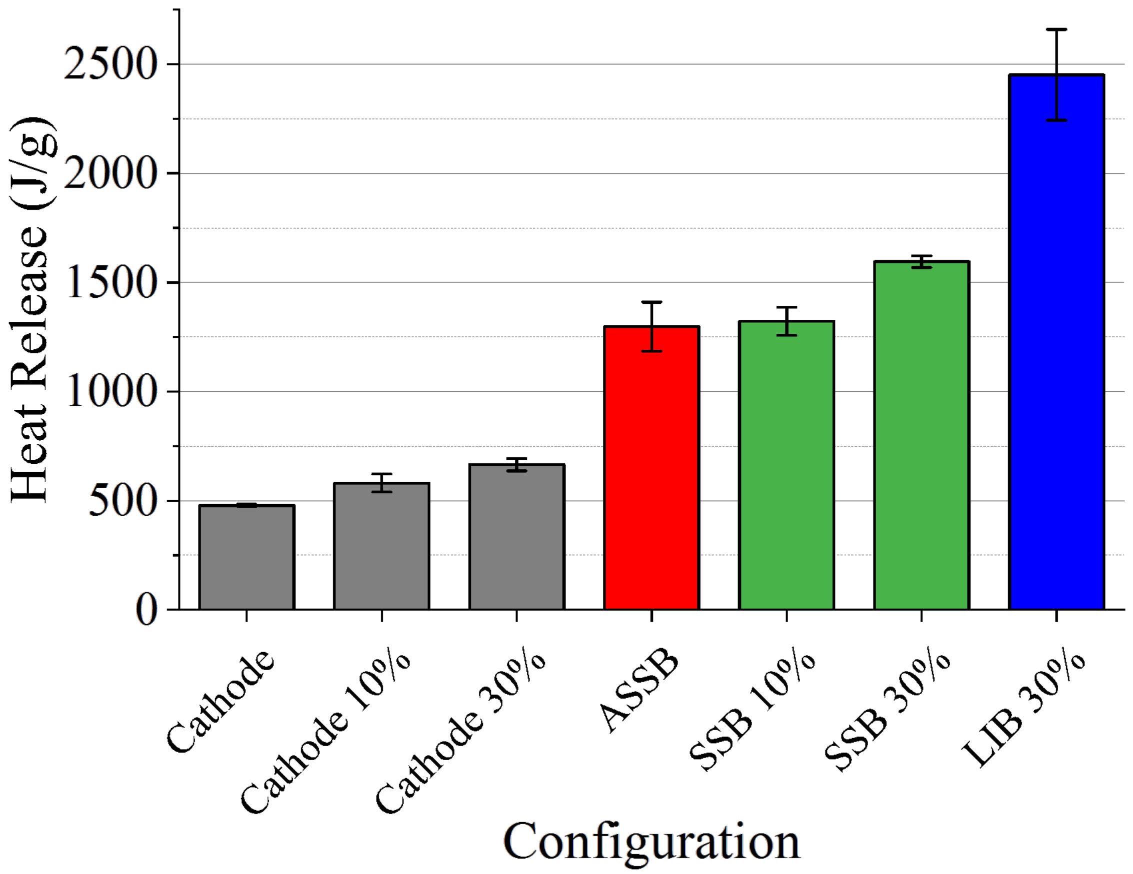
- Sample pan inner diameter ~5.5 mm
- SE thickness 0.5-0.7 mm (comparable to Present Day format)
- Cathode at 100% SOC (identical to previous work)
- N-to-P ratio 1-to-1 (identical to previous work)

Heat Release Dependent upon Amount of LE

- 10% VF of liquid electrolyte has little to no effect on overall heat release compared to the ASSB

