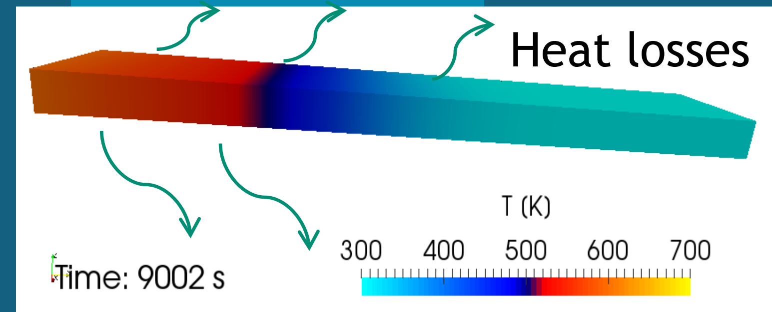
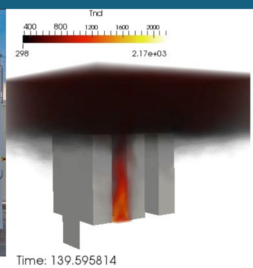
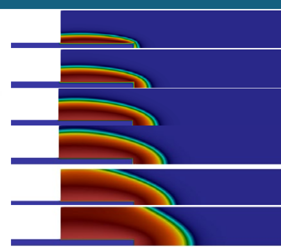
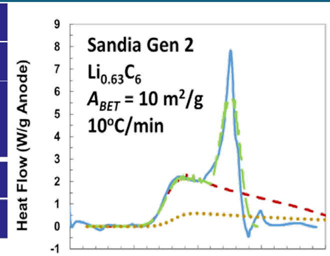
Predictive modeling for energy-storage safety in abnormal thermal scenarios









PRESENTED BY

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Office of Electricity Peer Review
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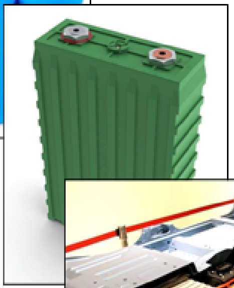
Validated reliability and safety is one of four critical challenges identified in 2013 Grid Energy Storage Strategic Plan

- Failure rates as low as 1 in several million,
- Potentially many cells used in energy storage.
- Moderate likelihood of ‘something’ going wrong,

A single cell failure that propagates through the pack can have an impact even with low individual failure rates

How do we decrease the risk?

Single Cell
~0.5-5 Ah



Strings and large
format cells
~10-200 Ah

EV Battery Pack 100s-
1000s cells
10-50 kWh

Stationary storage
system 1000s or more
individual cells
MWh+

www.nissan.com
www.internationalbattery.com
www.samsung.com
www.saft.com

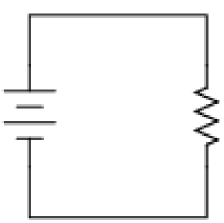
Approaches to designing in safety

The current approach is to test our way into safety.

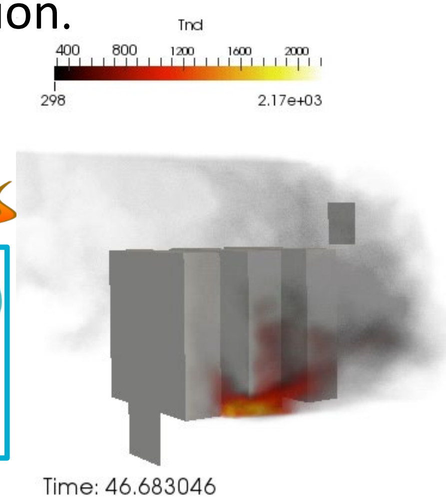
- Large system (>1MWh) testing is difficult and costly.

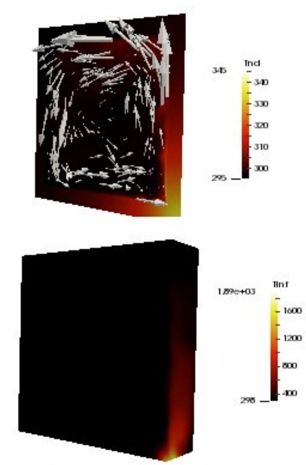
Supplement testing with predictions of challenging scenarios and optimization of mitigation.

- Develop multi-physics models to predict failure mechanisms and identify mitigation.
- Build capabilities with small/medium scale measurements.
- Still requires some testing and validation.



