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UNDERSTANDING THE THERMAL BEHAVIOR AND SAFETY OF SILICON-GRAPHITE ANODES

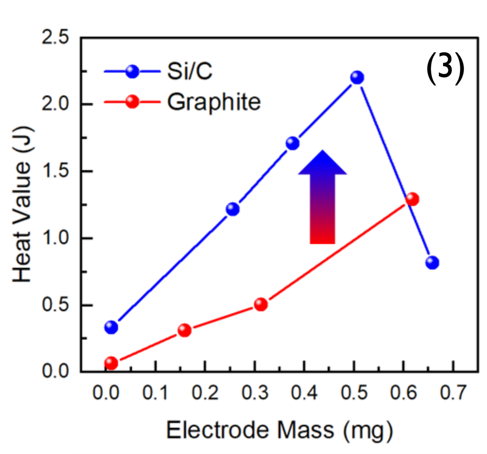
Bryan R. Wygant,[1*] Randy Shurtz,[2] Loraine Torres-Castro[3]

[1]Nanoscale Sciences, [2]Fire Science and Technology, [3]Power Sources Research and Development, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA,
*bwygant@sandia.gov

Background

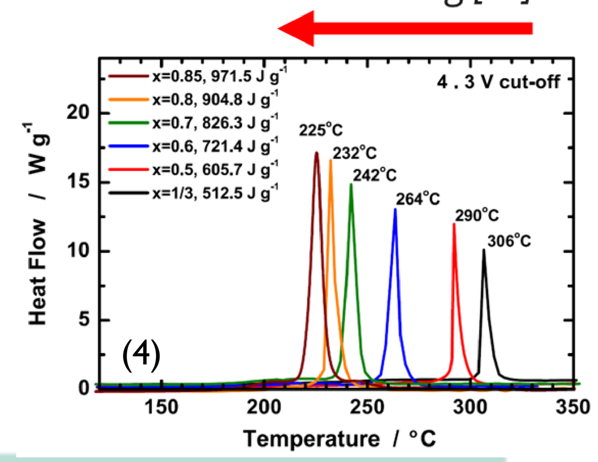
Project Goal	Use ***microcell safety testing*** to understand how Si content impacts the ***safety of Si/graphite anodes*** when paired with an energy dense cathode and balance safety and performance.
Current Practice	Large format batteries subjected to destructive tests require larger quantities of materials and infrastructure to safely conduct, ***slowing the rate at which testing proceeds.***
Why SNL?:	SNL has ***established expertise in many forms of battery testing*** and staff with experience in microcell safety testing.
Innovation	This work ***bridges the gap*** between small-scale electrode-only safety testing and full-cell testing, ***improving the speed and efficiency of safety testing***. Earlier work from SNL has demonstrated the value of this approach.
Impact	These results will be interesting to: battery scientists, safety researchers, and battery manufacturers. This provides ***foundational knowledge to improve the safety of two emerging battery chemistries.***
Alignment	This ***innovative*** microcell approach improves our ability to study the safety of emerging battery chemistries, improving the ***security*** and ***reliability*** of future energy technologies. Inherently safer batteries reduce cost, allowing for the development of more ***affordable*** energy storage technologies.

Before they're commercialized, can we determine the relative safety during thermal runaway for Si/graphite||NMC811 batteries?

