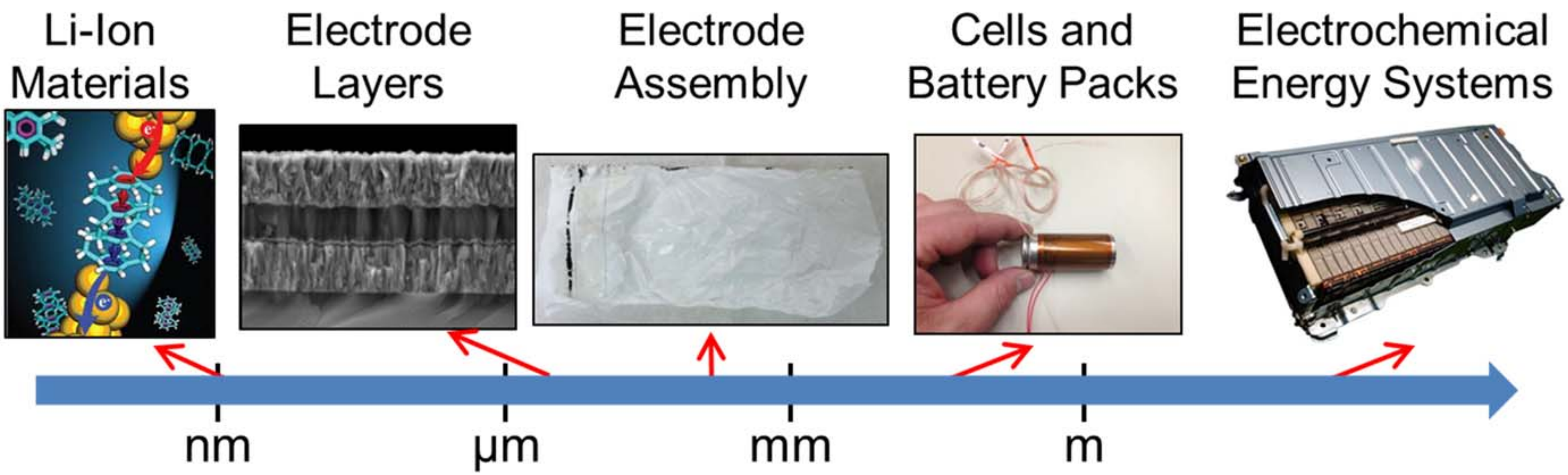
Safety of Li-ion Batteries: A Thermal Engineering Perspective



Ankur Jain

Assistant Professor

Mechanical and Aerospace Engineering Department

The University of Texas at Arlington

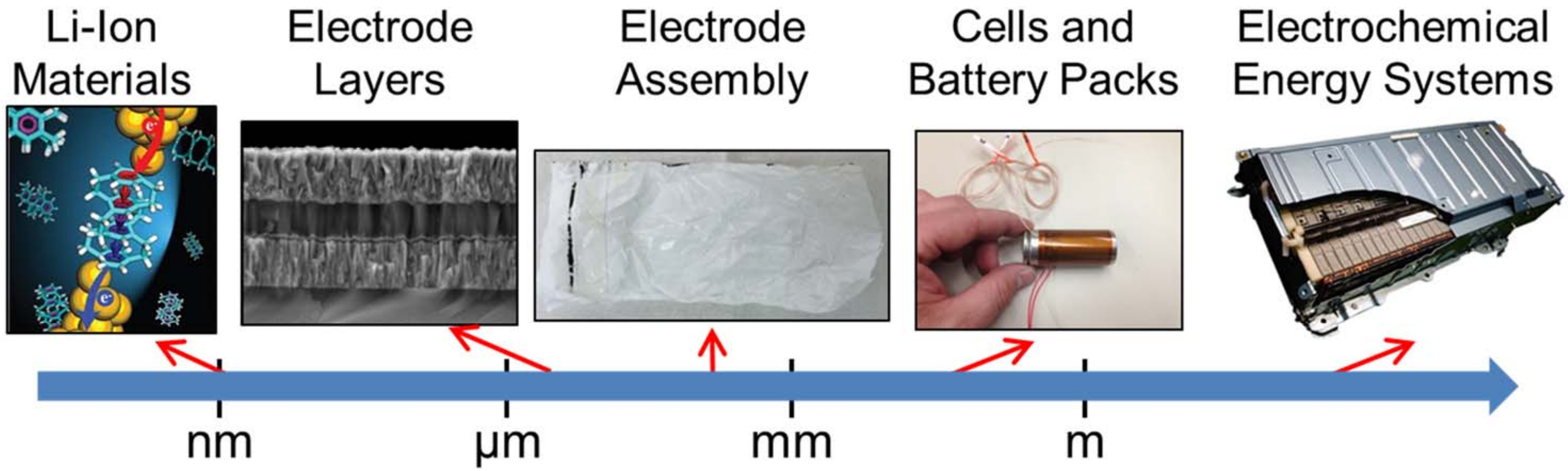
Email: jaina@uta.edu, Web: www.uta.edu/mtl/

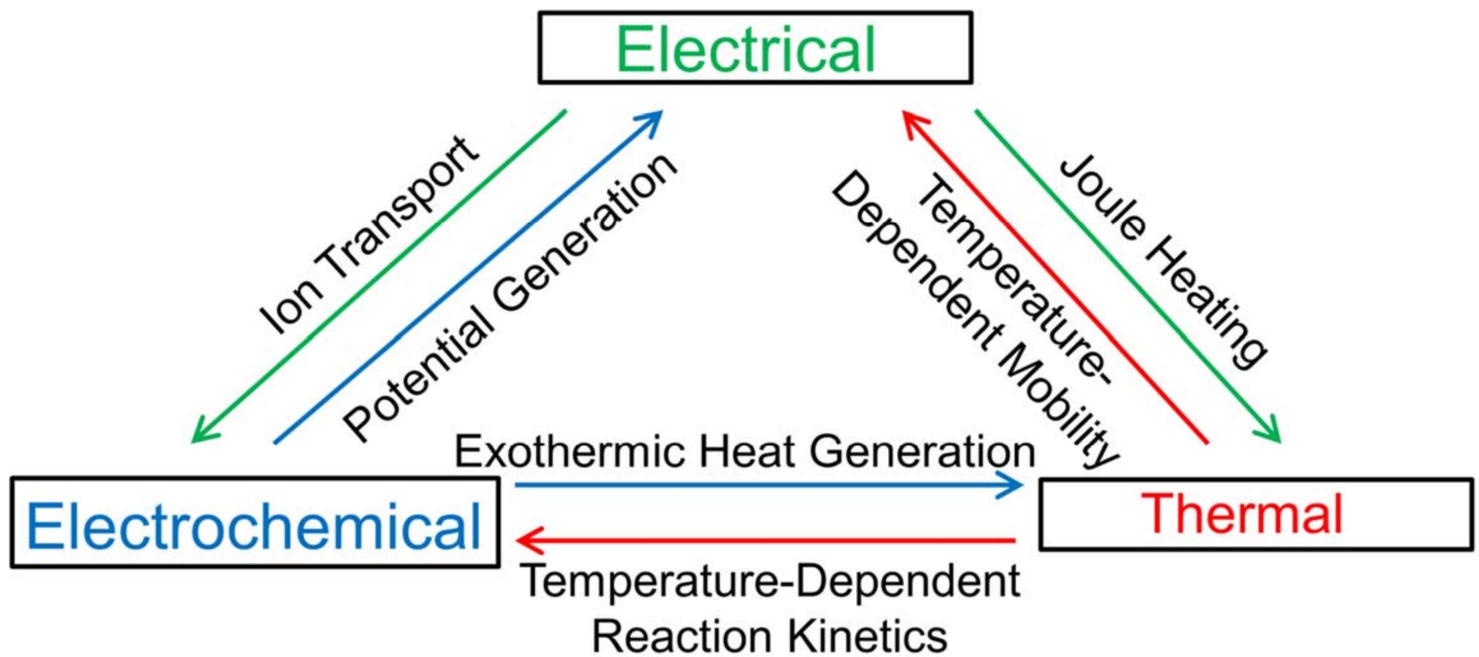
Microscale Thermophysics Laboratory at UTA

- Mission: To Understand and Optimize Heat Transfer in Engineering and Biological Materials, Processes and Systems.
- Research directions: Thermal Measurements and Modeling, Electrochemical Energy Conversion & Storage, Microscale Heat Transfer.
- Sponsors:

NSF · Office of Naval Research Science & Technology (ONR) · Department of Energy · IUSSTF · MICROFABRICA · ORAU · INVENTEK CORPORATION

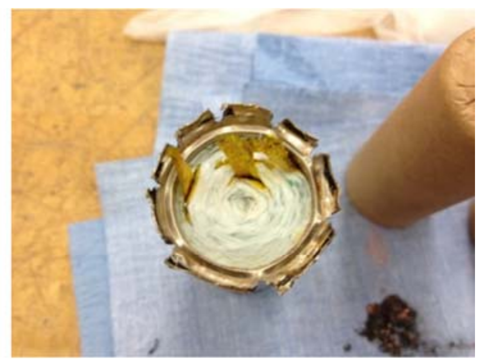
Li-ion Cell: A Multiphysics Multiscale System

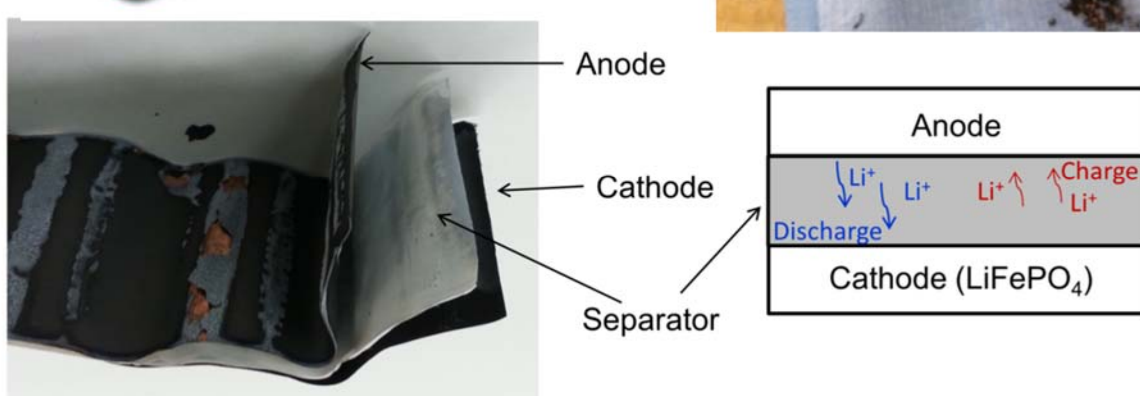




Thermal Concerns in Li-ion Batteries

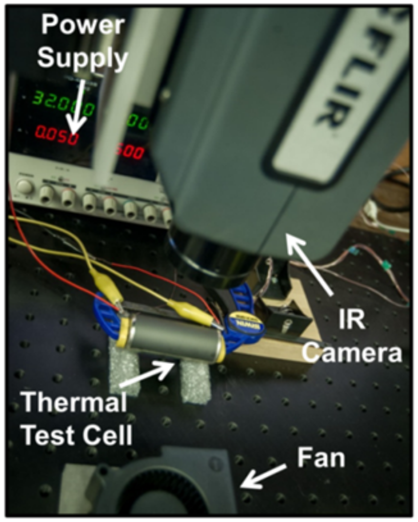
- <u>Fundamental Heat Transfer Questions of Much Practical Relevance</u>:
    - How much heat is generated in a Li-ion cell and how?
    - What is the nature of thermal conduction through the Li-ion cell?
    - How does one optimize heat generation and conduction processes?
    - How does one thermally interrogate the cell?
    - How does one reconcile thermal and electrochemical trade-offs?