Simulated short circuit



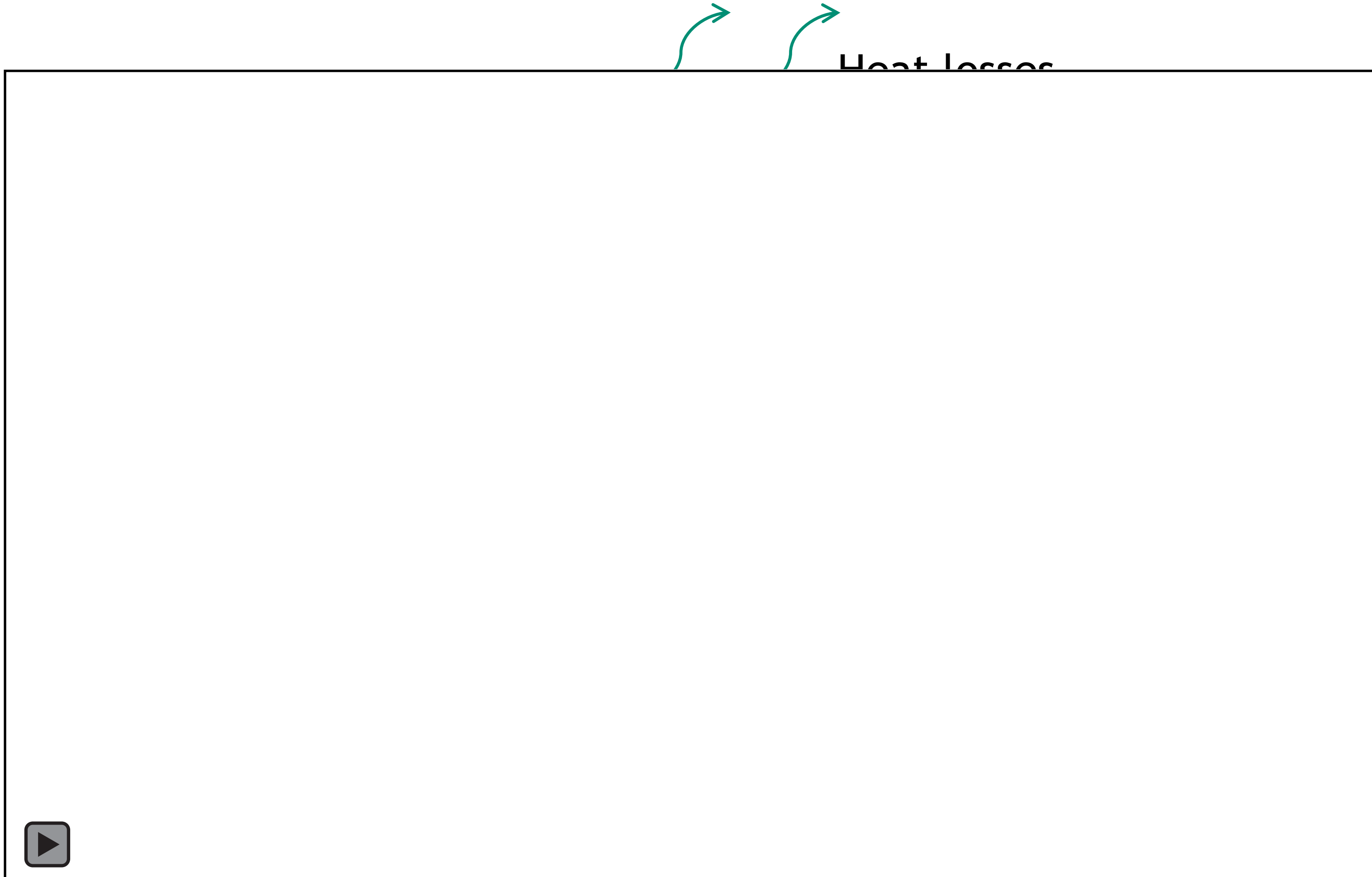


Simulating cascading failure of cell stack

Short circuit simulated in first cell acts as boundary condition

Lamb, J., et al. (2015). J. Power Sources **283**: 517-523.

Simulating cascading failure of cell stack



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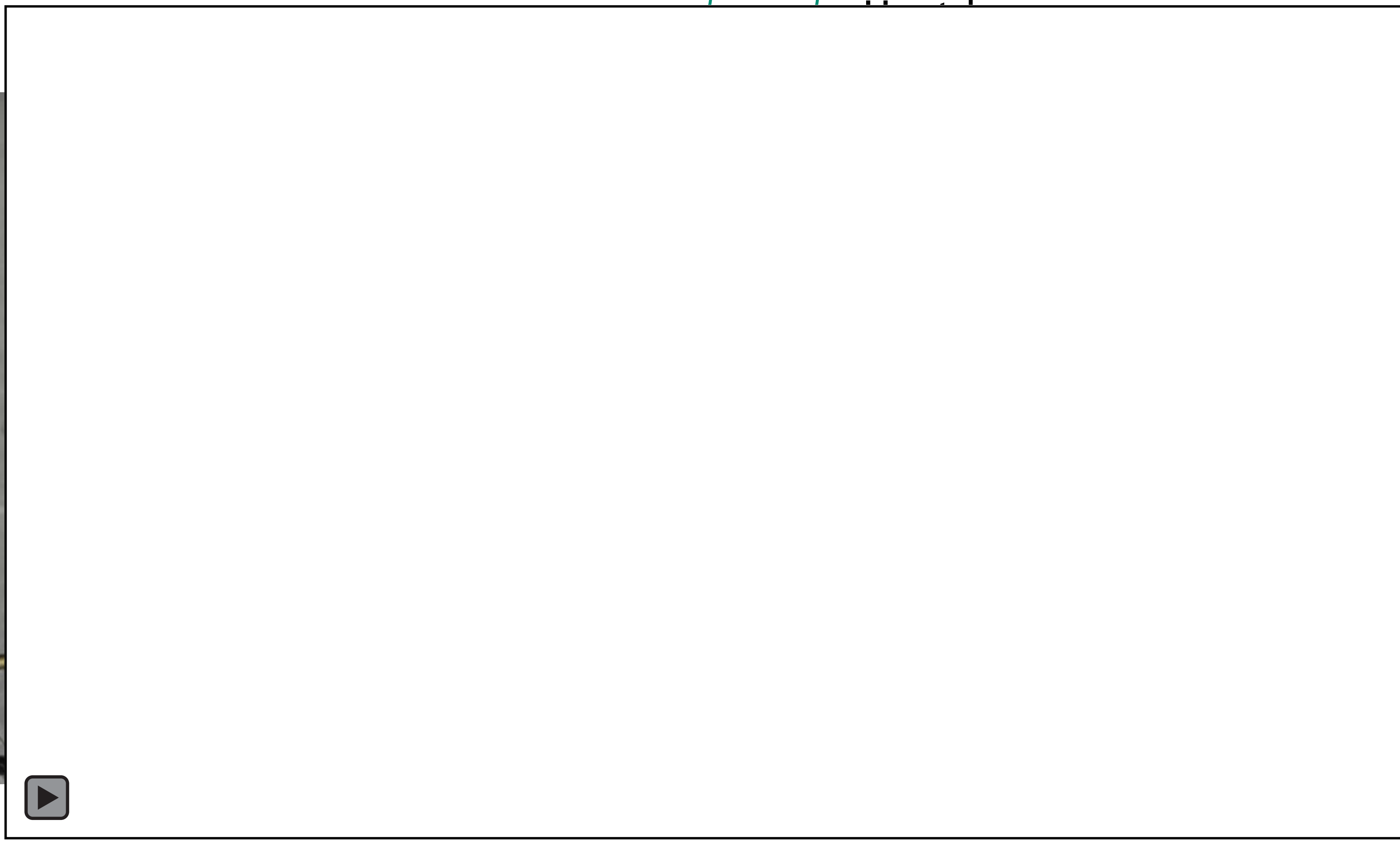


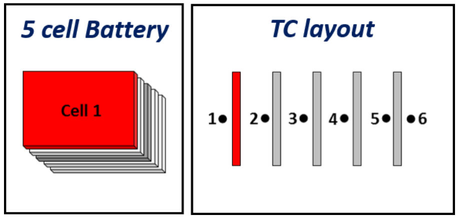
Lamb, J., et al. (2015). J. Power Sources **283**: 517-523.

Cascading runaway:
From temperature measurements to understanding heat release

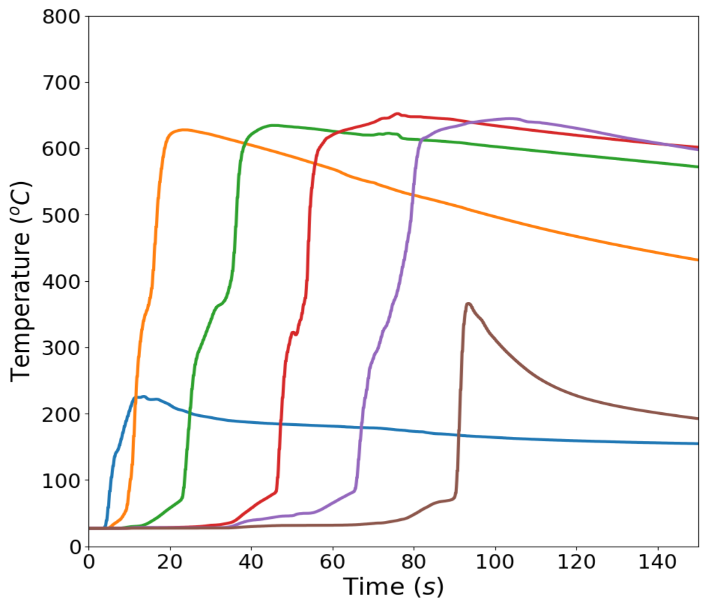
Propagation data from Sandia (Lamb, et al. (2015) and Torres-Castro) for 5 x cells.