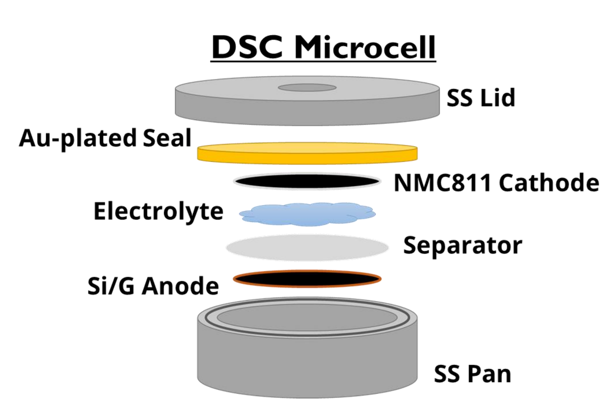


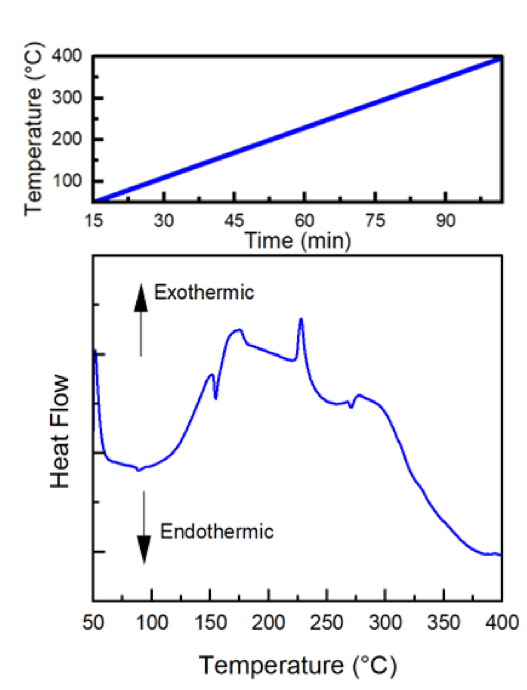
Increased energy density could be detrimental to safety in event of failure

Increasing [Ni]



DSC Analysis and Microcells



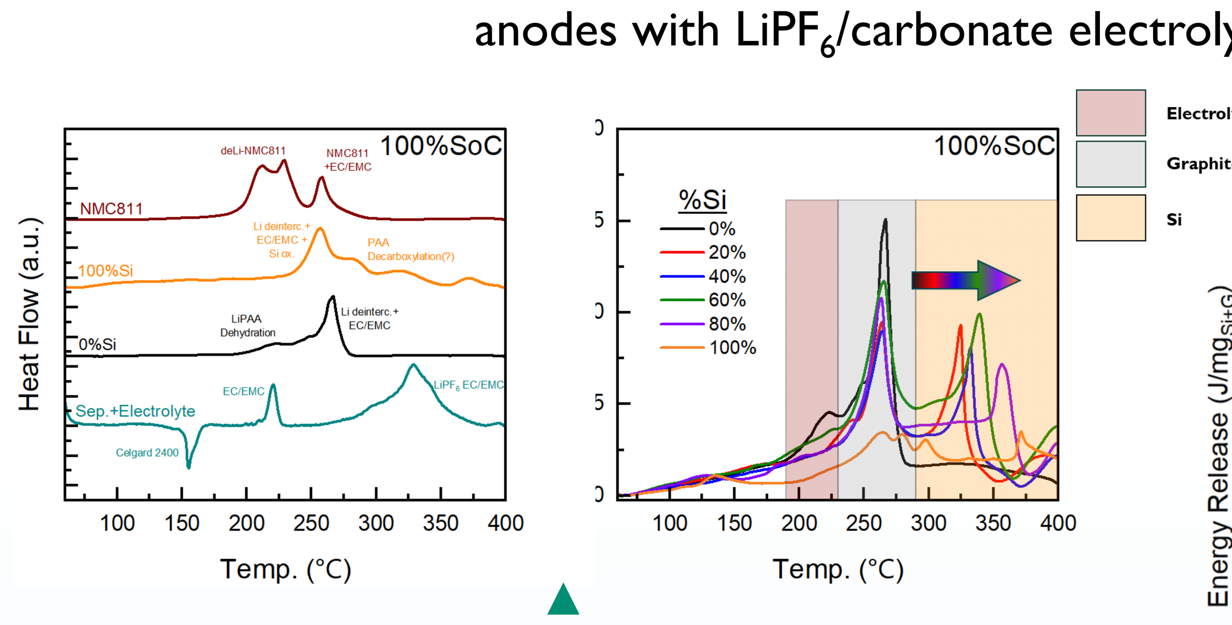


Differential Scanning Calorimetry (DSC)

Increase external temperature of sample sitting on thermocouple;
measure amount of heat required to increase the temperature of the sample relative to a reference