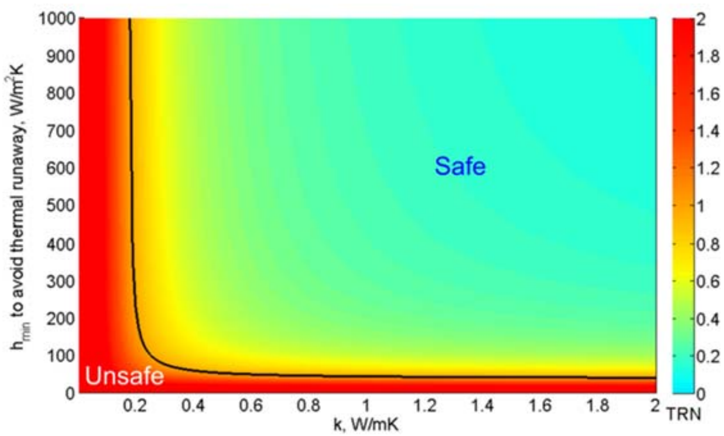


Outline

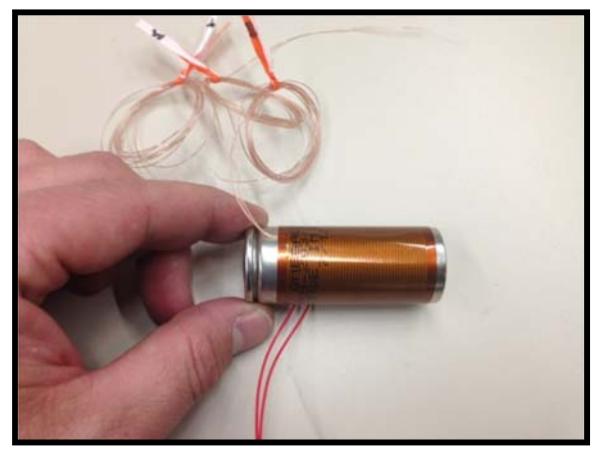
1. Non-invasive core temperature measurement
(Thermal x-ray)



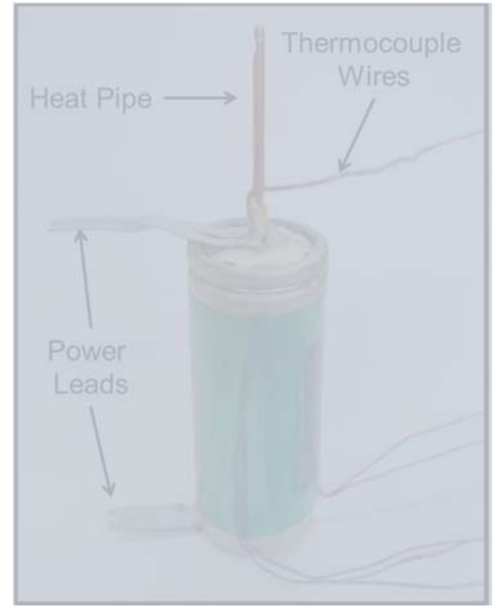
2. Prediction of thermal runaway
(When is a battery at risk of exploding?)



3. Material-level thermal transport measurements
(Why does a cell get so hot?)

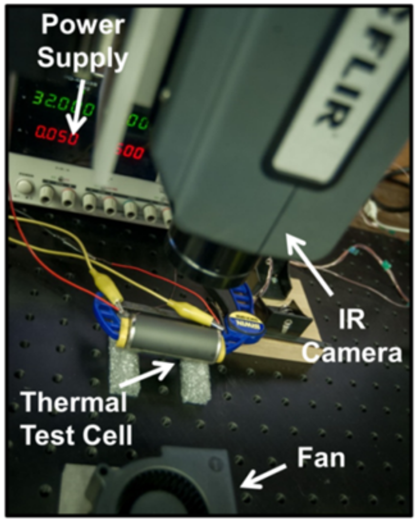


4. Heat pipe based cooling
(How to passively cool a cell)

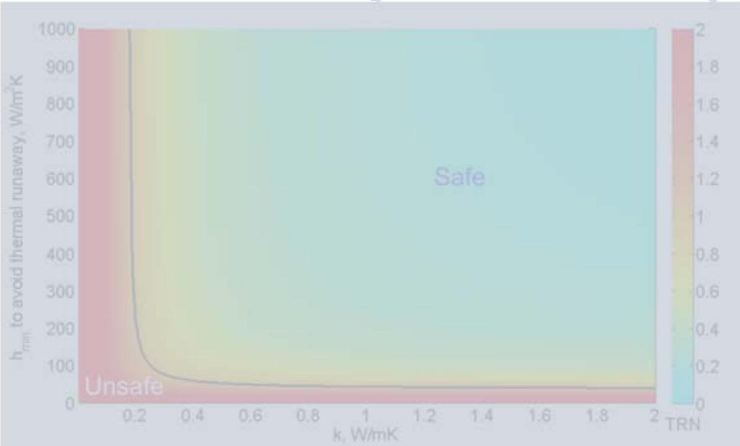


Outline

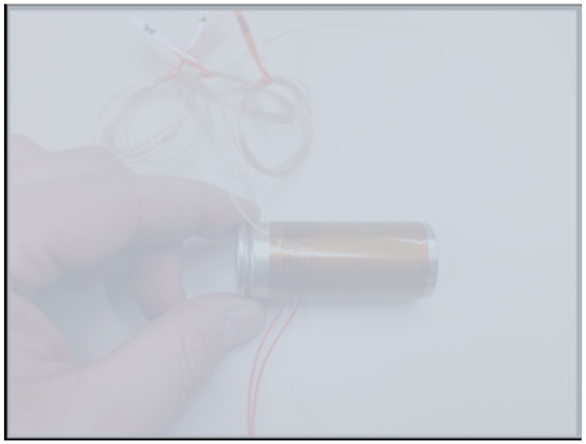
1. Non-invasive core temperature measurement
(Thermal x-ray)



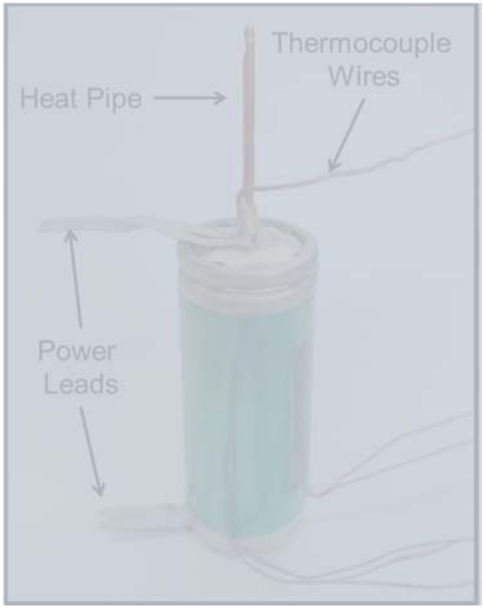
2. Prediction of thermal runaway
(When is a battery at risk of exploding?)



3. Material-level thermal transport measurements
(Why does a cell get so hot?)



4. Heat pipe based cooling
(How to passively cool a cell)

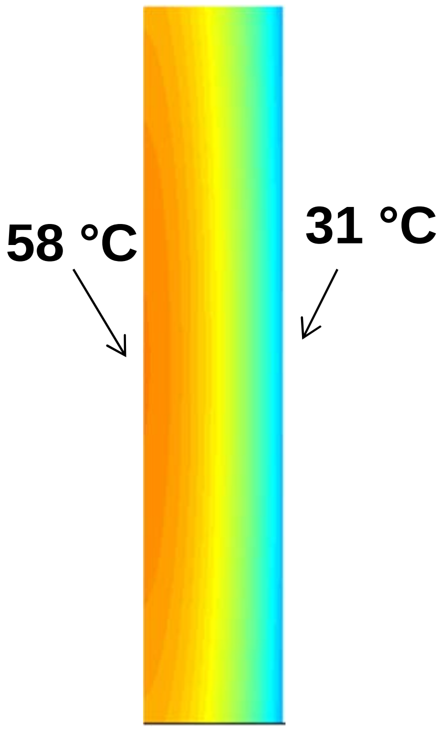


Measurement of Internal Temperature

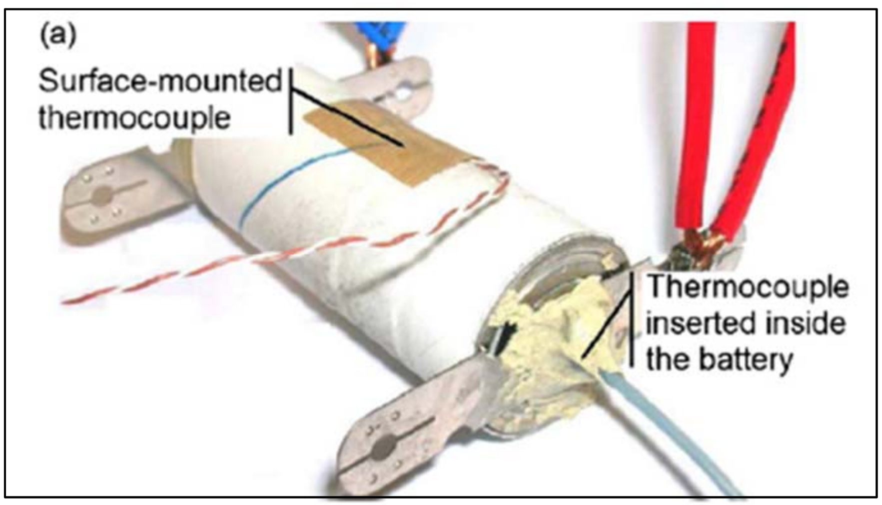
- Surface temperature measurement is a poor indicator of core temperature.

- A non-invasive method for core temperature measurement is very desirable.

- Such ‘x-ray’ capability exists for other physical properties such as stresses, but not for temperature.



Shah, *et al.*, *J Power Sources*, 2014



Forgez, *et al.*, *J Power Sources*, 2010

Anthony, *et al.*, *J Power Sources*, in review, 2016

Non-Invasive Core Temperature Measurement

- We have shown that the core temperature of a heat-generating cylinder in steady state is given by

$$T_{core} = \frac{1}{2\pi}\int_0^{2\pi} T_0(\theta)\,d\theta + \frac{QR^2}{4k_r}$$

where $T_0(\theta)$ is the temperature around the outside surface of the cylinder.

