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Investigation of Exothermic Reaction Pathways in Solid-State Batteries: Implications for Safety

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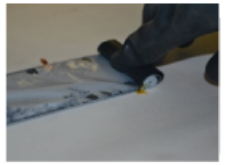
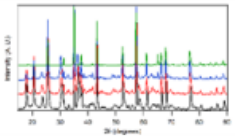
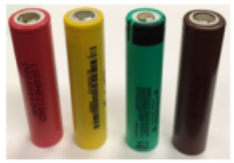
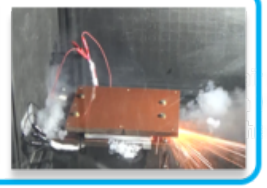
Sandia Addresses all Aspects of Safety & Reliability for Battery Energy Storage

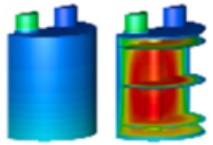
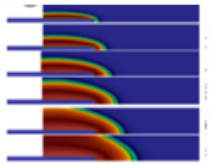
Materials R&D

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

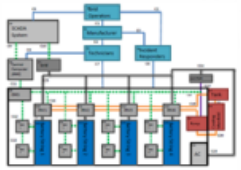
Cell and Module Testing

- 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

Solid-State Batteries, Why the Excitement?

Two Primary Advantages

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

Solid-state battery:
main industrial players – geographical overview

(Source: Solid-State Battery 2021 report, Yole Développement, 2021)

Non exhaustive list of companies
Companies working on key technology building blocks such as Li-metal anodes are also included here.

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

Are Solid-State Batteries Inherently Safe?

Motivation for Thermal Modeling Study

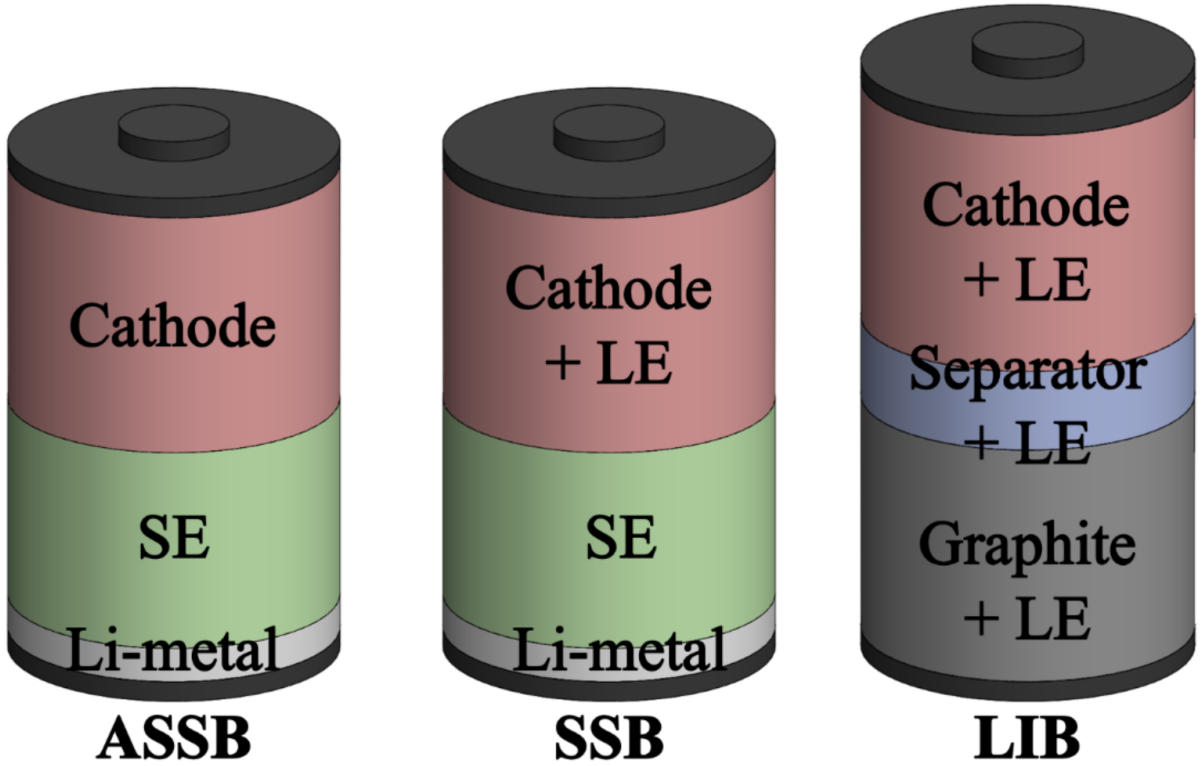
1. Probe the assumption of inherent safety in All-Solid-State Batteries (ASSB)
2. Quantify the safety impact of liquid electrolyte in Solid-State Batteries (SSBs)