- At some VF, increasing liquid electrolyte does increase overall heat release

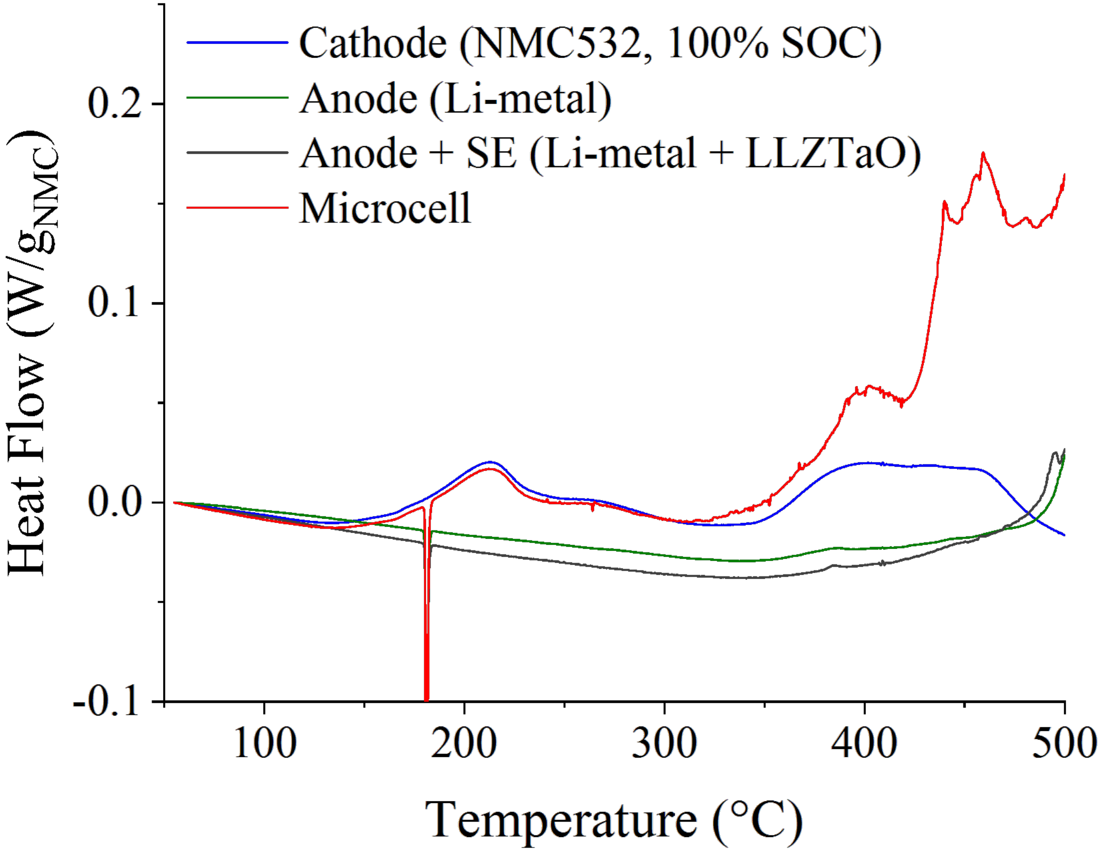
- The overall heat release of the LIB is much higher than the SSB



Li Metal Combined with Cathode Significantly Increases ASSB Heat Release

- Without Li-metal (or with only Li-metal), the high temperature exotherms remain relatively small

- With the cathode in proximity of Li-metal (separated by SE), the exothermic heat release increases by 130%