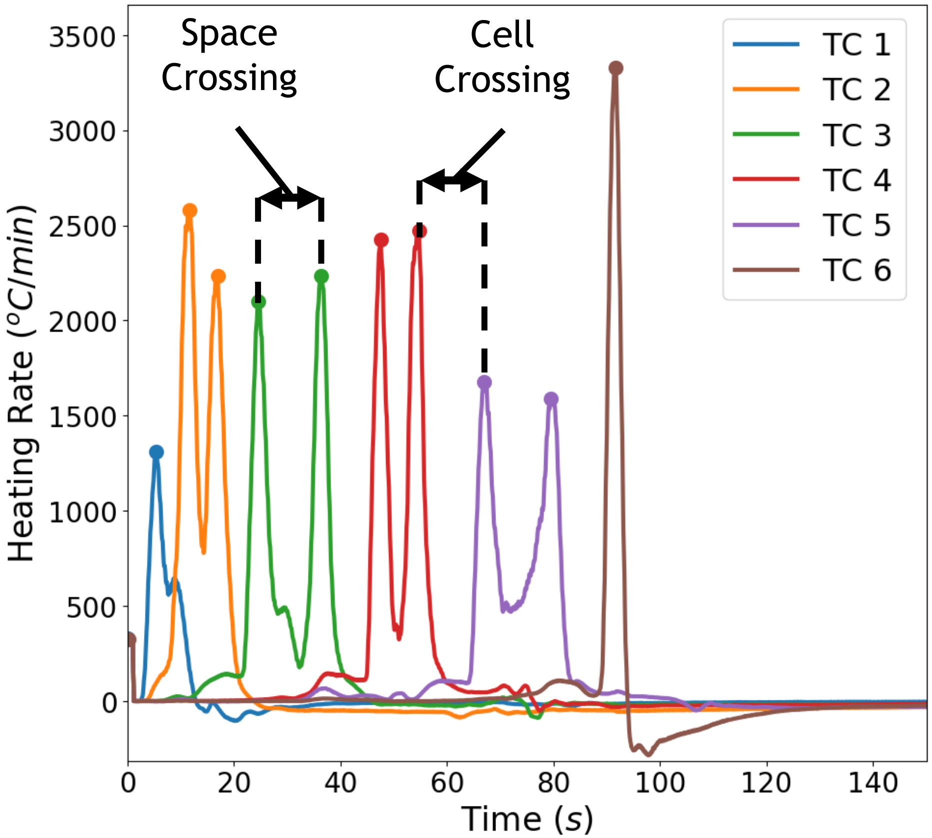
Extracted heating rate from thermocouples.

Peak heating rates → cell thermal runaway



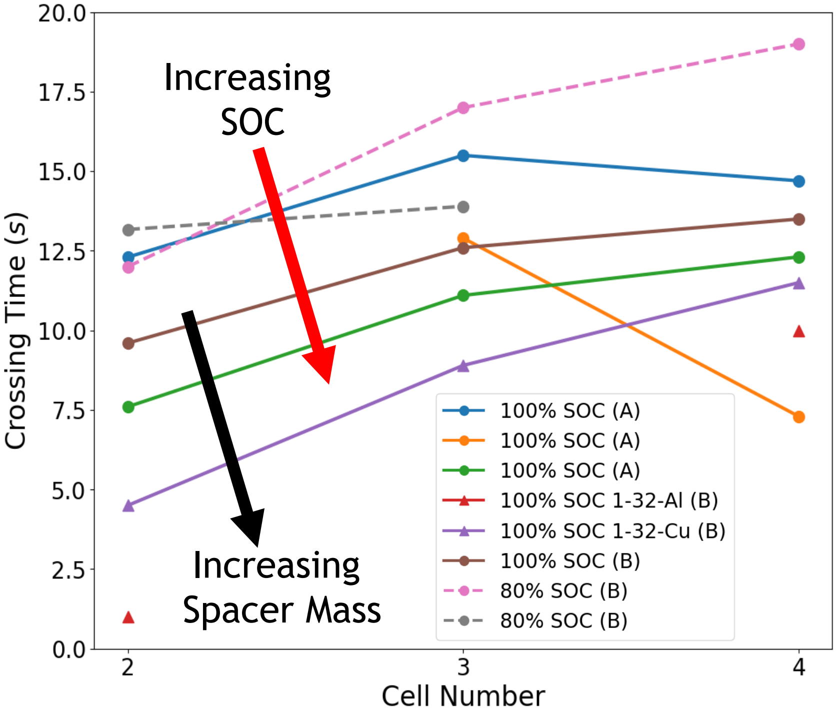
Measured temperatures in cascading failure: Time separation associated with intercell-thermal resistance



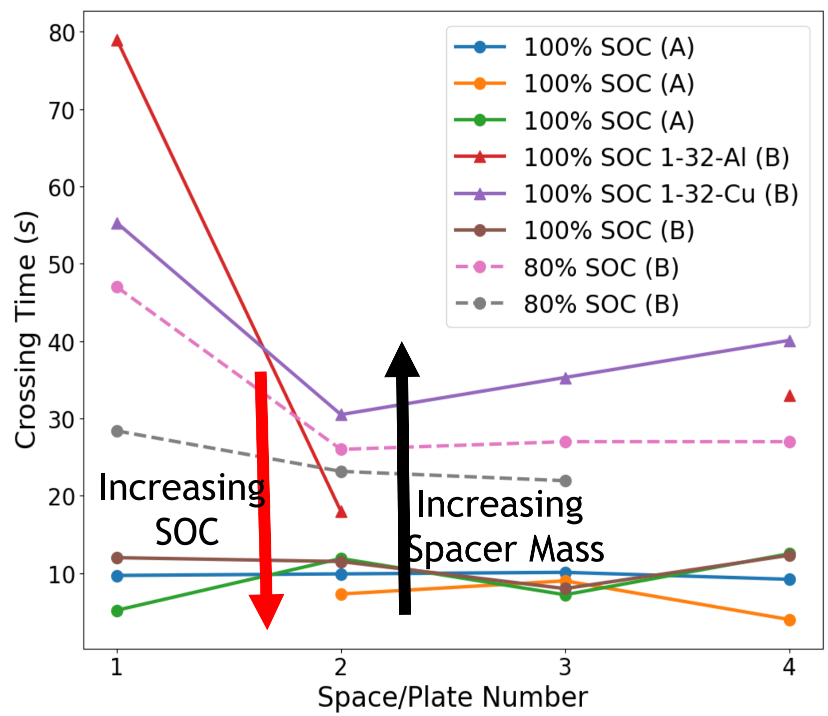


Data mining: cell crossing and gap crossing times.