- Similarly, in transient conditions, we have shown that

$$T_{core}(t) = T_{1,core}(t) + T_{2,core}(t) = \left[\frac{QR^2}{4k_r} + \sum_{n=1}^{\infty} A_n \exp\left(-\alpha_r \lambda_{0n}^2 \cdot t\right)\right] + \sum_{n=1}^{\infty} B_{0n}(t)$$

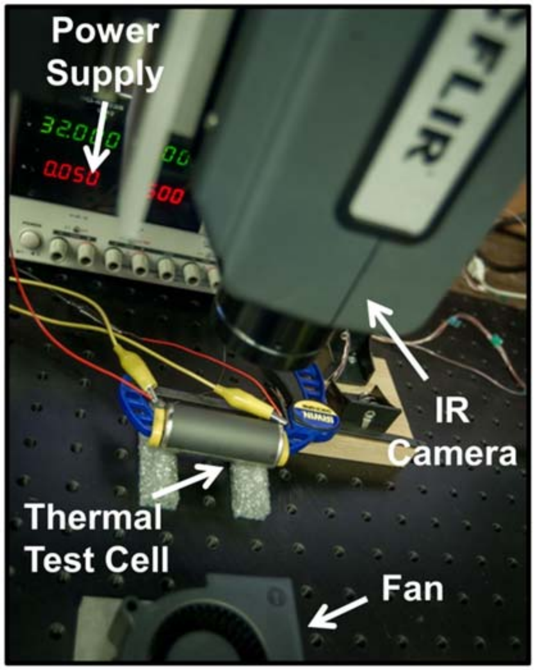
where
$$A_n = \frac{-\frac{Q}{4k_r}\int_0^R \left(R^2 - r^2\right)\cdot rJ_0\left(\lambda_{0n} r\right)dr}{N_{r,n}} \quad B_{0n}(t) = \frac{\alpha_r \lambda_{0n} R J_1\left(\lambda_{0n} R\right)}{N_{r,n}}\int_0^t w_{0I}(\tau)\exp\left[-\alpha_r \lambda_{0n}{}^2 (t-\tau)\right]d\tau \quad w_{0I}(\tau) = \frac{1}{2\pi}\int_0^{2\pi} T_0(\theta,t)\,d\theta$$

- These equations show that the core temperature can be determined using appropriate integrals of measured surface temperature, either in steady state or in transient.

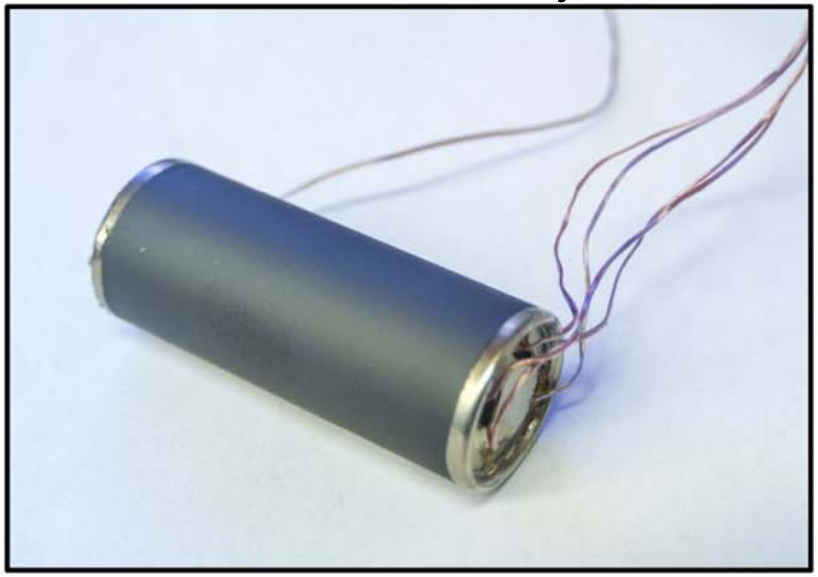
Anthony, *et al.*, *Int. J. Heat Mass Transfer*, 2016
Anthony, *et al.*, *Sci. Rep.*, 2016

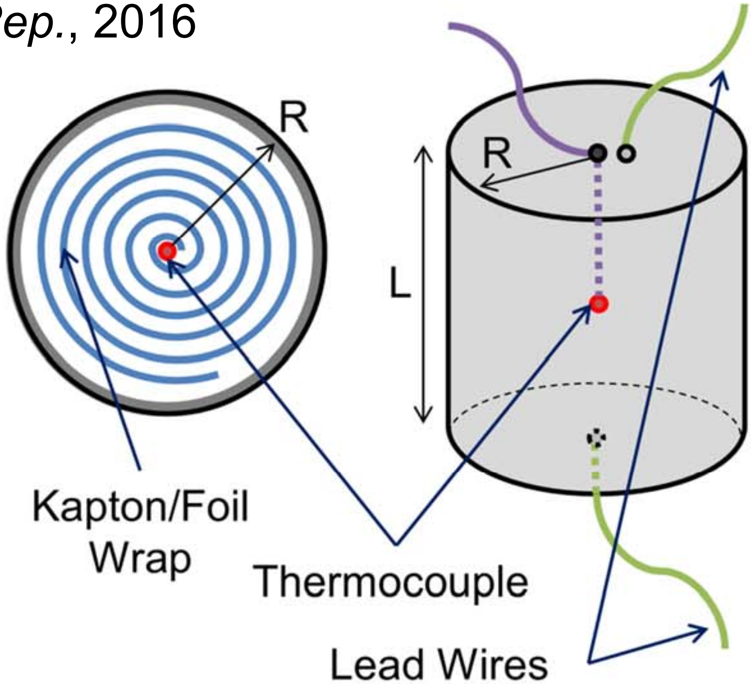
Non-Invasive Core Temperature Measurement

- A thermal test cell similar in construction and thermal properties as a 26650 Li-ion cell.
- IR camera for surface temperature measurement.
- Theoretical models from last slide used to determine T_{core} and $T_{core}(t)$ in various operating conditions.
- Embedded core thermocouple for measurement validation.



Anthony, *et al.*, *Int. J. Heat Mass Transfer*, 2016
Anthony, *et al.*, *Sci. Rep.*, 2016



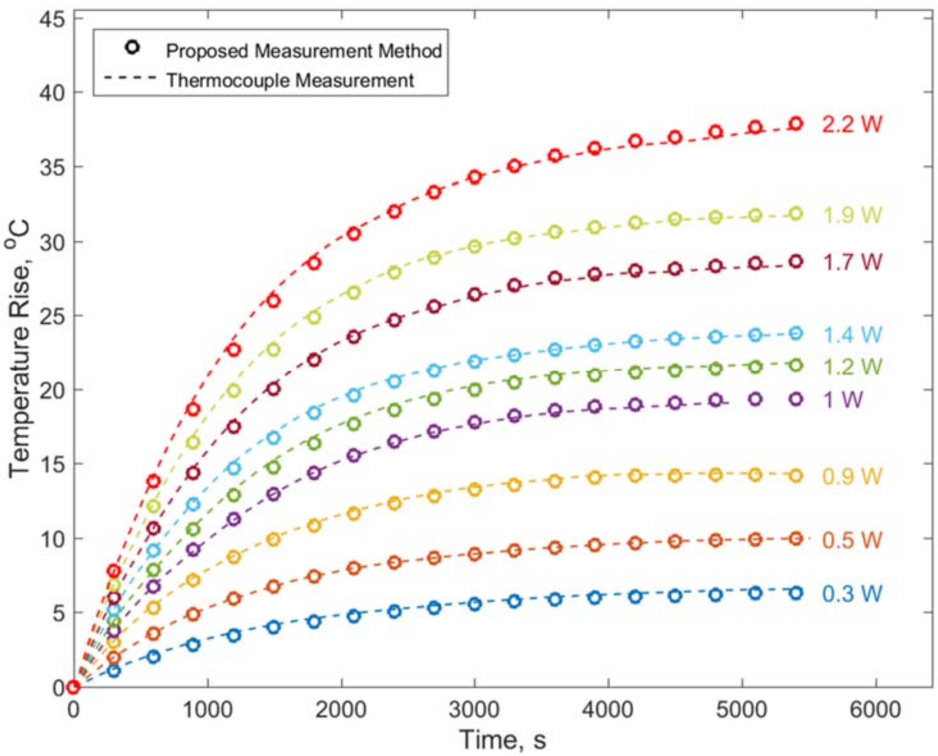


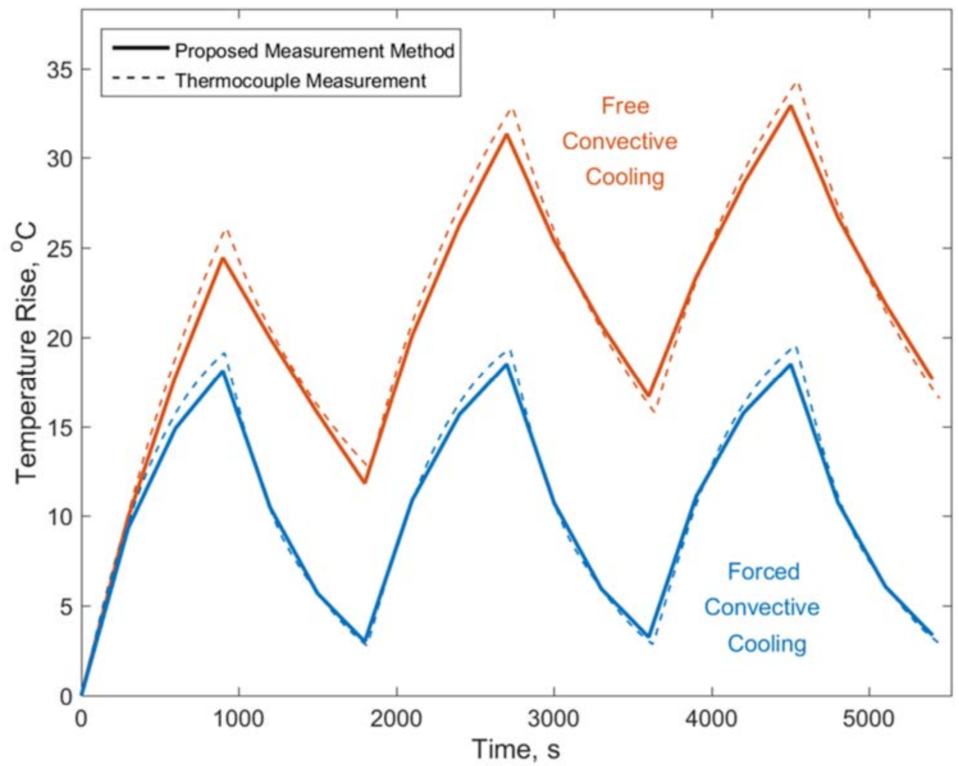
Non-Invasive Core Temperature Measurement

- Very good agreement between this measurement method and measurement from embedded thermocouple.

- Able to capture temperature at steady-state and during transients.

- Good agreement for ON-OFF type of heating typical for cyclic charge/discharge.