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



Thermodynamic Modeling Suggests that SSB with low amount of LE may have similar safety as ASSB

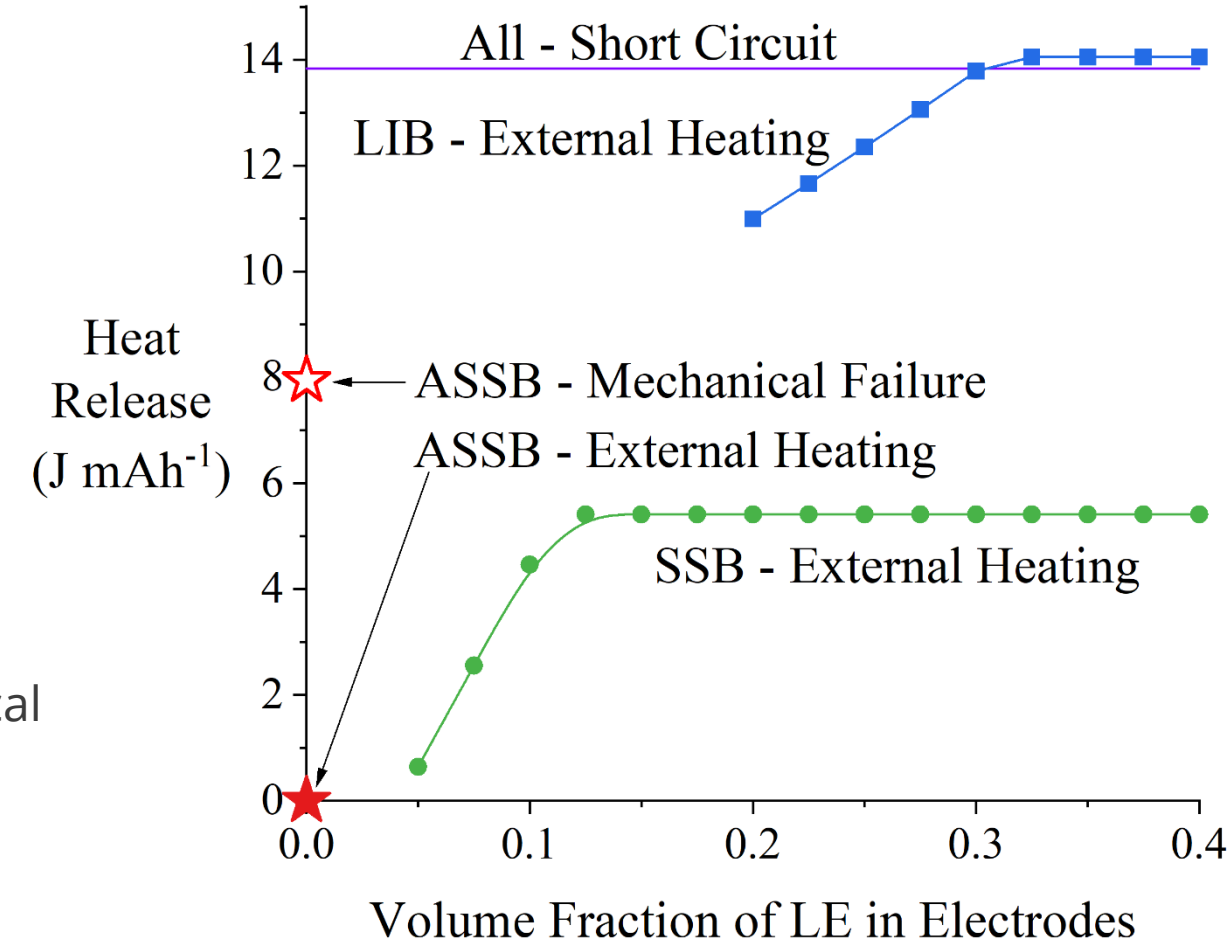
All: short circuit heat release equal among configurations