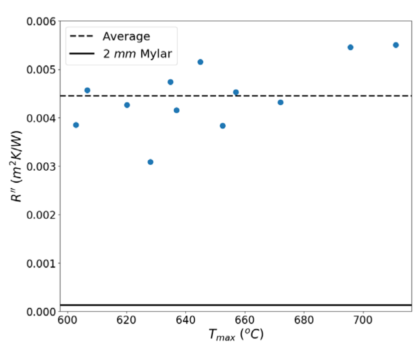
Timing for propagation front to cross a single pouch cell



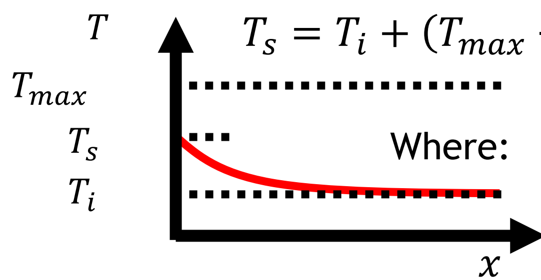
Timing for propagation front to cross spacers



- Using measured T_{max} and Δt_{lag}, compute contact resistance, R''



$$T_s = T_i + (T_{max} - T_i)[1 - \exp(\eta^2)\,\mathrm{erfc}(\eta)]$$



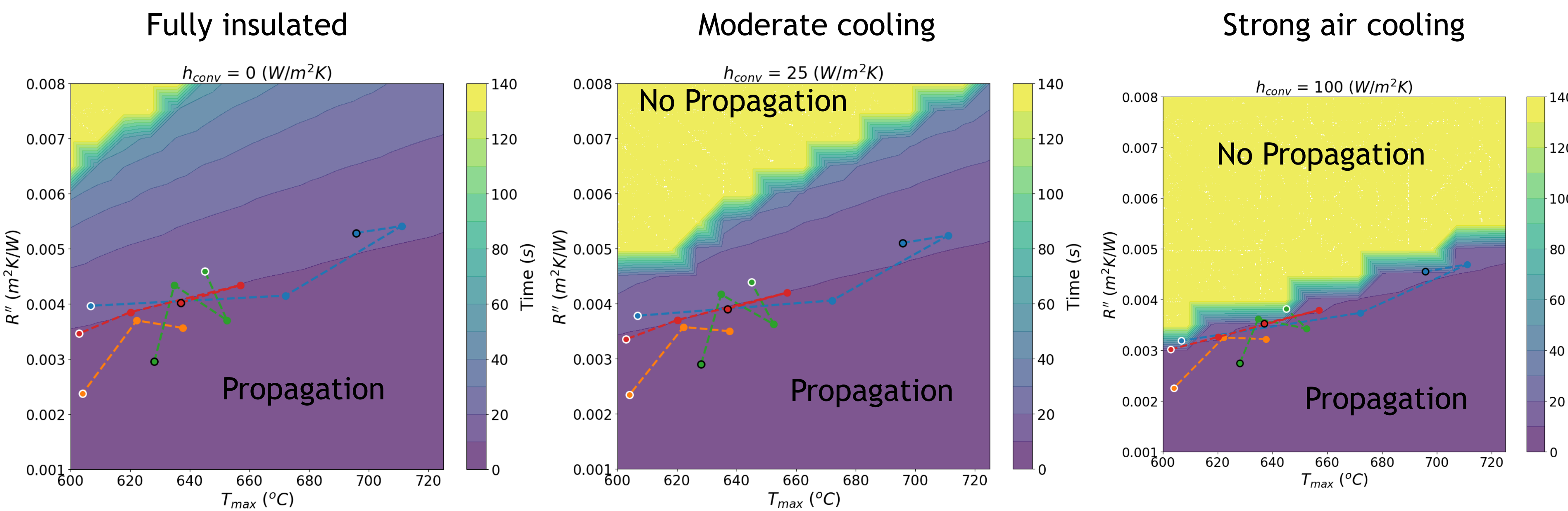
Where: $\eta = \frac{h\sqrt{\alpha t}}{k}$ and $R'' = \frac{1}{h}$

Limits of cascading thermal runaway

Including cooling defines propagation limits: Finite-element heat-transfer model

Model maps delay in propagation: yellow region is infinite delay—*failure to propagate*.

- R” is thermal resistance between cells - enhanced by spacers in experiments.
- T_{max} is indication of total heat release -depends on SOC



Convection cooling and conduction through stack results in failure to propagate for some scenarios.

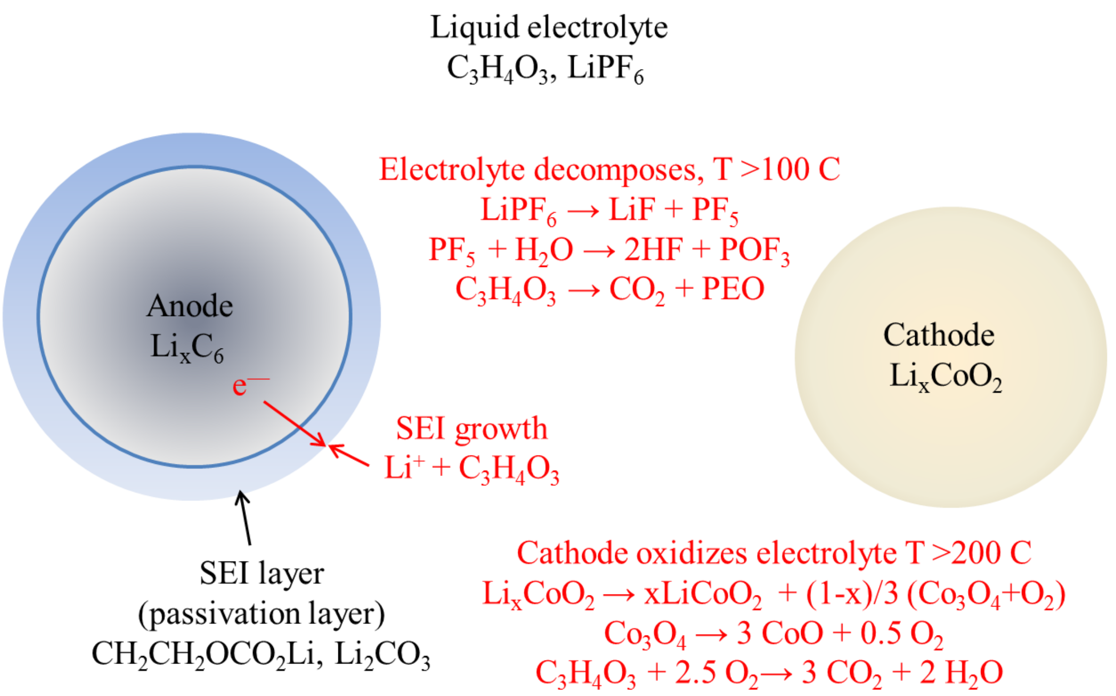
Consider cost tradeoff : cooling versus thermal resistance.

The drive to greater energy density and efficiency

Increased energy densities and other material advances lead to more reactive systems – greater efficiency / less losses.

- Charged batteries include a ‘fuel’ and ‘oxidizer’ all internally.