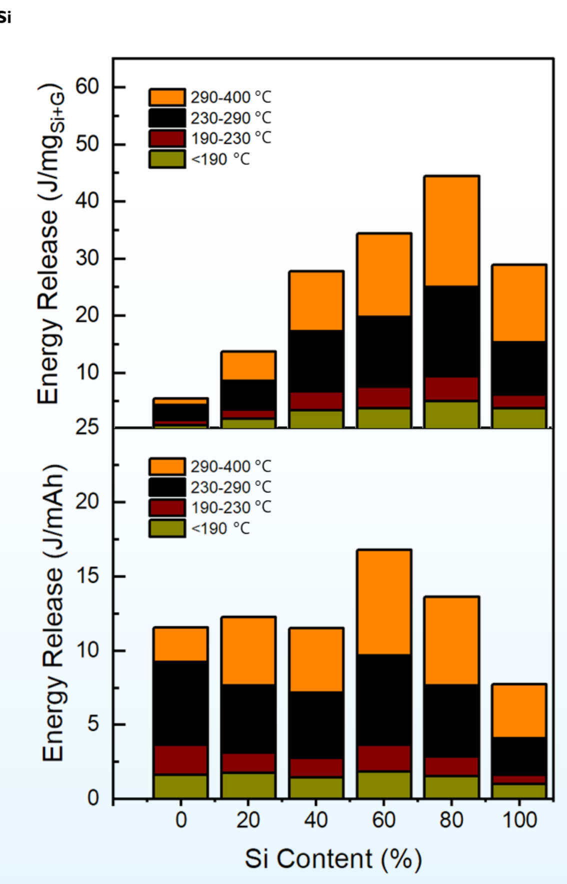
Electrode DSC Results

Began by testing thermal response of 100% chemically lithiated Si/G anodes with $LiPF_6$/carbonate electrolyte



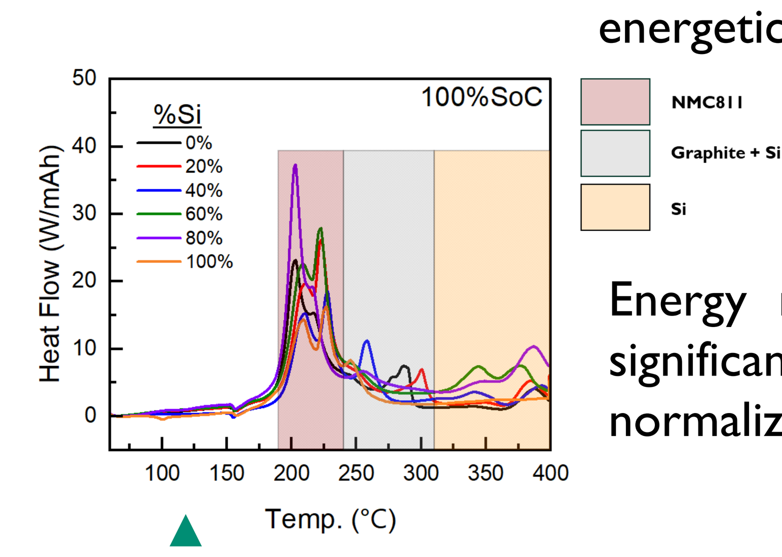
Li-C and Li-Si show similar response at ~260°C, but an additional peak >300°C is visible in the composites

Energy Release plateaus or peaks around 60% Si, with most release from the lower temperature peak