ASSB: (solid star) no relevant heat release pathways

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

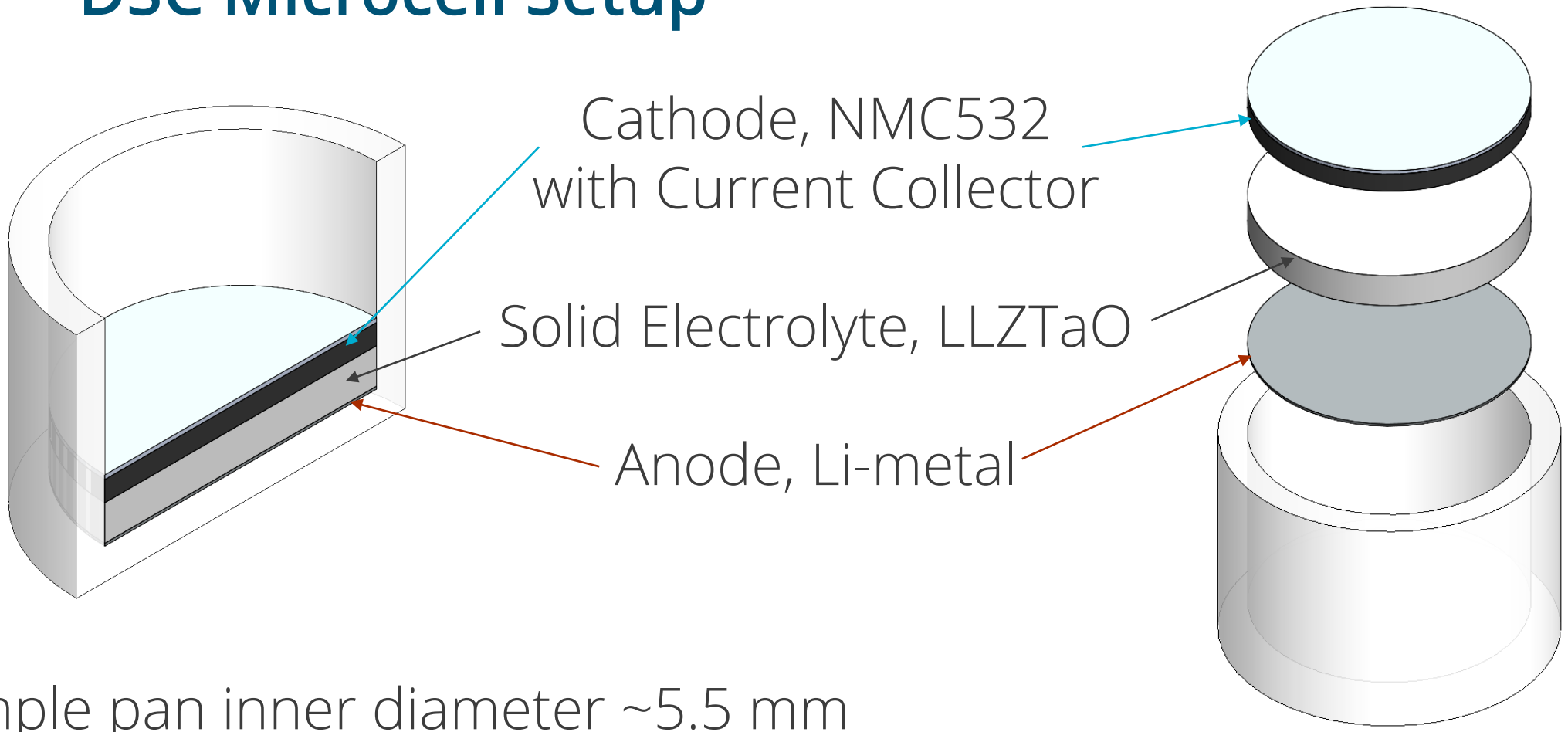
SSB: Heat release reduction <12% VF

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.