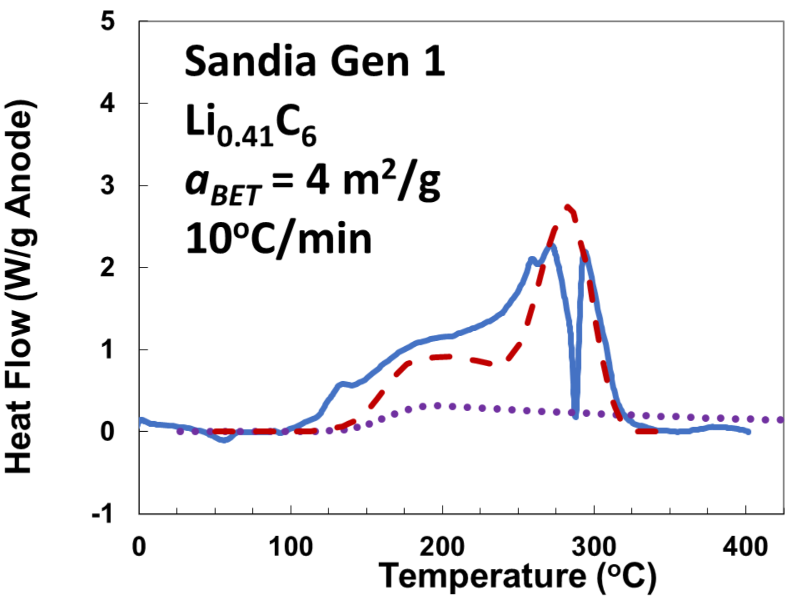
- Li-Ion electrolyte, packaging, and other materials are often flammable.
- External heating or internal short circuits can lead to thermal runaway.

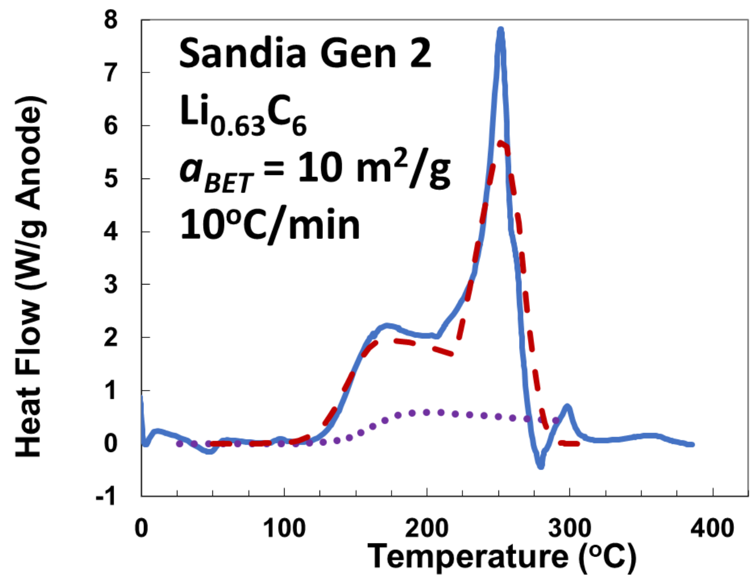


Anode-electrolyte calorimetry suggests several regimes during thermal runaway: initiation, plateau and runaway

- Anode-electrolyte reactions generate heat:
  - could raise cell temperatures ≈650°C
  - Nominal reaction:

$$2LiC_6 + EC(liq) \rightarrow 2C_6 + C_2H_4(g) + Li_2CO_3(cr)$$





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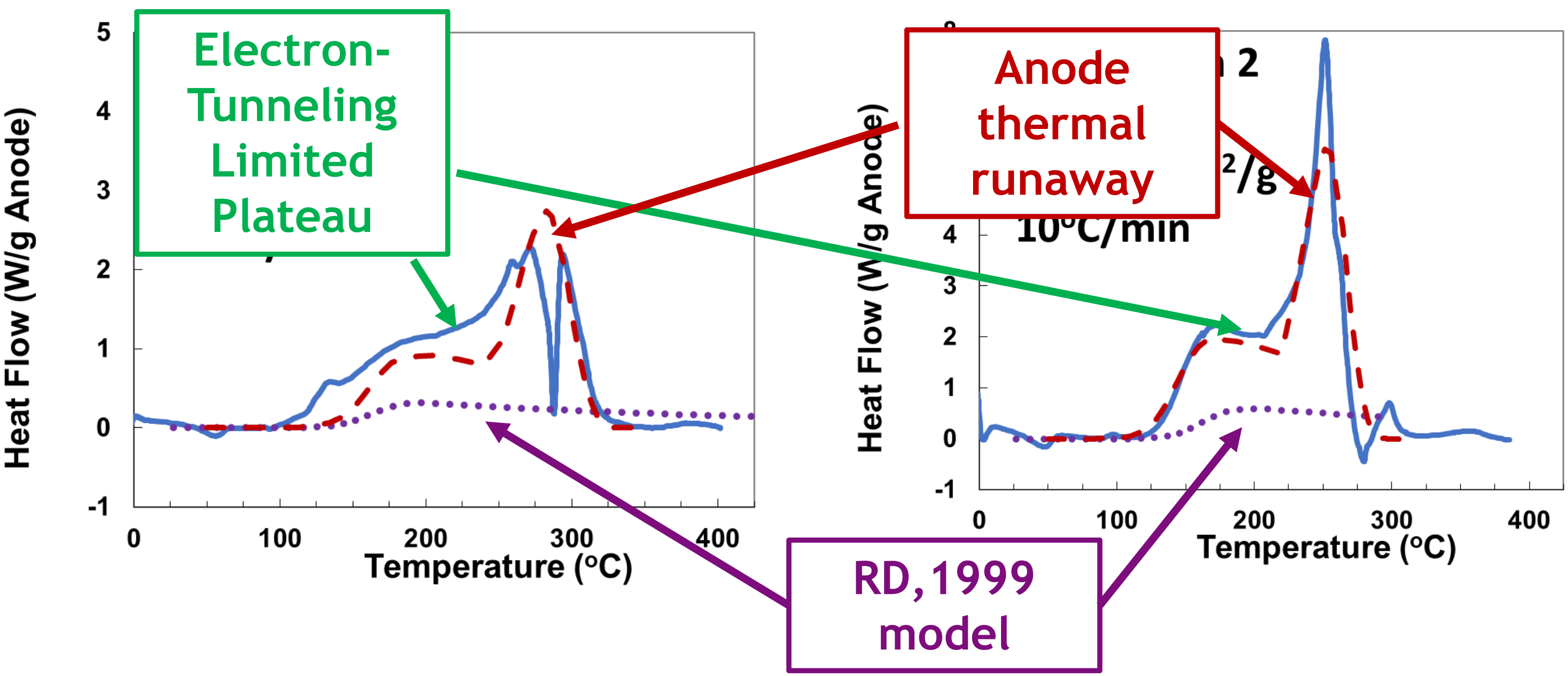