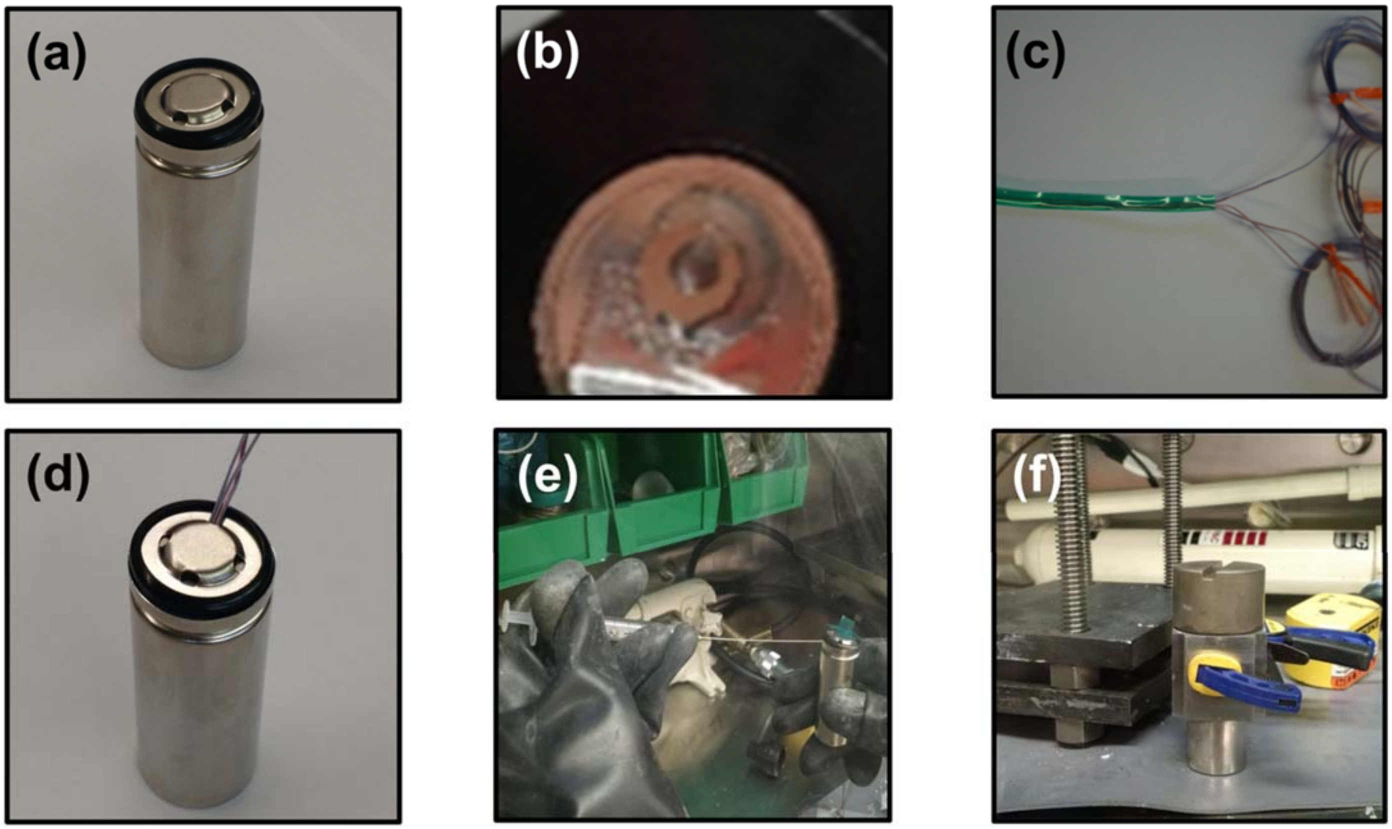


Anthony, *et al.*, *Int. J. Heat Mass Transfer*, 2016
Anthony, *et al.*, *Sci. Rep.*, 2016

Core Temperature Measurement in a Li-ion Cell

• 26650 Li-ion cells with embedded thermocouples were assembled .

• Internal temperature was predicted during realistic discharge processes and validated against embedded thermocouple measurements.



Fabrication Steps

Final Cell

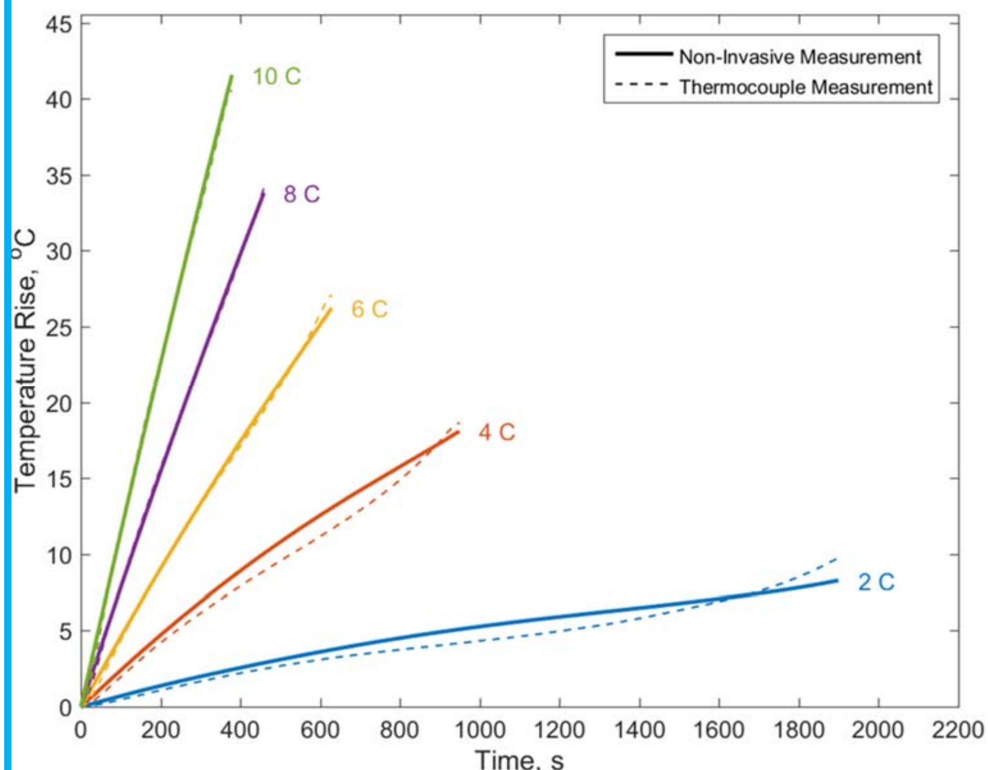
Anthony, *et al.*, *Int. J. Heat Mass Transfer*, in review, 2017

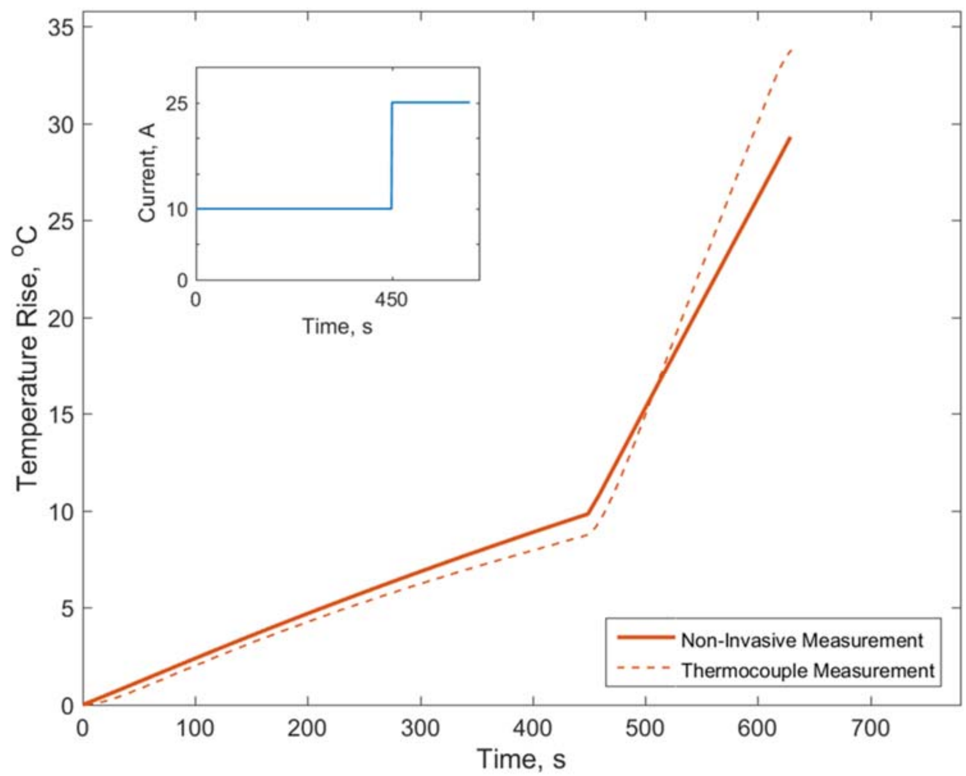
Measurements on 26650 Li-ion Cell

- Core temperature is measured on a 26650 cell instrumented with an internal thermocouple, up to 10C discharge rate.

- Good agreement between predicted temperature and internal thermocouple measurement over entire discharge period.

- We are working towards core temperature prediction during thermal runaway.



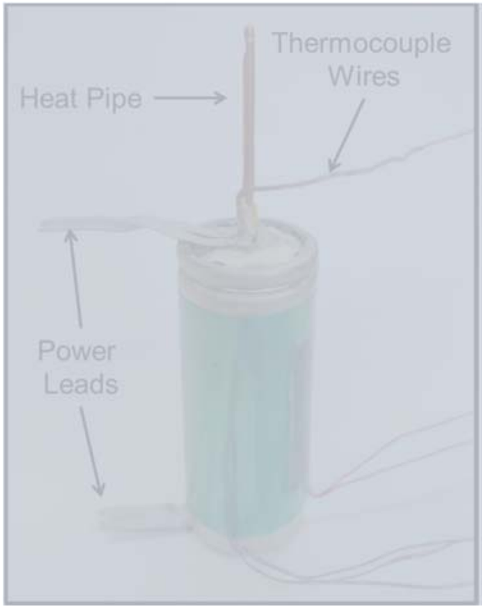


Anthony, *et al.*, *Int. J. Heat Mass Transfer*, in review, 2017

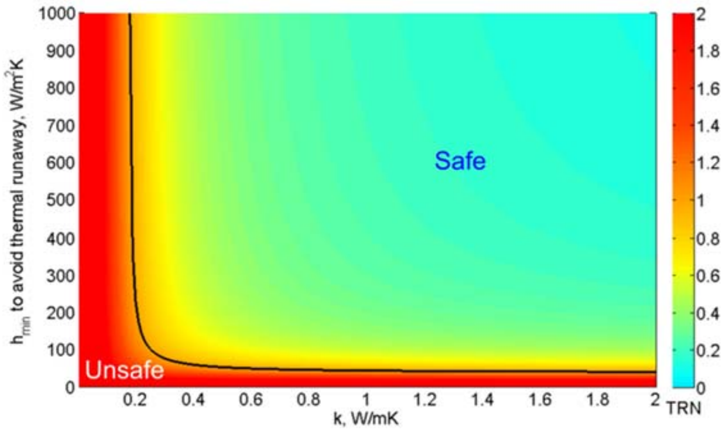
Outline

1. Non-invasive core temperature measurement *(Thermal x-ray)*

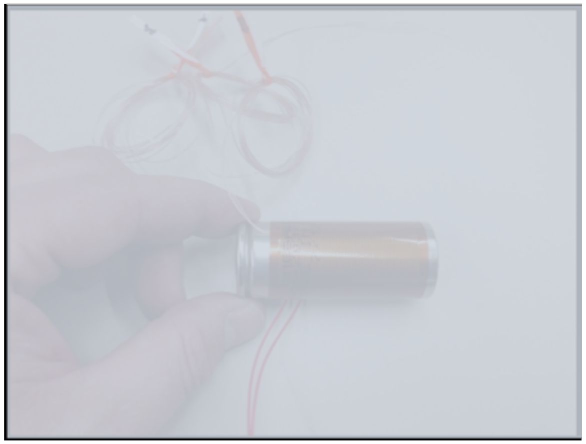
4. Heat pipe based cooling *(How to passively cool a cell)*