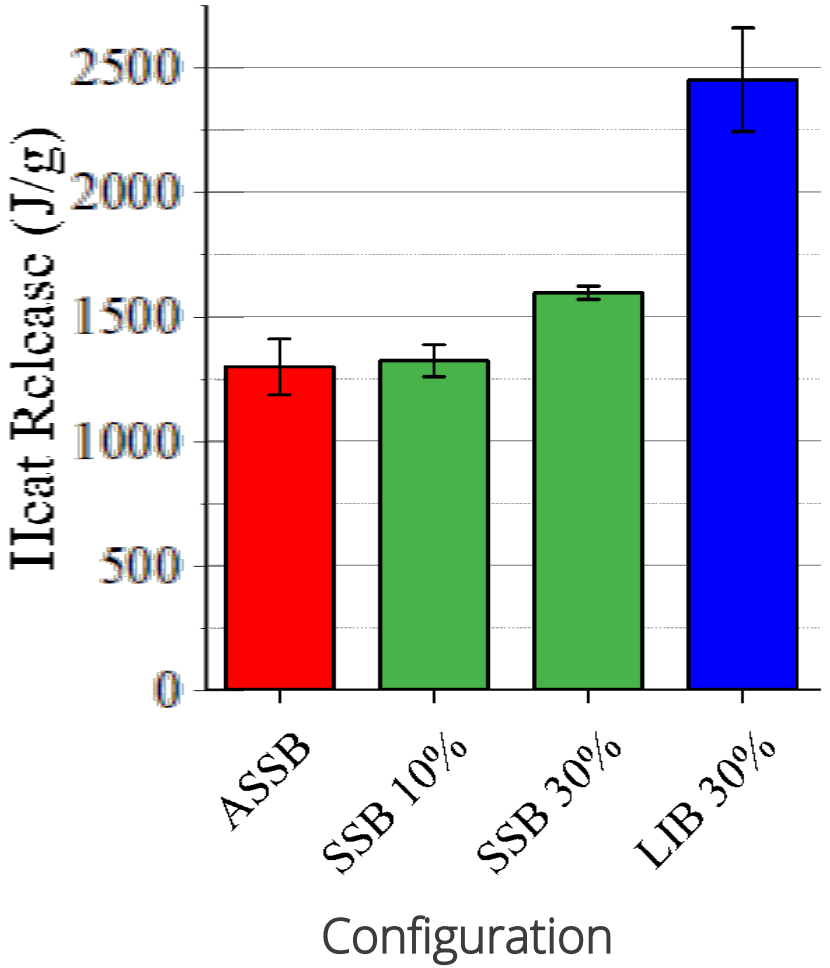
DSC Microcell Setup



- Sample pan inner diameter ~5.5 mm
- SE thickness 0.5-1.0 mm
- Cathode at 100% SOC (delithiated, identical to previous work)
- N-to-P ratio 1-to-1 (identical to previous work)

DSC Experiments Show 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



DSC Exothermic Reactions Decoupled through Materials Characterization

DSC halted at critical temperature and cathode harvested for XRD analysis

<u>ASSB & SSB</u>

350 °C

445 °C

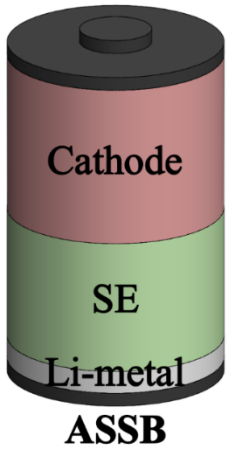
550 °C

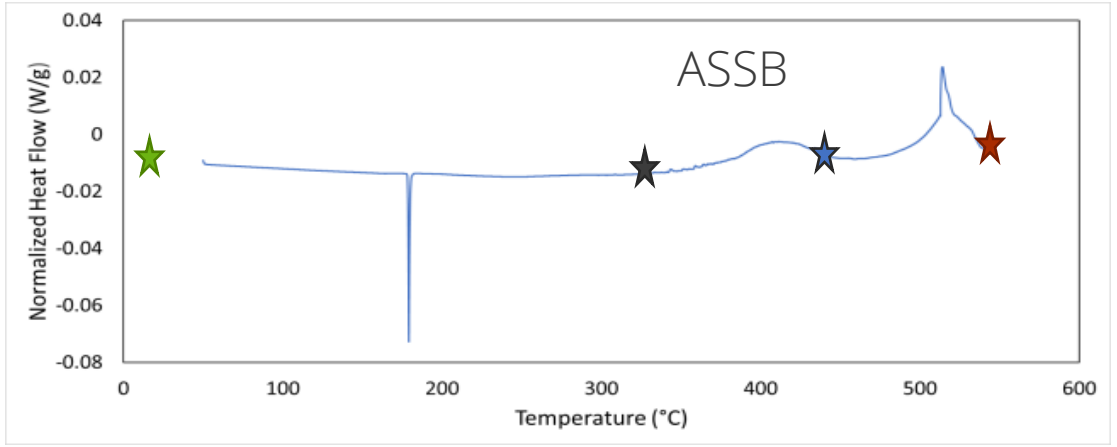
<u>LIB</u> – Reaches peak and end of largest exotherm at lower temperature