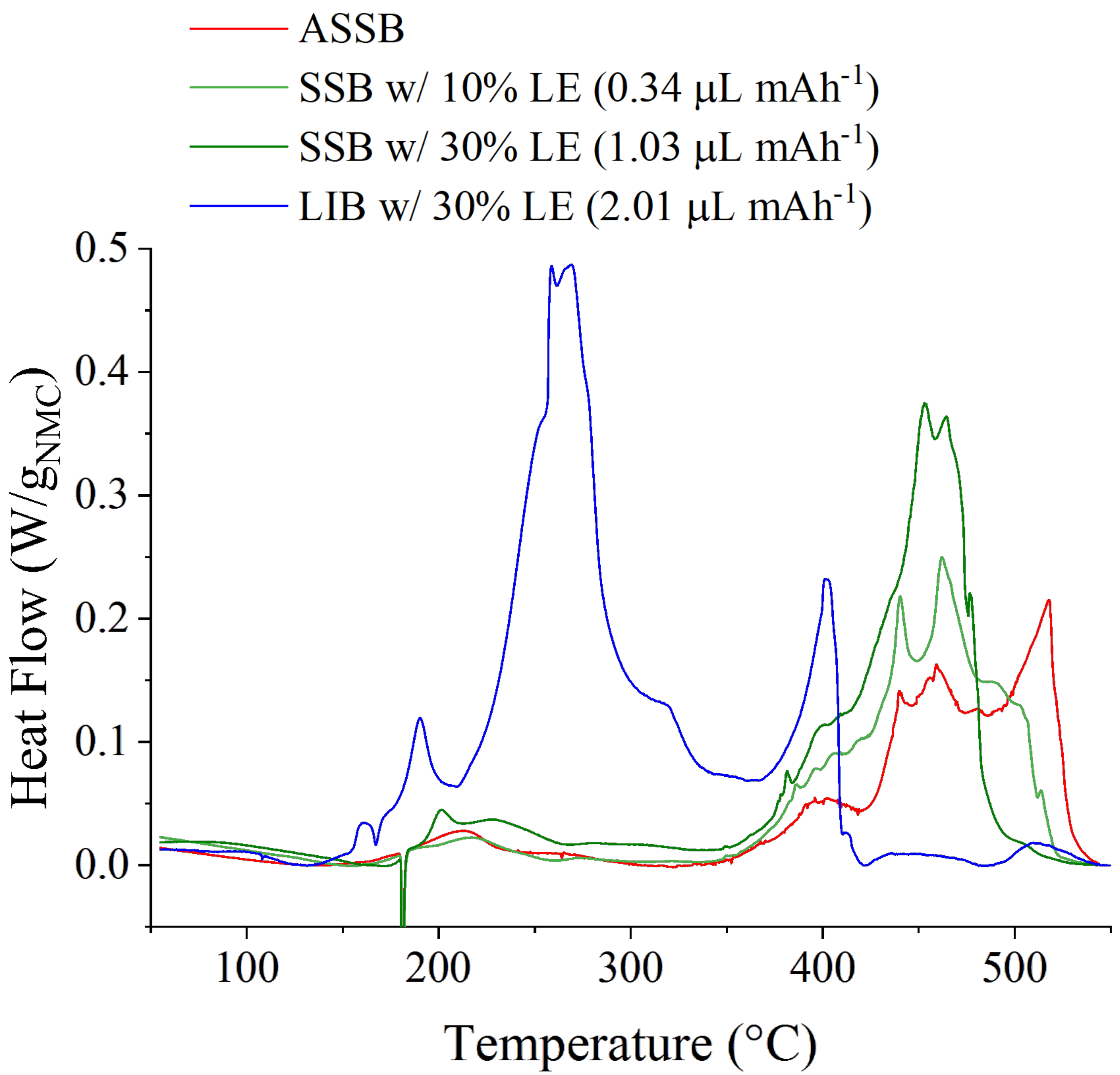


LE Volume affects Peak Exotherm Temperature but Not SSB Onset Temperature

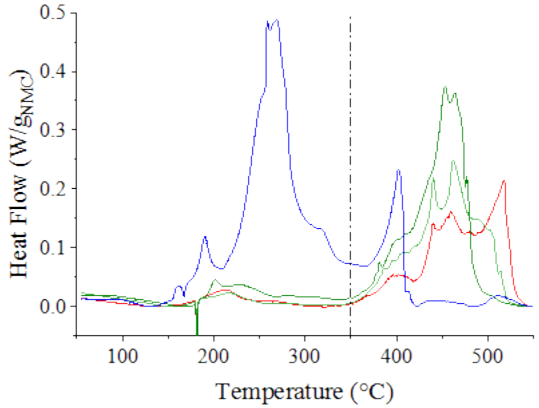
- For ASSB and SSB, large exotherms occur at high temperatures relative to the LIB

- For the SSB, onset temperature to large exotherms remains around 350 °C, regardless of LE volume