2. Prediction of thermal runaway
(When is a battery at risk of exploding?)

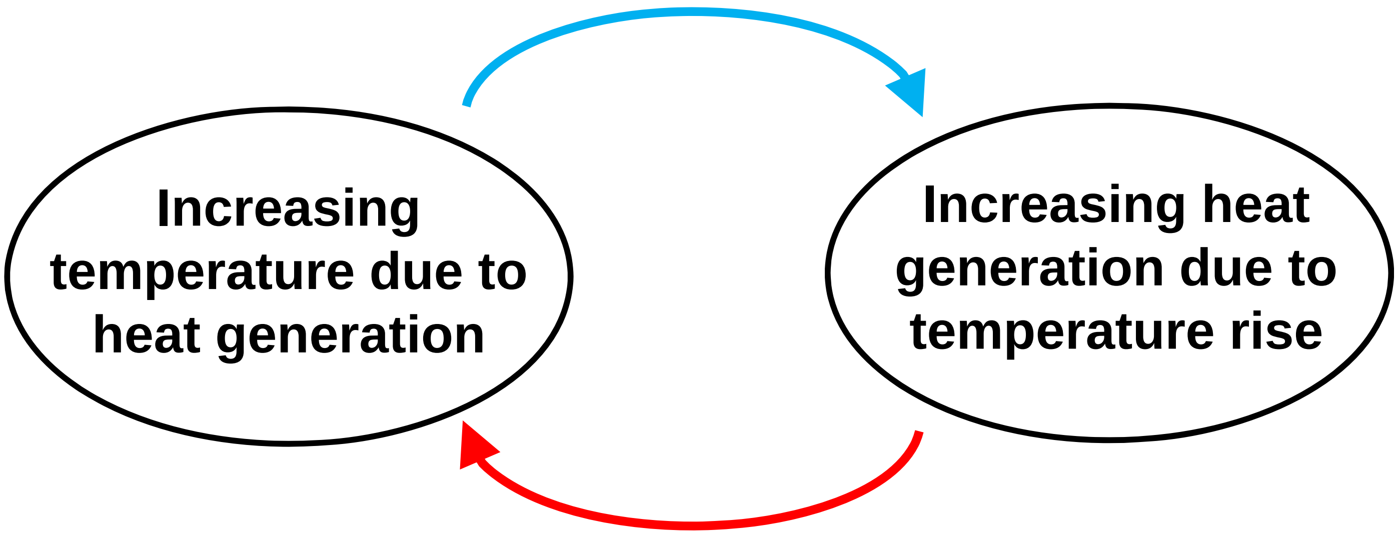


3. Material-level thermal transport measurements *(Why does a cell get so hot?)*



Thermal Runaway Prediction

- Heat accumulation in a Li-ion cell results in thermal runaway.



$$\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}\right)+\frac{Q(T)}{k_r}=\frac{1}{\alpha_r}\frac{\partial T}{\partial t}$$

Governing Energy Equation

$$T(r,t)=\sum_{n=1}^{\infty}C_n J_0\left(\frac{\mu_n r}{R}\right)\cdot exp\left[\alpha\left(\frac{\beta}{k}-\frac{\mu_n^2}{R^2}\right)\cdot t\right]$$

General Solution

- This shows that in order for the cell temperature to stay bounded,

$$TRN \equiv \frac{\beta \cdot R^2}{k_r \mu_1^2} < 1 \qquad \beta = \frac{dQ}{dT}$$

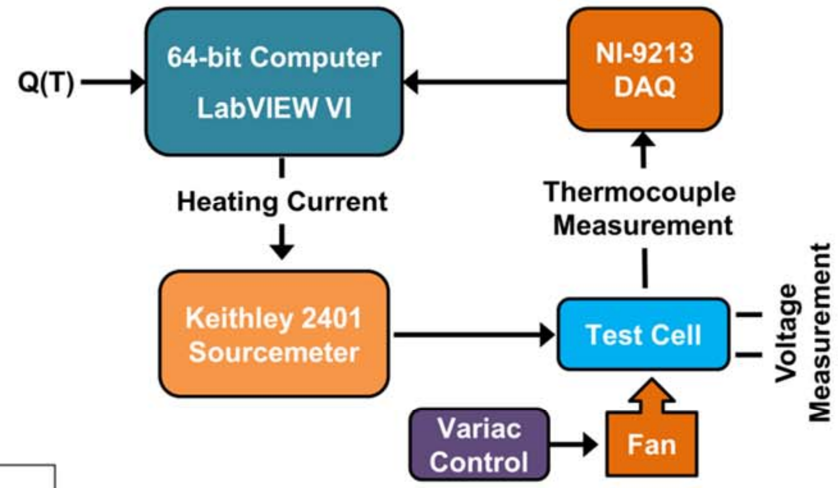
- *TRN* is a fundamental, non-dimensional number that governs whether thermal runaway occurs or not.

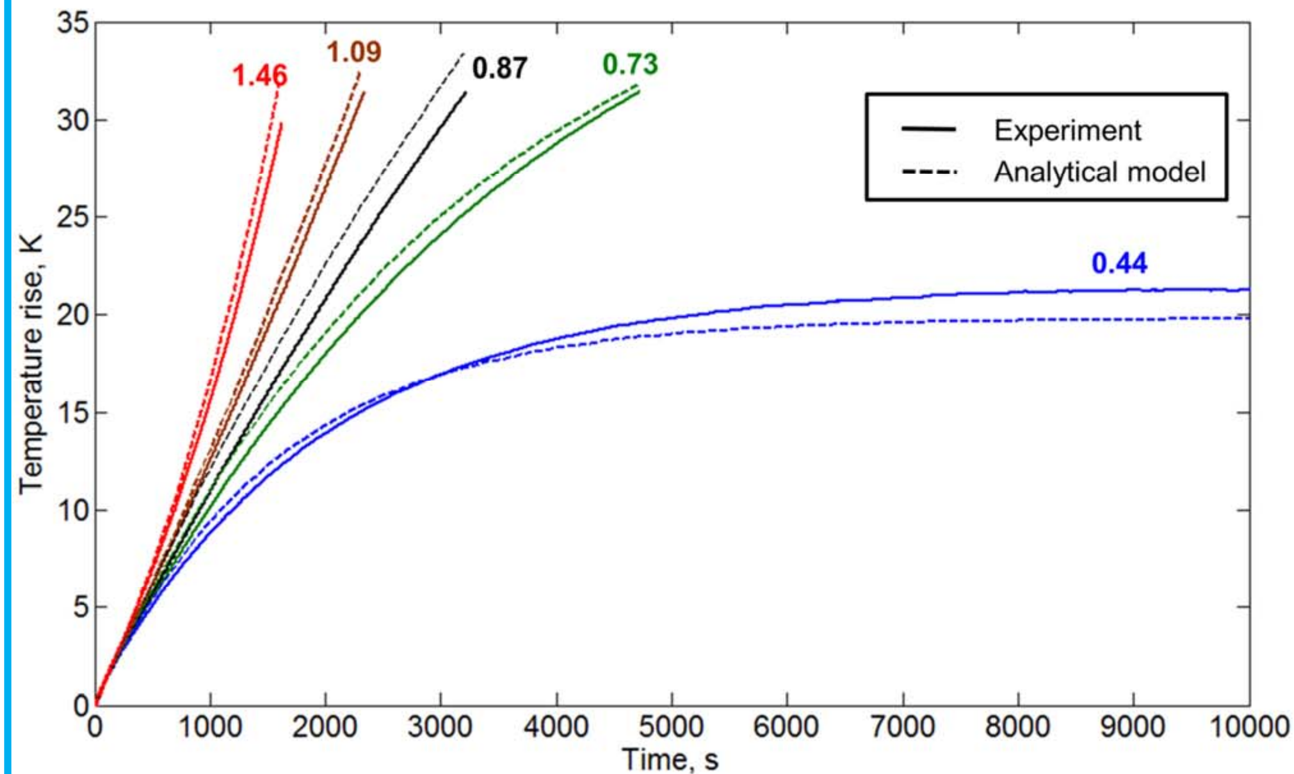
Shah, *et al.*, *J. Power Sources*, 2016

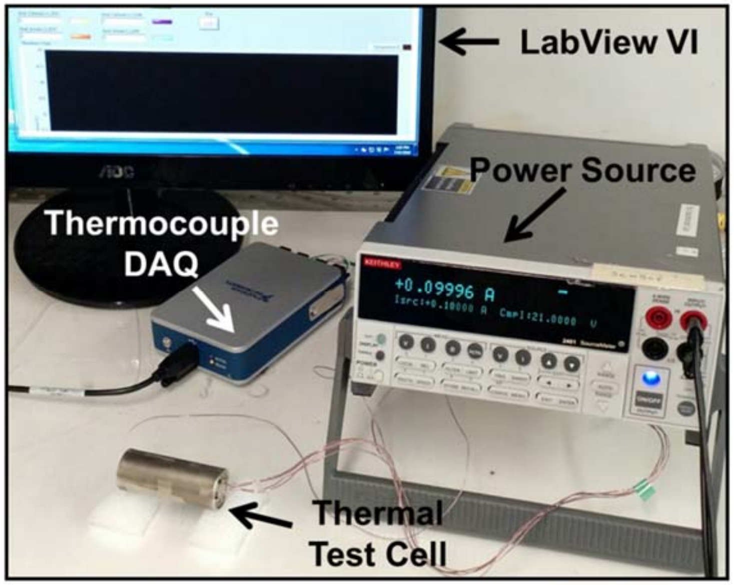
Experimental Validation

• Experimental data confirm this theoretical prediction for a variety of cases.

• Thermal runaway is seen to occur only when *TRN*>1.







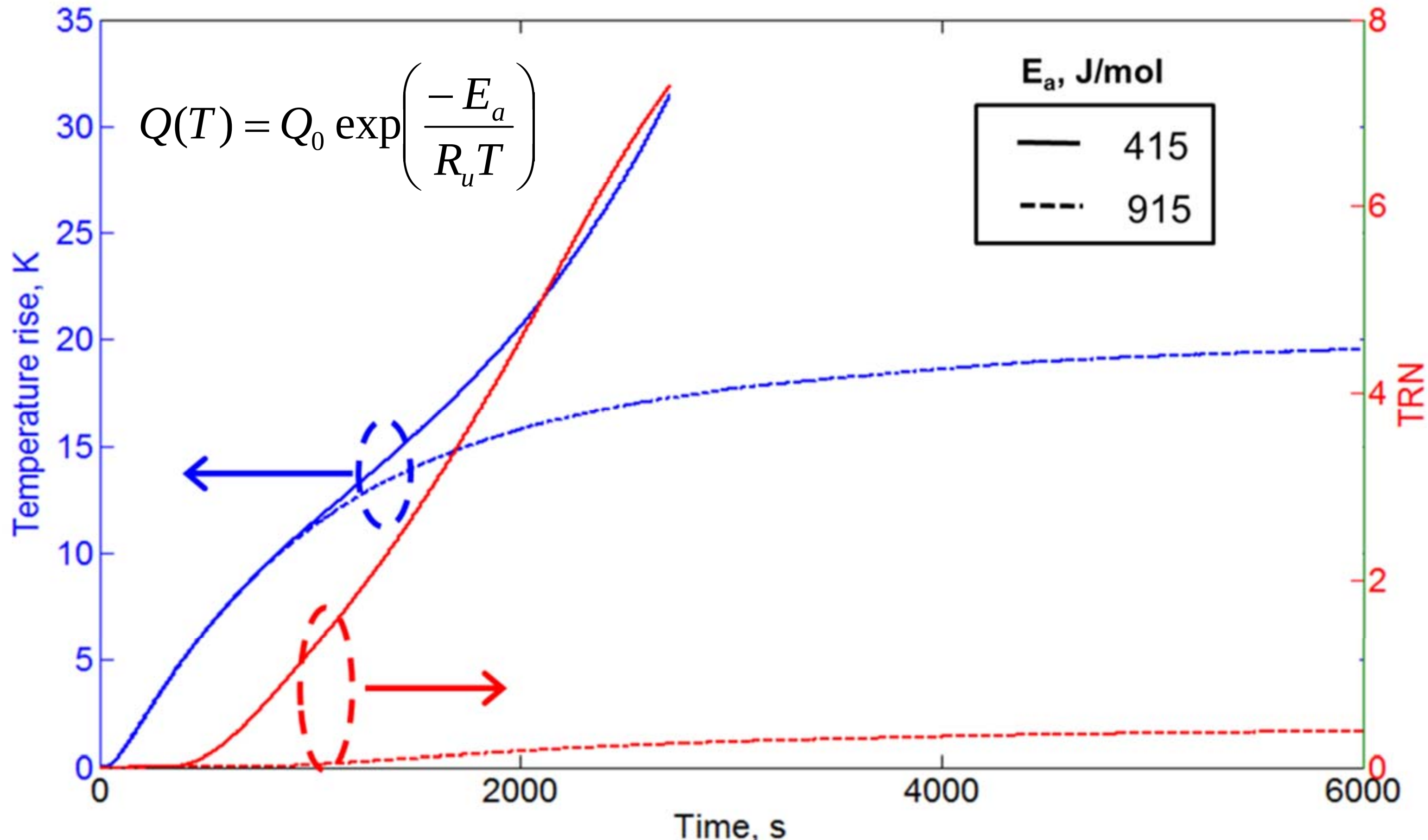
Shah, *et al.*, *J. Power Sources*, 2016