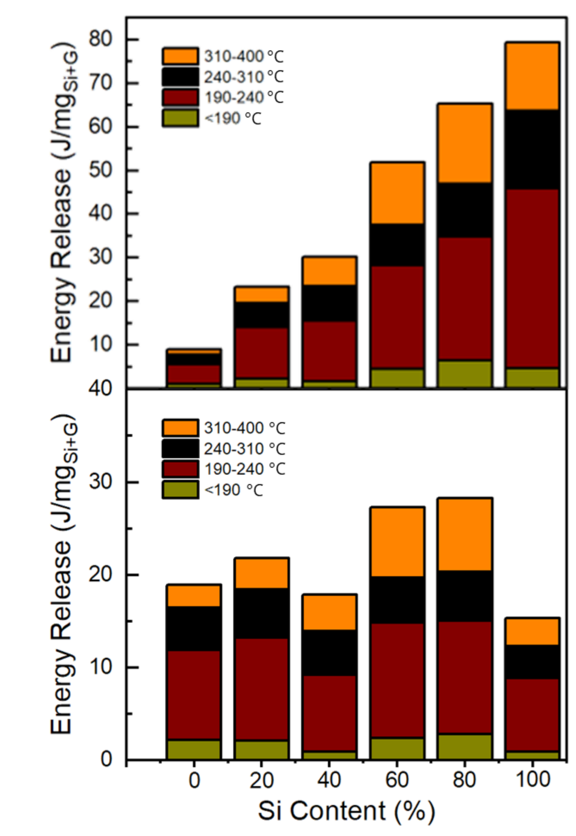
Microcell DSC Results

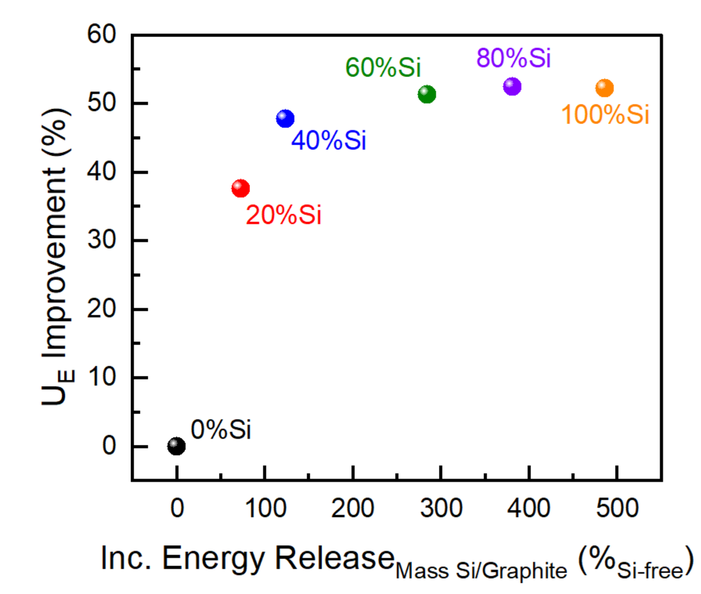
Microcells containing Si/G, NMC811, polymer separator, and electrolyte show more energetic responses



Microcells similar to electrodes, but most of the heat flow occurs during NMC811 and electrolyte decomposition

Energy release differs significantly based on normalization



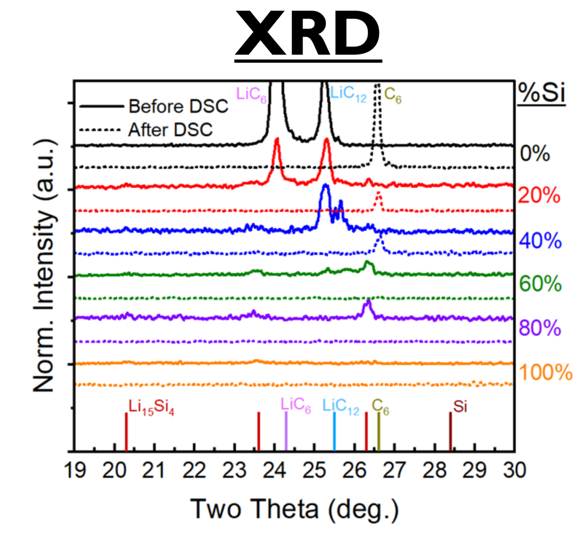


By energy released (relative to graphite) against the % improvement in energy density (U_E), we can determine that **20-40% Si** provides *best* balance of safety and performance