A comprehensive model for anode-electrolyte thermal runaway

$$-\frac{dx_{\mathrm{i}}}{dt} = x_{\mathrm{i}} \overbrace{\frac{a_e}{a_0}}^{\text{Edge Area Effect}} \overbrace{\frac{m_E}{(m_{50}+m_E)}}^{\text{Limiting Electrolyte}} A_2 \exp\left(-\frac{E_2}{RT}\right) \overbrace{\exp(-z_t)}^{\text{Electron-Tunneling Limiter}}$$

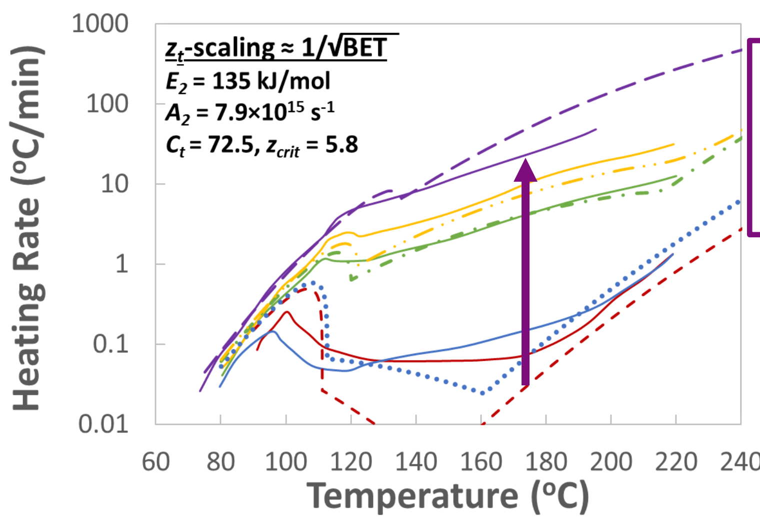
$$\overbrace{\frac{dz_t}{dt}}^{\text{Barrier Growth}} = -\frac{dx_i}{dt} \overbrace{\frac{C_t}{\left(\frac{a_{BET}}{a_0}\right)^{n_t}}}^{\text{Variable Area Effect}} \text{ for } \overbrace{z_t < z_{crit}}^{\text{Critical Barrier}}, \text{and } \overbrace{\frac{dz_t}{dt} = 0}^{\text{Allows Acceleration}} \text{ otherwise}$$

$$\mathrm{Q}\,[W/g] = -\frac{dx_{\mathrm{i}}}{dt}\frac{\Delta H_{rxn}}{W_a}$$

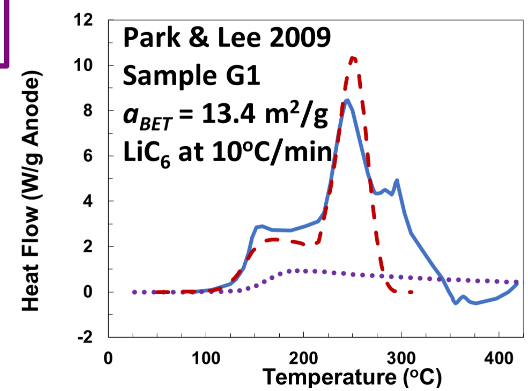
Heat Release with new ΔH_{rxn}

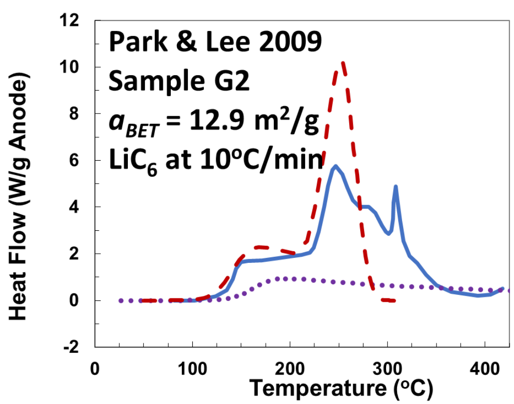
More predictions with comprehensive model:

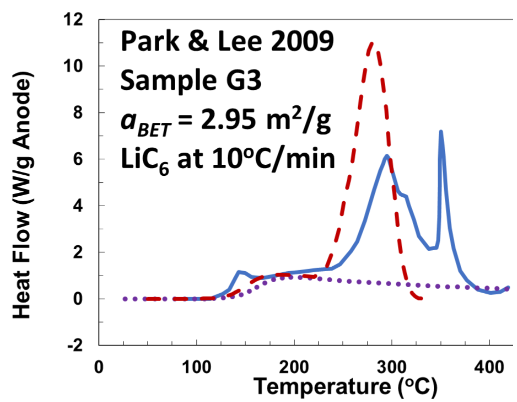
Predicting the full range of behavior over a range of particle sizes

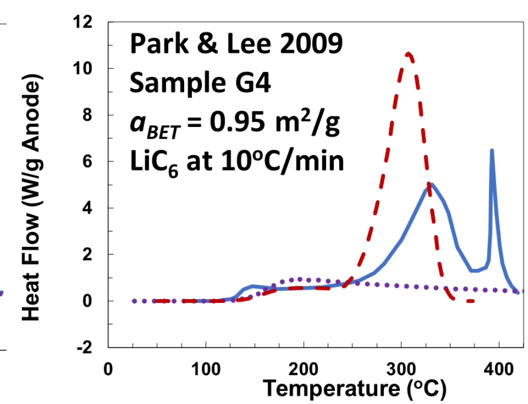


Increasing specific area





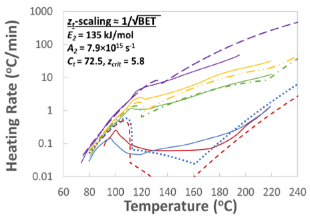


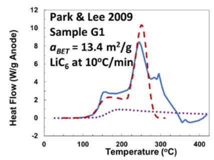


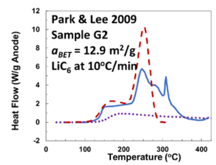
Increasing specific area

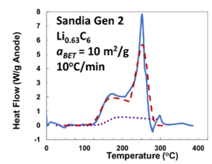
MANY predictions with comprehensive model: 24 x DSC, 5 x ARC