Battery Behavior in Realistic Conditions

• Electrochemical reactions in a battery follow Arrhenius kinetics.

• Experimental data show that temperature remains bounded while *TRN*<1, but thermal runaway occurs once *TRN* exceeds 1.

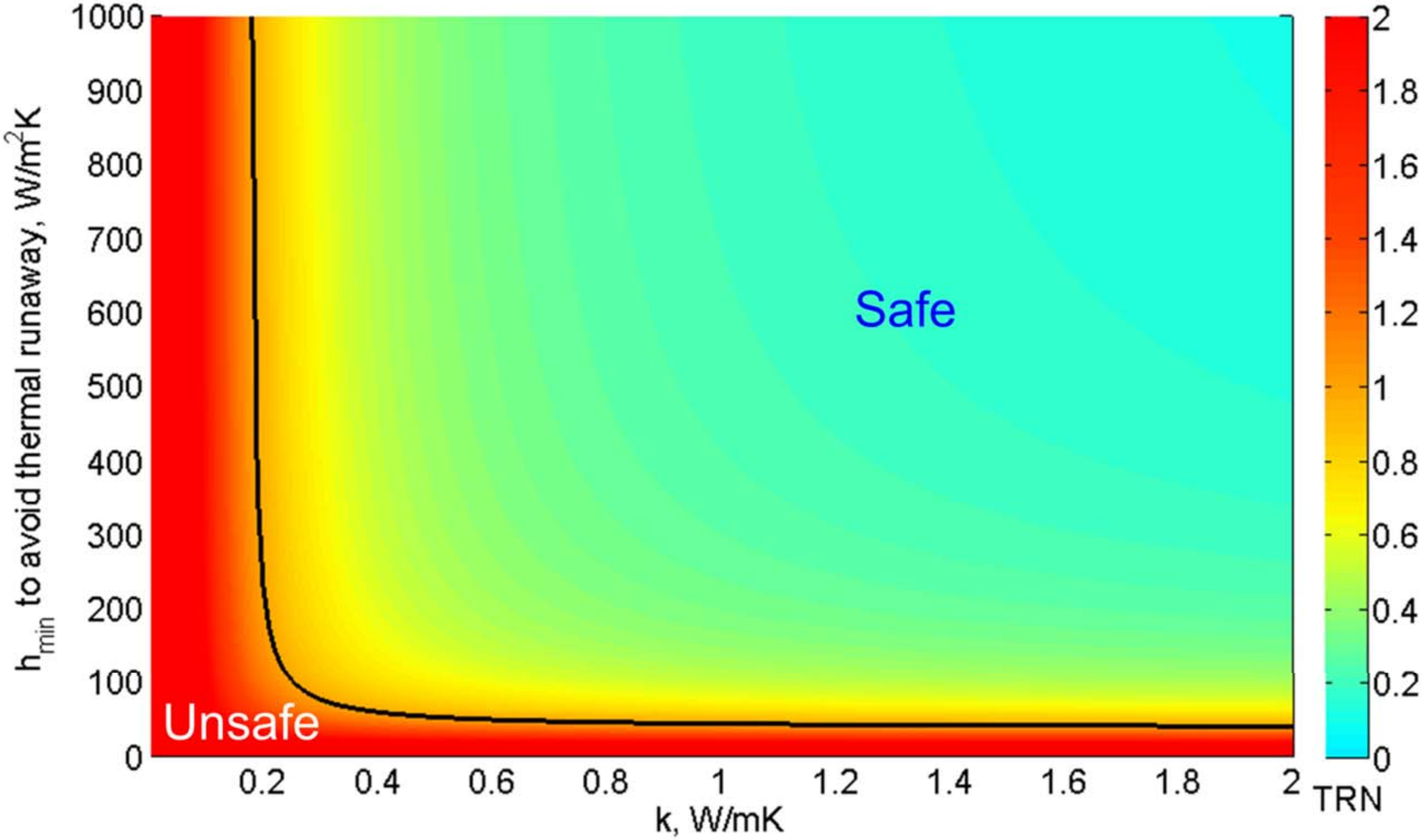
• Data indicates the possibility of pro-active prediction of onset of runaway.



Shah, *et al.*, *J. Power Sources*, 2016

Prediction of Safe/Unsafe Thermal Design Space

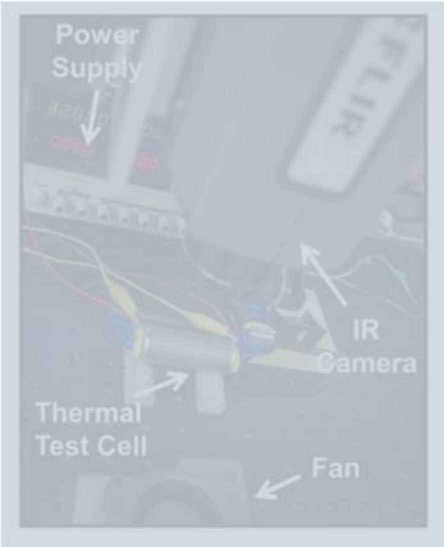
• The experimentally-validated model can predict safe and unsafe regions in the thermal design space.



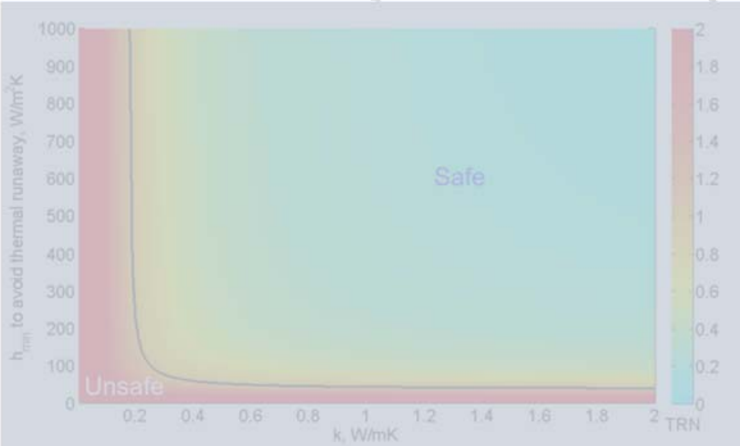
Shah, *et al.*, *J. Power Sources*, 2016

Outline

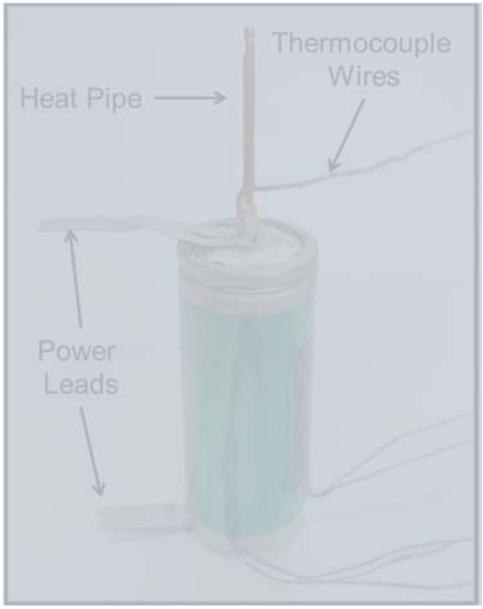
1. Non-invasive core temperature measurement
(Thermal x-ray)



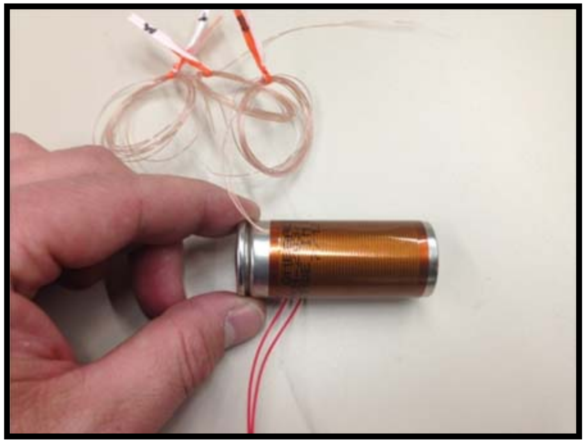
2. Prediction of thermal runaway
(When is a battery at risk of exploding?)



4. Heat pipe based cooling
(How to passively cool a cell)

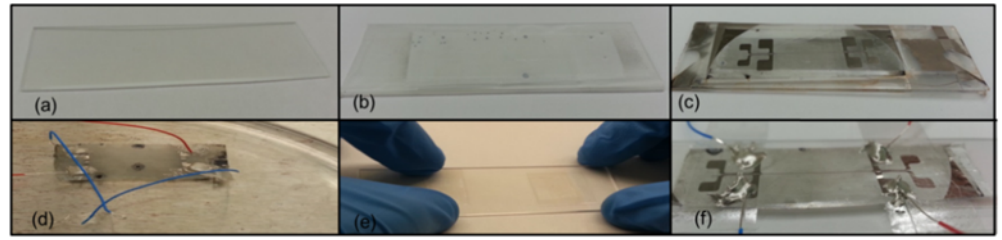


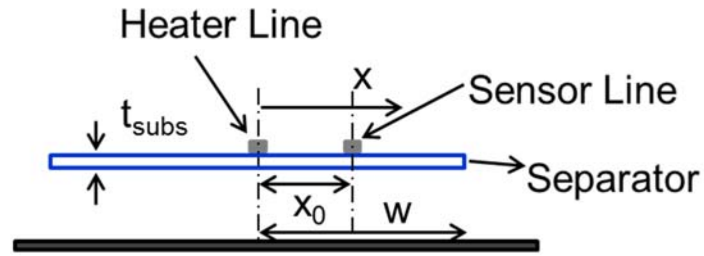
3. Material-level thermal transport measurements
(Why does a cell get so hot?)