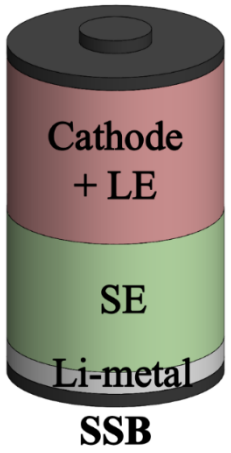
212 °C

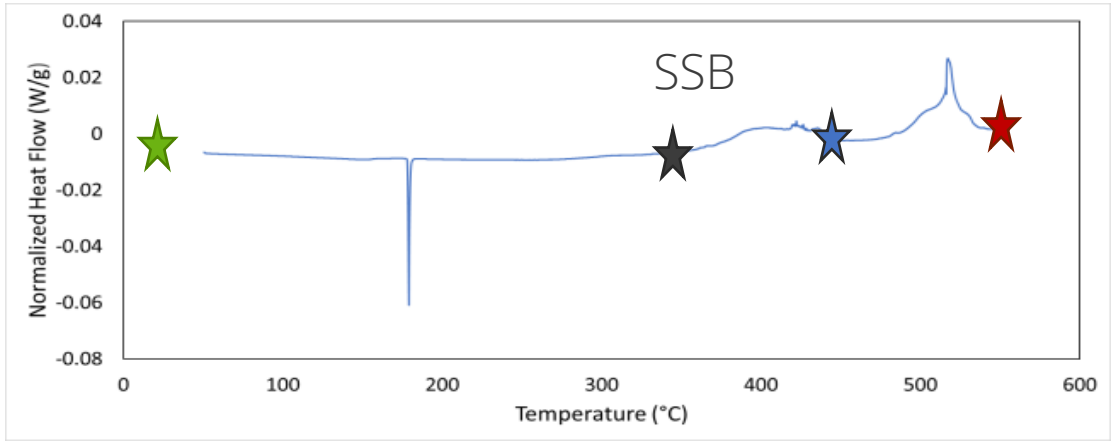
262 °C

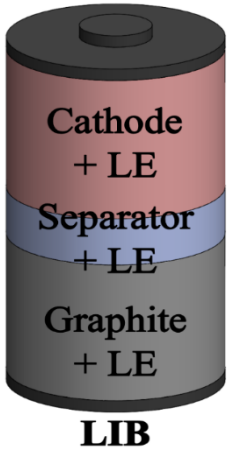
312 °C

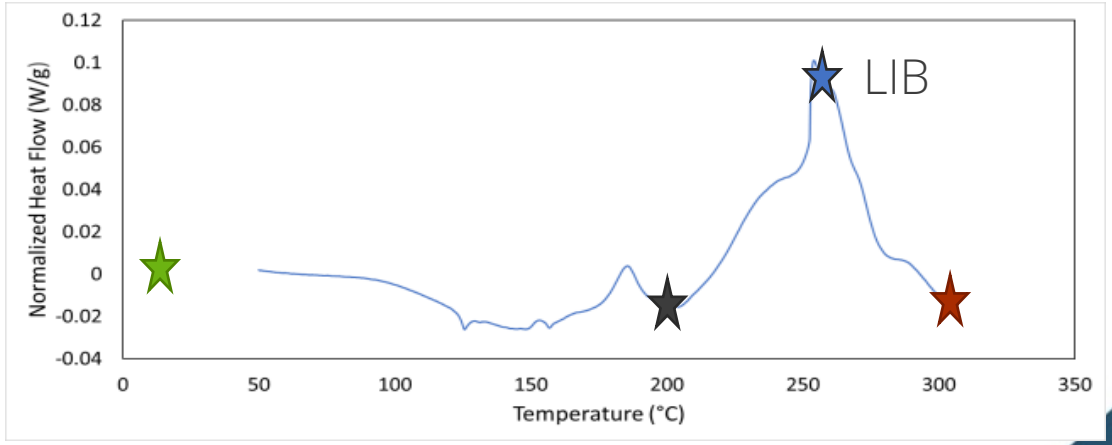