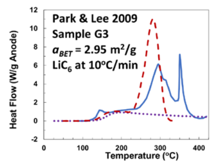
Shown earlier

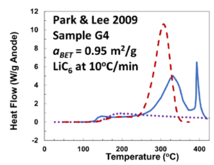


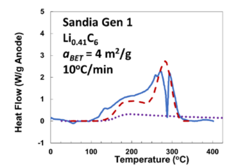




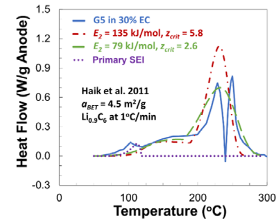


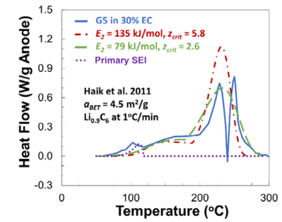


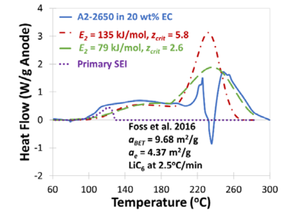


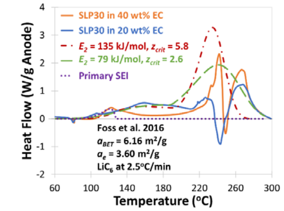


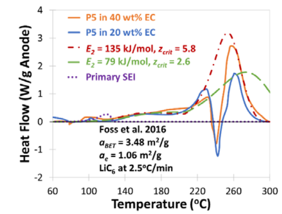
Detailed area measurements

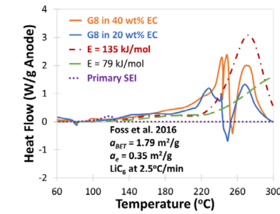




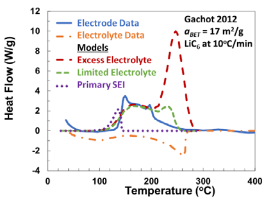


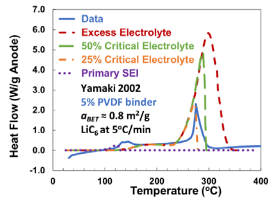


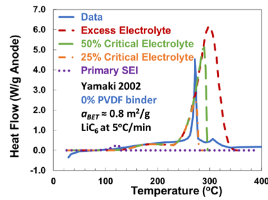




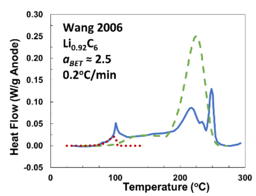
Limiting Electrolyte

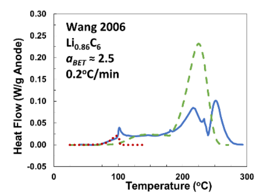


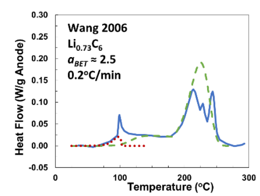


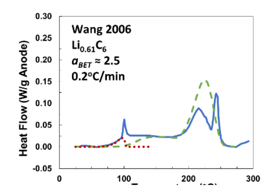


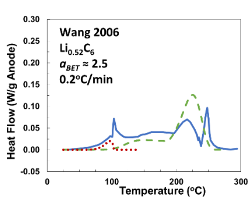
State of Charge

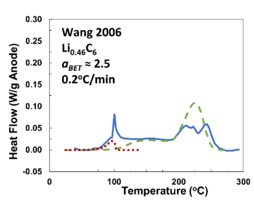


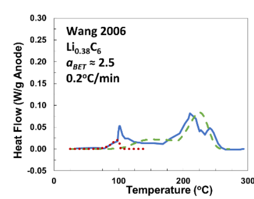


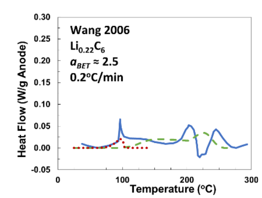


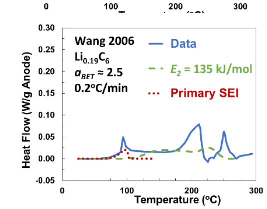




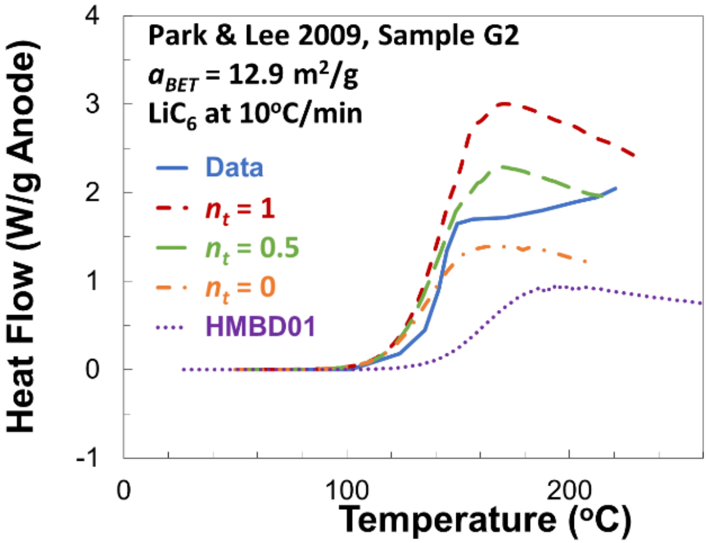


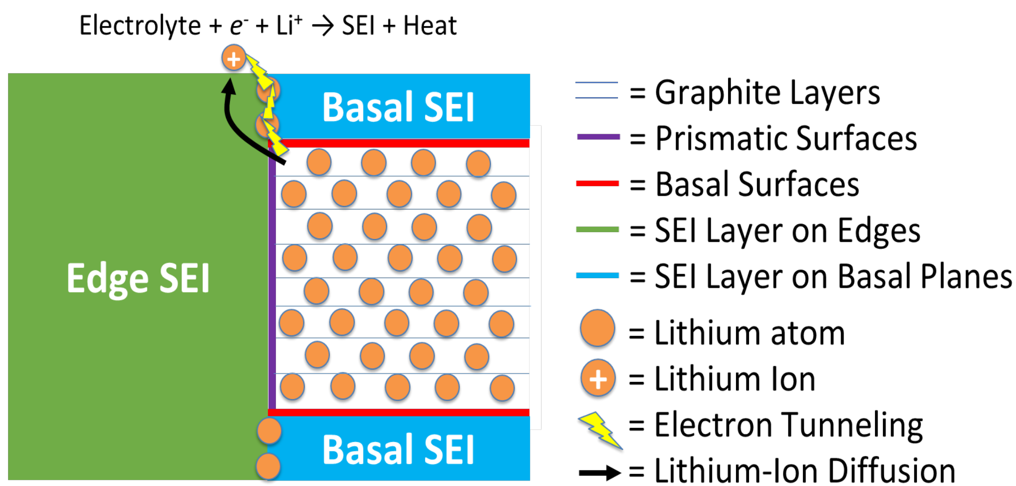






What have we learned from initiation and plateau regime? Area dependence



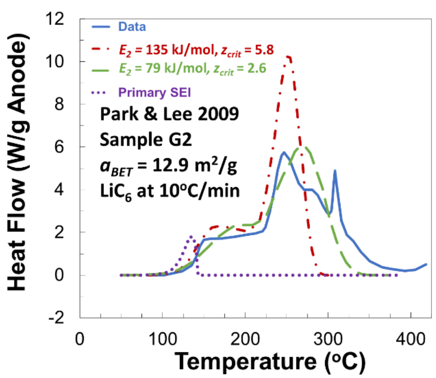


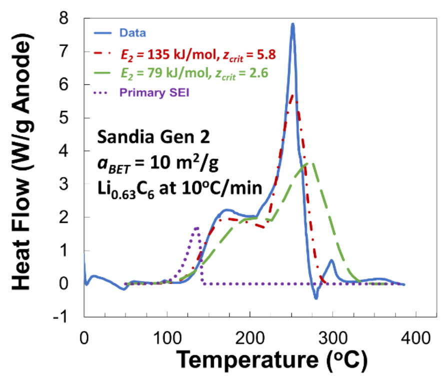
a) Prismatic and basal SEI differ in composition and thickness
b) Defect formation favored at grain boundaries and/or the basal-prismatic interface
c) Defects include neutral Li atoms and other features that promote tunneling
d) Tunneling barrier is inversely proportional to the length of the defect-rich interfaces