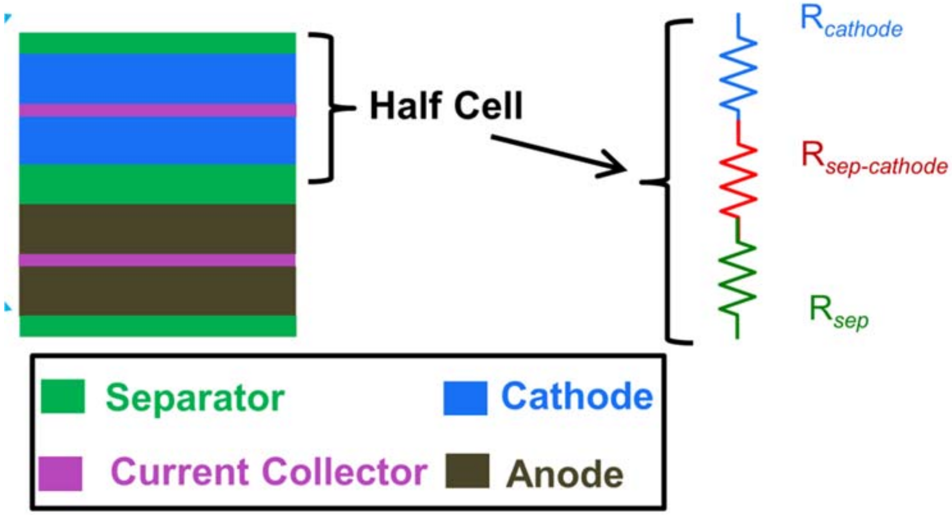


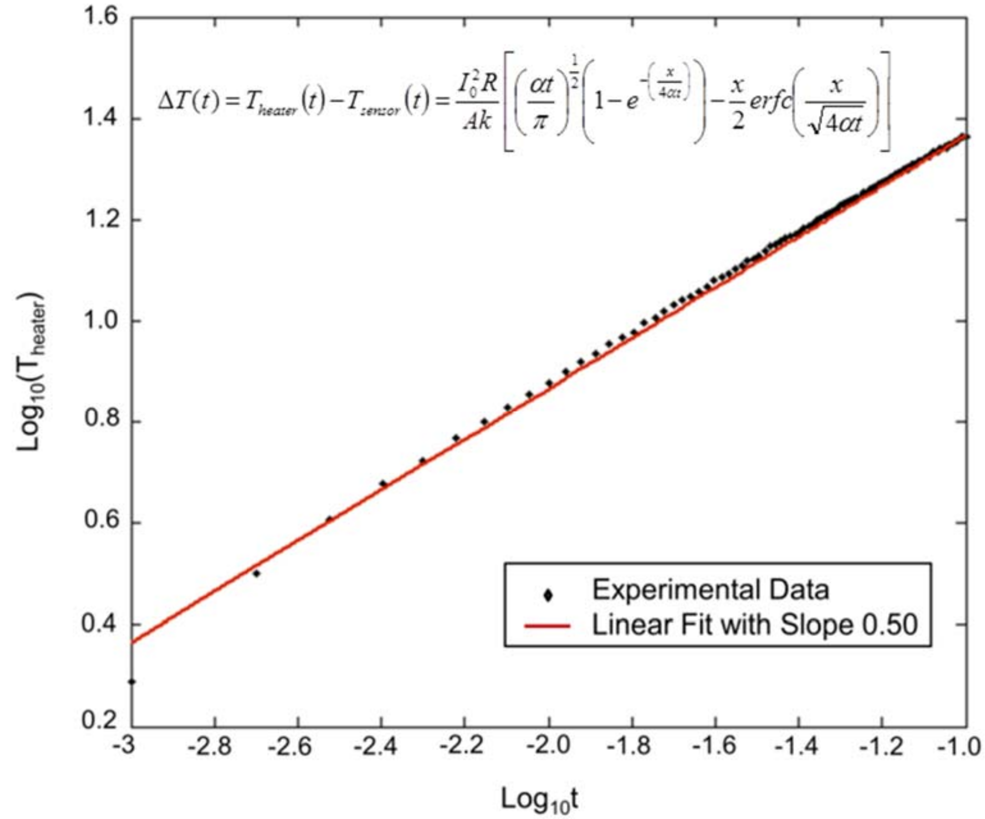
Measurement of Material-level Thermal Transport

- Measurements show that thermal conductivity of even the least conducting material in a Li-ion cell is greater than the measured cell-level thermal conductivity.
- This indicates that interfacial thermal resistances in a Li-ion cell may be important.







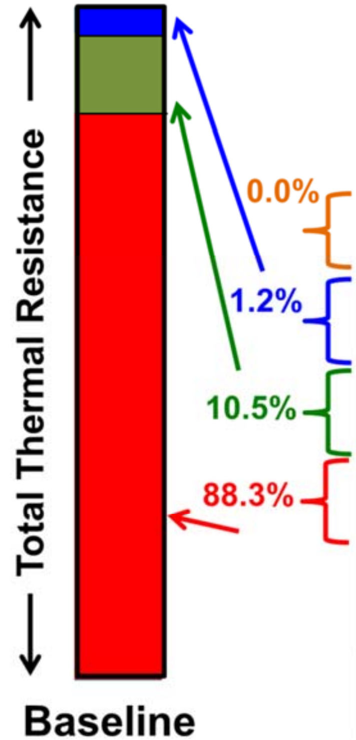


Vishwakarma, *et al.*, *J Power Sources*, 2014

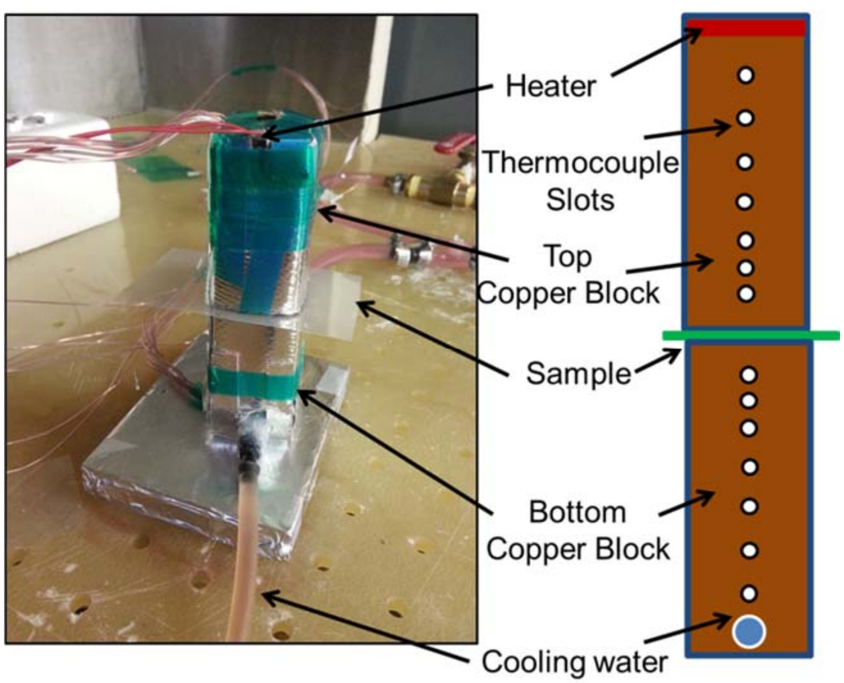
Measurement of Material-level Thermal Transport

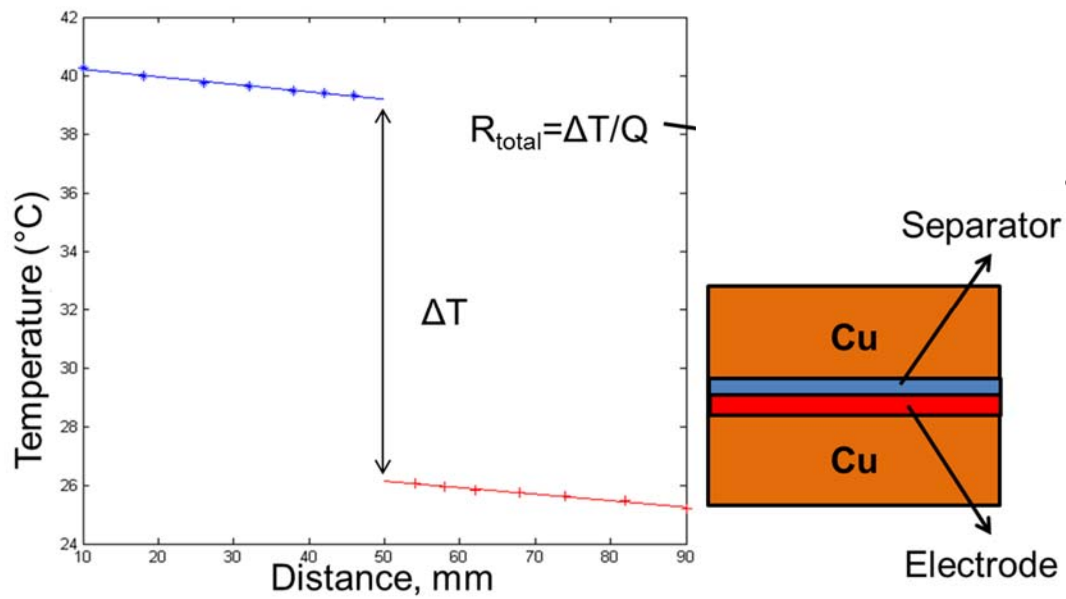
- Separator-cathode thermal contact resistance contributes ~88% of total thermal resistance in a Li-ion cell.

- Measurements in good agreement with acoustic mismatch theory for interfacial phonon transport.