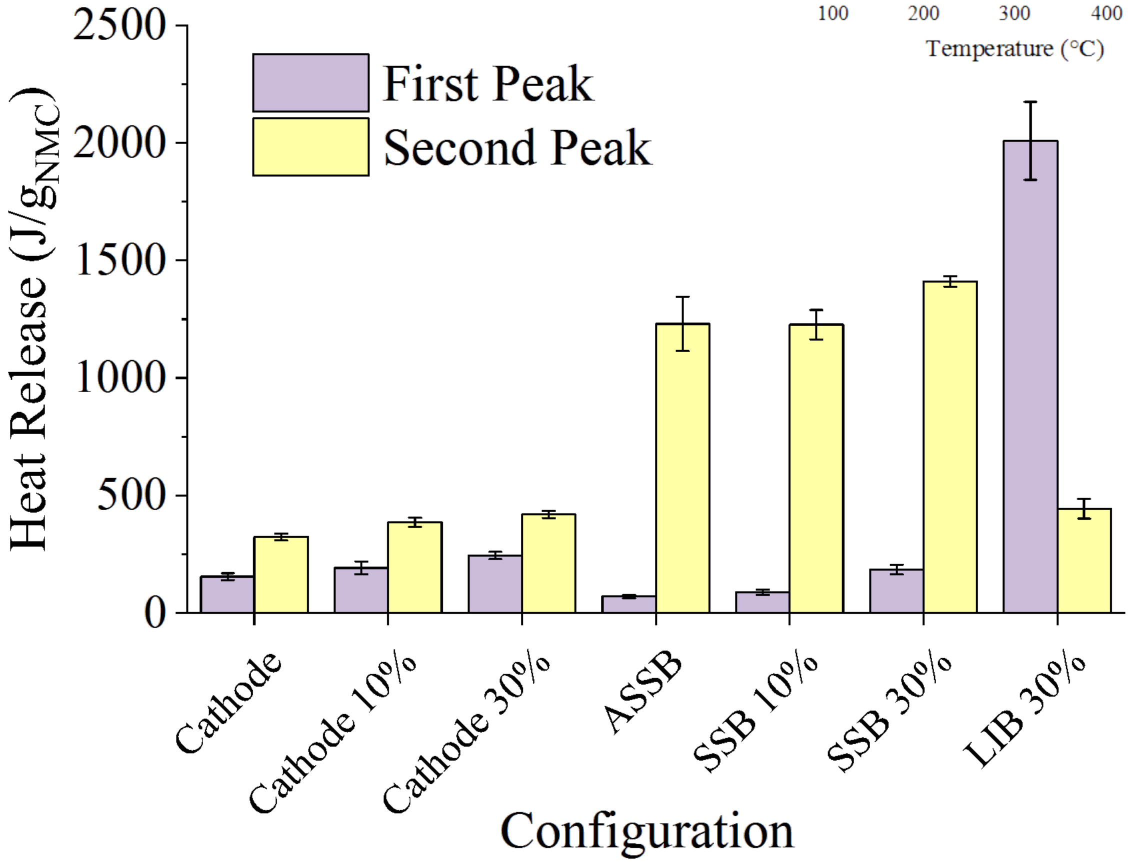
- As LE volume increases, peak heat flow moves to lower temperatures and a small exothermic spike develops around 200 °C



Separating Heat Release Into Two Peaks



- First peak heat release is much lower for the ASSB and SSB compared to LIB, regardless of LE volume
- Indicates thermal runaway onset temperature for SSB is likely much higher than for LIB