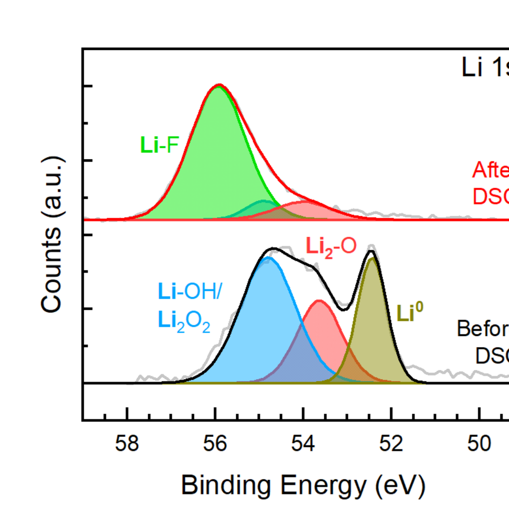
See Randy Shurtz's poster for modeling of the DSC behavior of Si/G anodes/microcells!

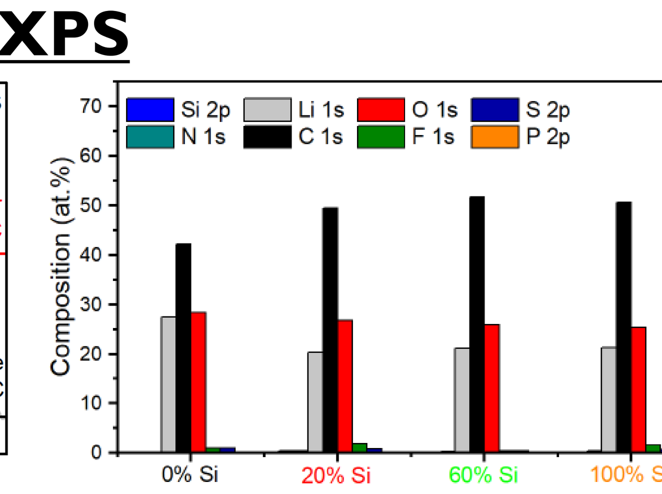
Materials Characterization

XRD

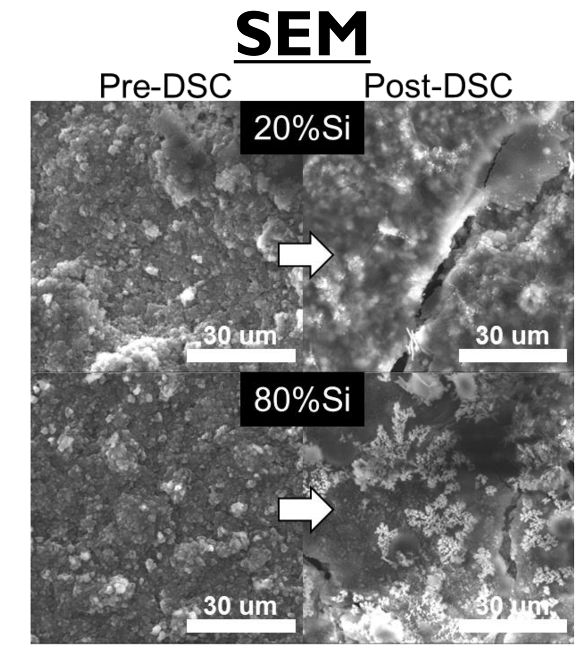


XPS





SEM



X-ray diffraction spectroscopy (XRD) confirms presence of fully- and partially-lithiated graphite in the samples before DSC

X-ray photoelectron spectroscopy (XPS) confirms the presence of reduced Li in the samples, and a native surface rich in C, Li, and O

Scanning electron microscopy (SEM) shows formation of thick surface coating following DSC testing of anodes

Conclusions + Future Directions

1. DSC and microcells offer a robust means of determining the relative safety (related to thermal release) of Si/G vs. NMC811 batteries at small scale
2. Comparison of DSC from electrodes-only and microcell results highlights need for materials-level analysis and impact of normalization metrics
3. 20-40 %Si shows best balance of improved energy density relative to thermal release

Where next?

- Explore impact of Si/G ratios on the thermal behavior of larger format batteries (e.g., 18650 cells and accelerated rate calorimetry)
- Expand to alternative cathode chemistries (e.g., $LiFePO_4$, $Li(NiCoAl)O_2$, etc.) to explore interplay between cathode and Si/G

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