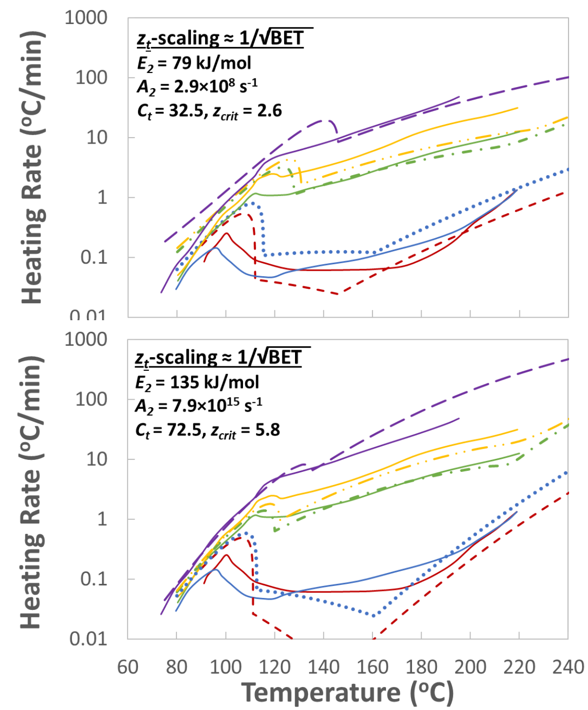
- Surface reaction rates correlated with super-linear edge-area scaling.
- Dependence of sqrt(area) for tunneling barrier suggests uneven coverage:
  - Likely linear structures involved
  - Other theoretical studies suggest neutral Li atoms in grain boundaries.

What have we learned about temperature dependencies? Activation energies, Tunneling barrier limits?

- Range of activation energies provide reasonable results in the plateau regime,
- Runaway and initiation are characterized by activation energies near 135 kJ/mol.







- Runaway well correlated by an area-dependent fraction of delithiation.
  - Not exactly a set temperature.
  - Endothermic exfoliation is sometimes observed/suspected.
  - Strains in 1.5% to 2% range: theoretical results suggest increased tunneling defects.

Publications and presentations

Journal Papers

- R. Shurtz, J. Engerer, J. C. Hewson, "Predicting high-temperature decomposition of lithiated graphite with electrolytes: I. Review of phenomena and a comprehensive model," submitted to Journal of the Electrochemical Society, September, 2018.
- R. Shurtz, J. Engerer, J. C. Hewson, "Predicting high-temperature decomposition of lithiated graphite with electrolytes: II. Predicting passivation layer evolution and the role of surface area," submitted to Journal of the Electrochemical Society, September, 2018.

Other Publications

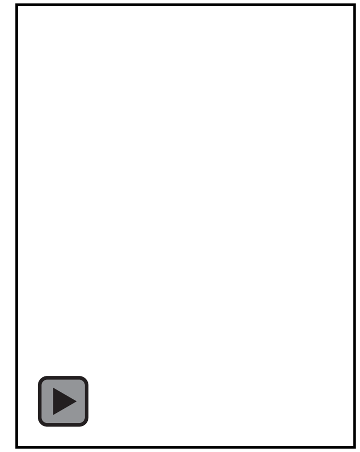
- J. C. Hewson, J. Lamb, W.-J. Lee, "Electrochemical energy storage and safety," in Battery Storage Systems. IEEE white paper, 2018.

Presentations at Technical Meetings

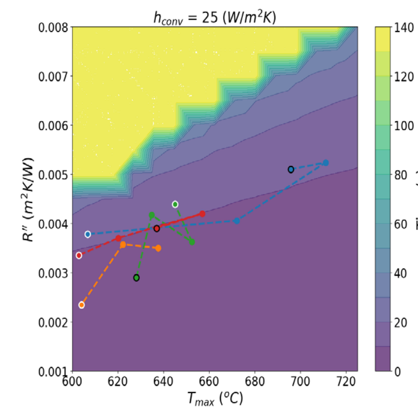
- (Invited) J. C. Hewson, "Energy storage material choices to avoid thermal runaway in lithium-ion batteries," Material Research Society Fall Meeting, November 29, 2017
- (Invited) J. C. Hewson, "Modeling the limits of thermal runaway in Li-ion packs and designing tests to measure those limits," Joint Army Navy NASA Air Force meeting, Special Fire Science Session, December 4, 2017.
- J. C. Hewson, R. Shurtz, "Predictive modeling for energy-storage safety in abnormal thermal scenarios," DOE-OE Energy Storage Peer Review Meeting, San Diego, CA, Oct. 10, 2017.
- J. C. Hewson, R. Shurtz, "Computer modeling to understand and prevent initial and cascading thermal runaway," Electrical Energy Storage Applications and Technologies, San Diego, CA, Oct. 12, 2017.
- R. Shurtz, J. C. Hewson, "Modeling Cascading Failure of Thermal Runaway in Stacks of Li-Ion Pouch Cells with Variation in Cooling Attributes," 233rd Electrochemical Society Meeting in Seattle, Washington, May 15, 2018.
- R. Shurtz, J. C. Hewson, "Modeling Thermochemical Sources for a Broader Range of Materials and Conditions," 233rd Electrochemical Society Meeting in Seattle, Washington, May 14, 2018.

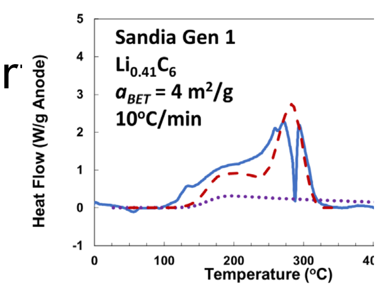
In closing

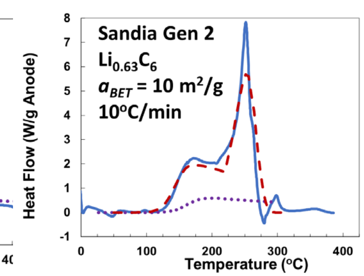
- Thermal runaway is a risk and potential barrier to development and acceptance.
- Heat release rates are moderate relative to potential dissipation.
- Multi-physics thermal models are identifying critical ignition and propagation trends.
- Quality measurements are key to parameter identification.
- Progress this term
  - Mitigate cascading failure through contact resistance.
    - Estimate contact resistance from measurements.
    - Identify cascading failure limits: cooling versus thermal resistance.
  - Anode-electrolyte modeling:
    - Relate chemical source to fundamental mater properties.
    - Predict high-temperature processes.



Moderate cooling







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