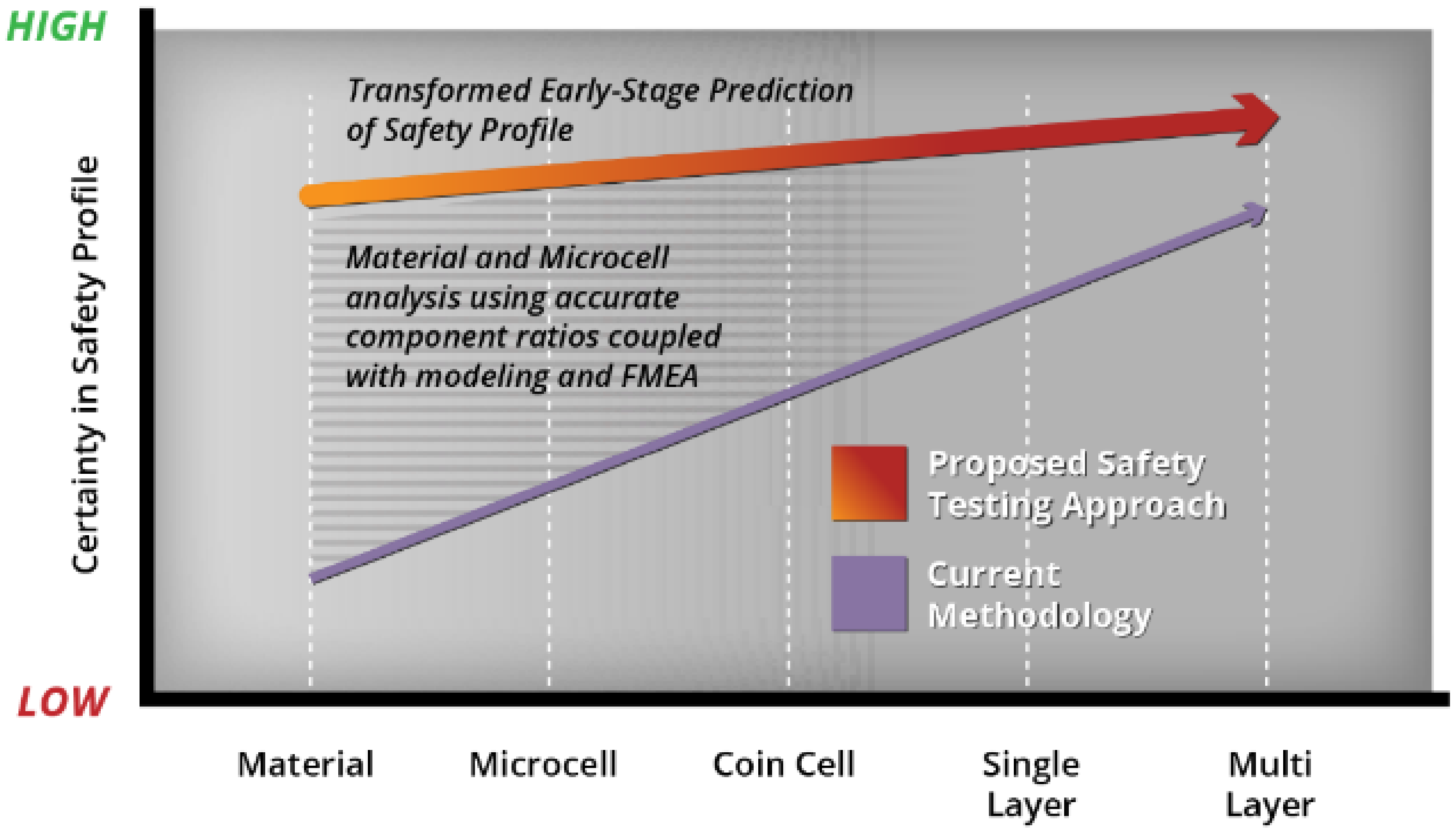


Summary – Experimental DSC

- Increasing the volume of LE in an SSB increases heat release
- Results indicate the onset to large exothermic events occurs at higher temperatures for SSBs compared to LIBs
- 10% volume fraction of liquid electrolyte in a SSB has minimal impact on heat release

ARPA-E Grant for Early-Stage Safety Prediction of Battery Chemistries

- Increase accuracy of initial–stage safety predictions from materials principles
- Incorporate findings into a Multi-Scale Safety Testing Manual that is easily accessible to all
- Expedite concept-to-commercialization by reducing safety risk in initial developmental stages



Request

Can I abuse your batteries?

- We would like to improve and expand this model through experimental verification and data analysis
- Seeking ≥ 1 Ah battery
- We are interested in all SSB and Li-metal anode configurations

Project Team

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Questions?

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