Baseline (Experiment A) $\mu Km^2/W$	Thermal Resistance
<1	Current Collector
11	Cathode
100	Separator
840	**Separator-Cathode Interface**
951	**Total Thermal Resistance**
0.24	**k_{eff} (W/mK)**

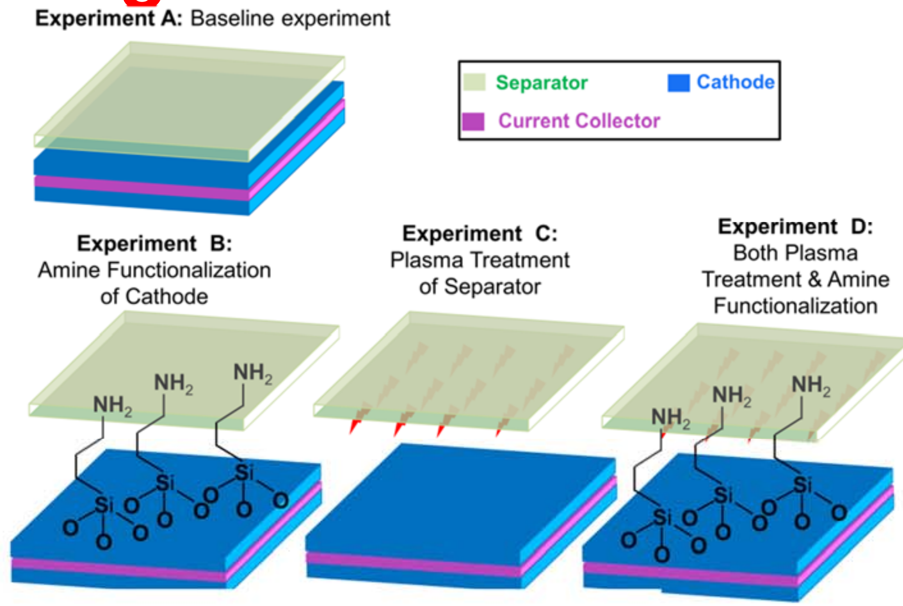


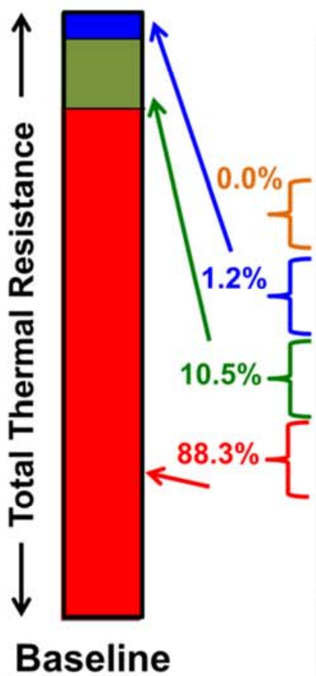


Vishwakarma, *et al.*, *J Power Sources*, 2015

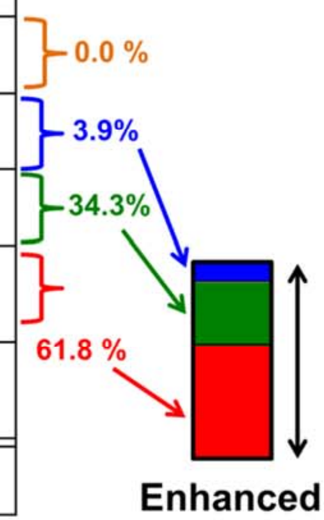
Enhanced Thermal Transport Through Interface Engineering

- Surface modification of separator/cathode resulted in significant reduction in separator-cathode thermal contact resistance.



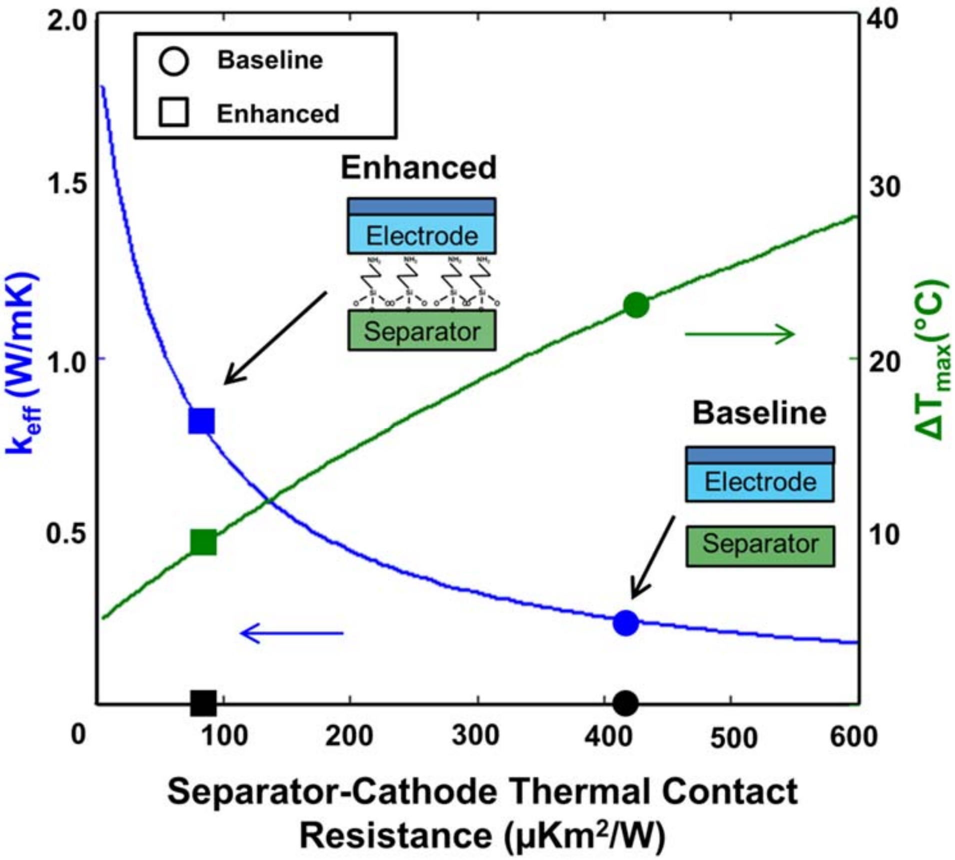


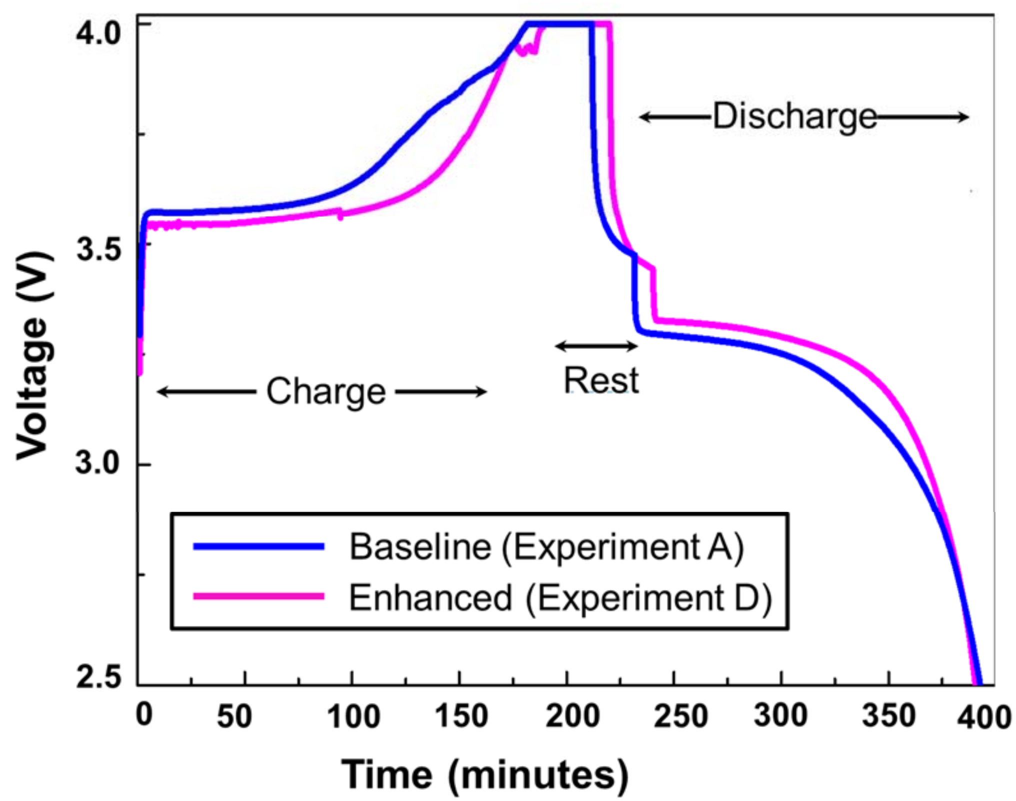
Baseline (Experiment A) μKm²/W	Thermal Resistance	Enhanced (Experiment D) μKm²/W
<1	Current Collector	<1
11	Cathode	11
100	Separator	100
840	Separator-Cathode Interface	180
951	**Total Thermal Resistance**	**291**
0.24	**k_{eff} (W/mK)**	**0.76**



Vishwakarma, *et al.*, *J Power Sources*, 2015

Thermal Enhancement without Electrochemical Deterioration





- This approach significantly improves thermal performance while preserving electrochemical performance.
- Large-scale implementation presents additional challenges.

Vishwakarma, *et al.*, *J Power Sources*, 2015

Summary

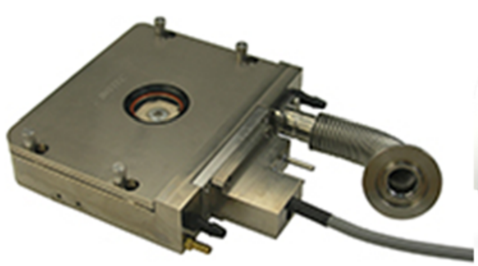
• Thermal engineering plays a key role in ensuring safety of Li-ion based electrochemical energy storage devices and systems.

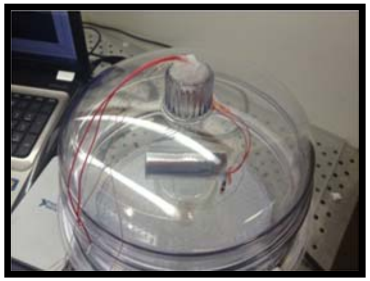
• Optimization of material-level thermal transport is important for device-level and system-level improvements in safety and performance.

• Synergistic partnerships between Universities, National Labs and companies is critical for transformative progress.

Facilities

- Thermal property measurement: Netzsch LFA467, Custom-built 1D Heat Flux System, CTherm TPS2200, TA Instruments Fox50.
- Thermal imaging: FLIR A6703sc mid-wave IR Camera, Meiji MT6000 fluorescence microscope, Fastec IL5 high speed camera.
- Electrochemical Measurements: Kikusui PFX2512 C/D system, VersaSTAT4 Potentiostat/Galvanostat.
- Electrical measurements and data acquisition: Multiple lock-in amplifiers, function generators, power sources, picoammeters, etc.
- Custom-built thermal characterization setup for cells/packs.
- Chemical handling: LC101 glovebox and Thermo Scientific 1300 chemical fume hood.
- Vacuum chambers: KL XTEMP−BX, Instec HCS662V
- Simulation & modeling: Advanced multiphysics simulation software, 256-core Xi computer workstation.
- Detonation facilities and high-rate cell cycling facilities (through collaborators).





Acknowledgments

A. Students:

Current:

1. Vivek Vishwakarma
2. Krishna Shah
3. Dean Anthony
4. Salwa Shaik
5. Mohammad Parhizi
6. Hardik Prajapati
7. Ratnesh Raj
8. Swapnil Luhar
9. Cody McKee
10. Divya Chalise
11. Chirag Waghela
12. Nicolas Long

Alumni:

1. Prof. Leila Choobineh (Asst. Professor, SUNY Polytechnic Institute, Utica, NY)
2. Dr. Stephen Drake (R&D Manager, Thermon Inc.)
3. Dr. Daipayan Sarkar
4. Mohammad Parhizi (MS, Ph.D. student, UTA)
5. Annas Javed (MS, Sr. Product Engr., Qualcomm)
6. Bhavik Patel (MS, Design Engineer, Siemens)
7. Arya Banait (BS, Grad Student, Stanford University)
8. Mark Robinson (BS, Transportation Tech. Serv.)
9. Jared Jones (BS/MS, Abbott Labs)

B. Collaborators: Prof. D. Wetz (EE, UTA), Prof. F. Liu (U. Mass.), Prof. D.K. Ezekoye (UT Austin), Dr. R. Prasher (LBNL), Dr. C. Daniel (ORNL), Dr. J. Ostanek, Dr. S. Miller, Dr. J. Heinzel (US Navy).

C. Funding: NSF (**CAREER**, CBET-TTP, **CBET-EFS**, ECCS-EPCN), **ONR**, **ONR-DURIP**, DoE, **IUSSTF**, ORAU, Microfabrica, Inventek.

Contact: jaina@uta.edu