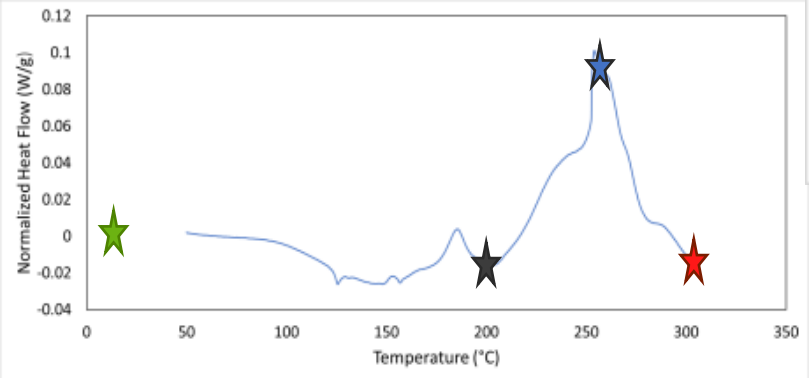
XRD of LIB Cathode Reveals Layered Structure Transitioning to Spinel

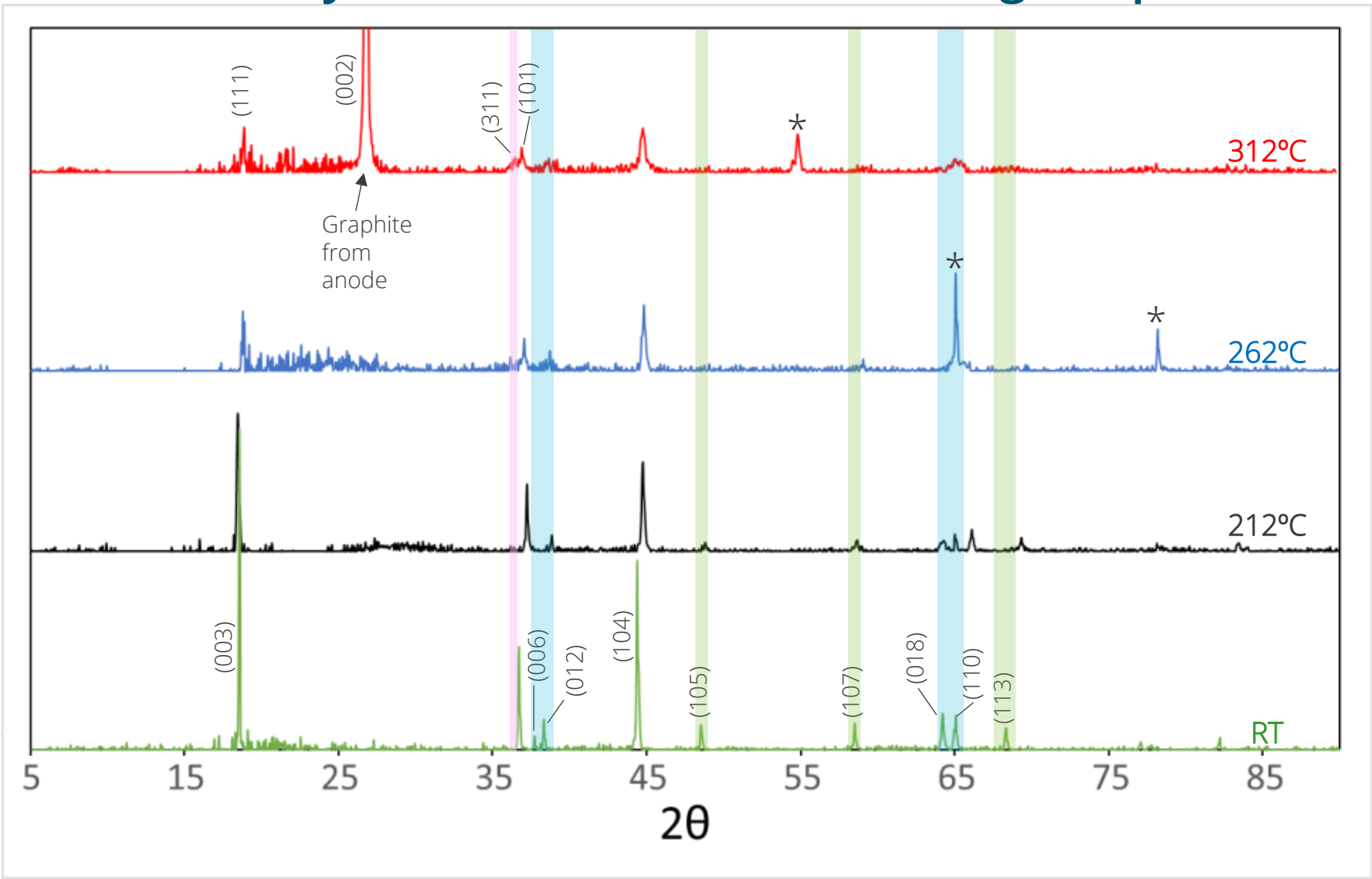
Layered Structure:
Distinguishable
(006) & (012)
(018) & (110)
(105)
(107)
(113)

Spinel Structure:
(311)

Spinel phase starting to form.

Exotherm peak occurs at significantly lower temp than for ASSB & SSB.

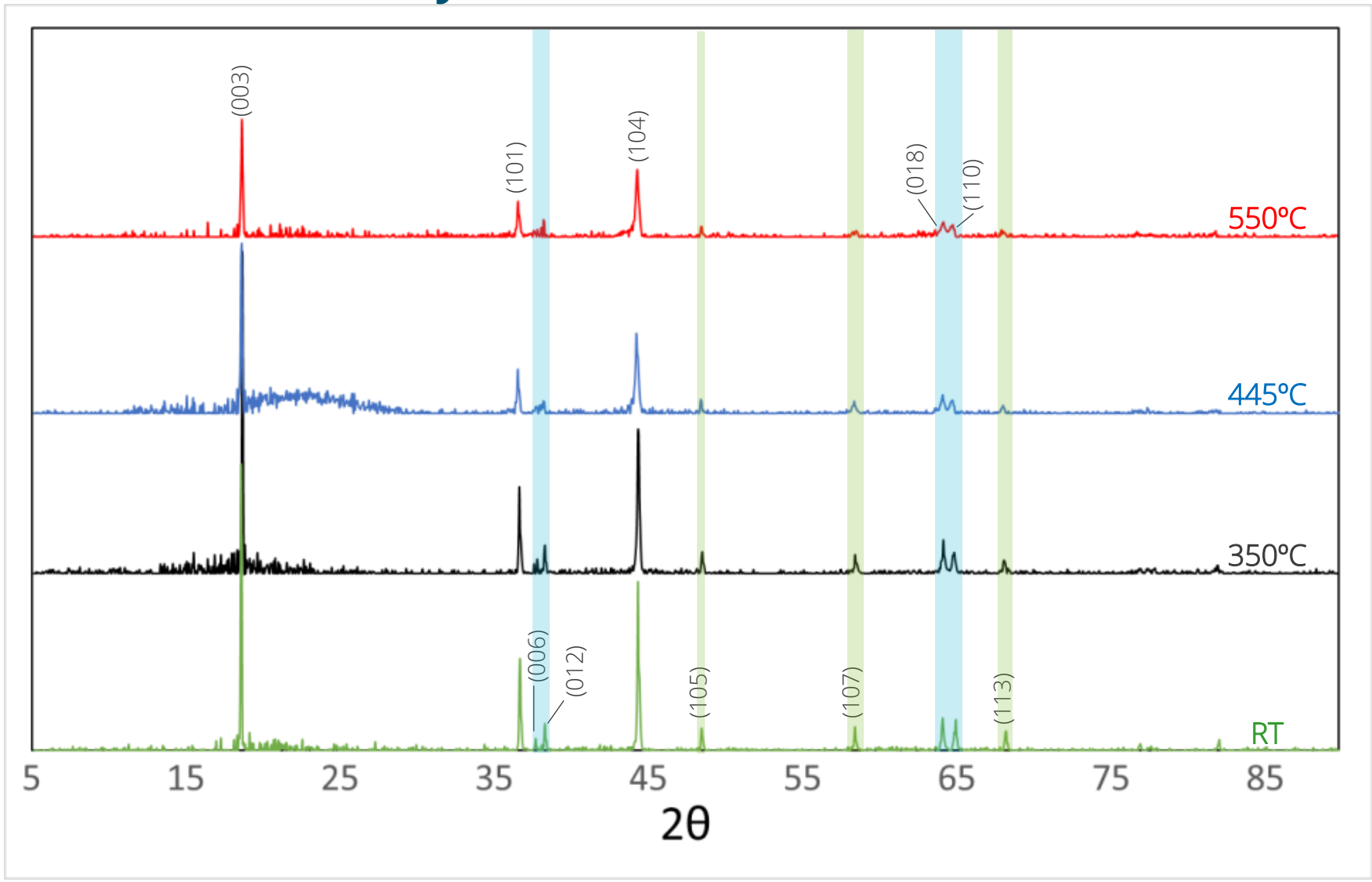


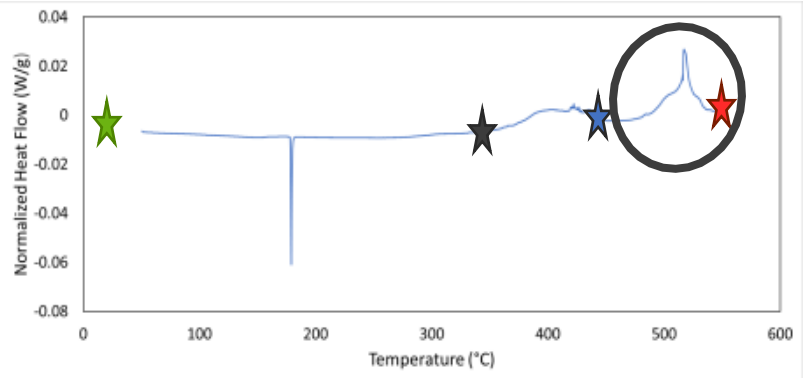


XRD of SSB10% Cathode Reveals Layered Structure at 550°C

Layered Structure:
Distinguishable
(006) & (012)
(018) & (110)
(105)
(107)
(113)

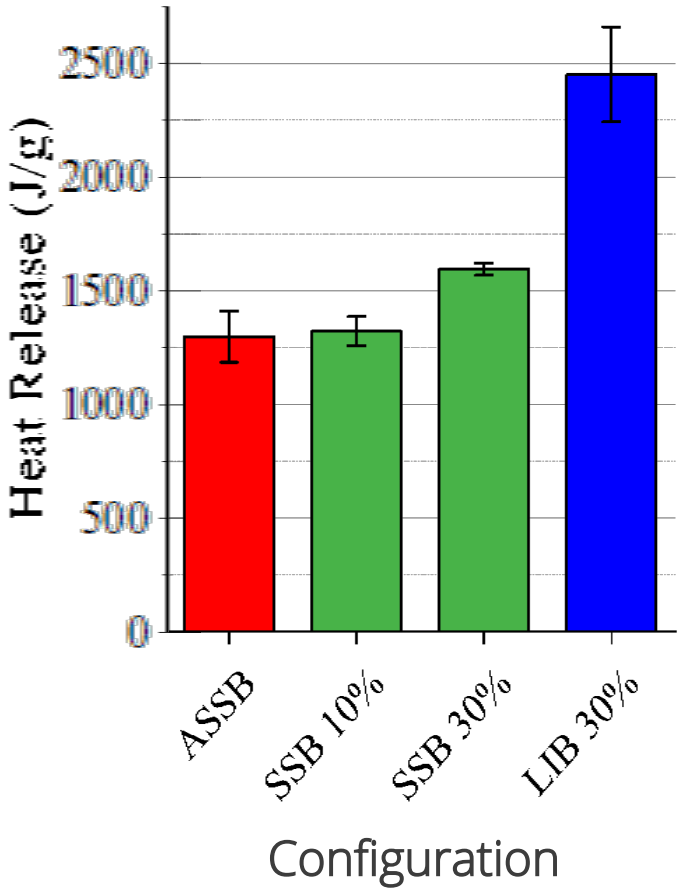
Remained in layered structure up to 550 °C.





Summary

- Safety Modeling: Could be possible to add some LE without increasing safety risk
- DSC Experiment: Addition of 10% LE to SSB does not show significant heat release relative to ASSB (0% LE)
- XRD Analysis: Cathode maintained layered structure in SSB but experienced degradation in LIB at lower temperatures



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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