PENNSTATE

Electrochemical Engine Center

Computer-Aided Engineering and Next Generation Development of Electric Drive Batteries

Chao-Yang Wang

Electrochemical Engine Center (ECEC)
The Pennsylvania State University
University Park, PA 16802 USA

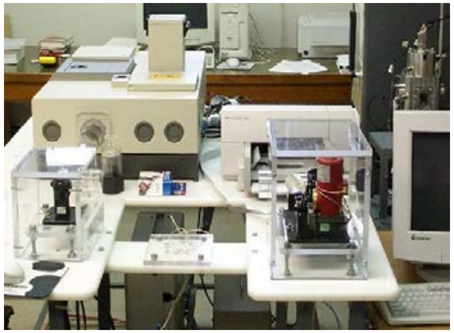
Outline

1. Background & Penn State Battery R&D
2. Computer-Aided Engineering of xEV Batteries
3. Next Generation of xEV Batteries
4. Summary

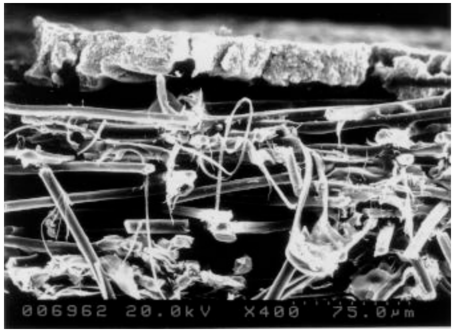
Electrochemical Engine Center

- Founded in 1997
- Engaged in battery and fuel cell research for vehicle electrification

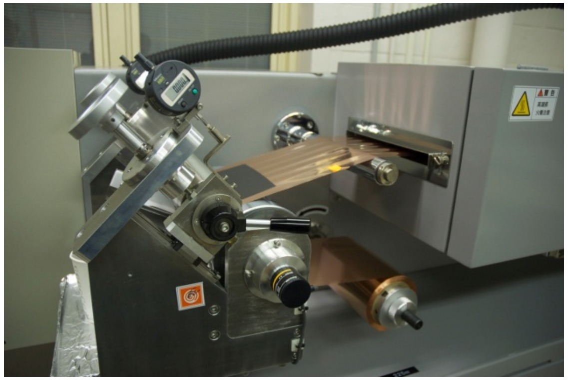


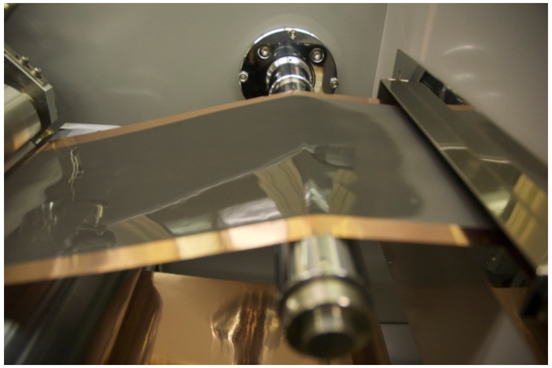



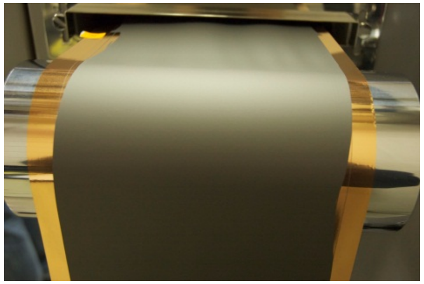


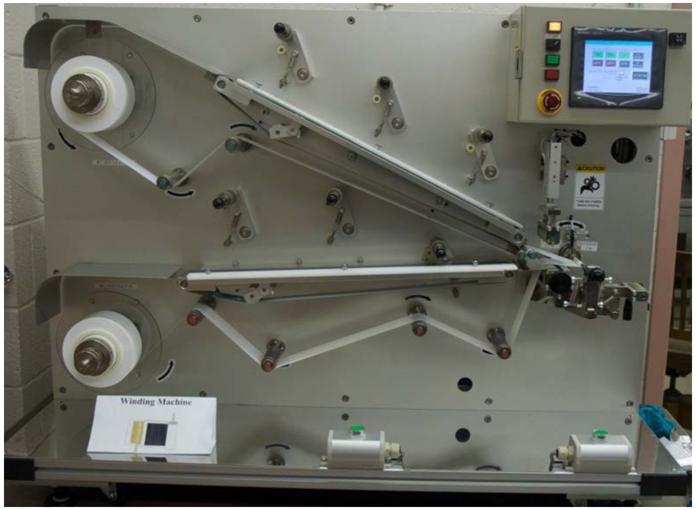



Lithium-Ion Battery Manufacturing Facility



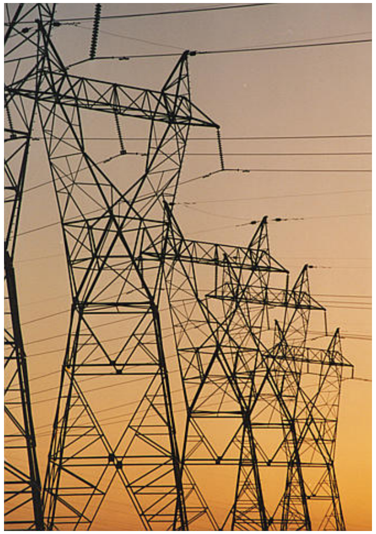






Energy Storage Technologies for a Sustainable Future

- Batteries for: PHEV, renewable energy storage, smart grids, etc.


- All-day power for iPhones, iPads, iPods, wireless society


Winning the Future with Clean Energy

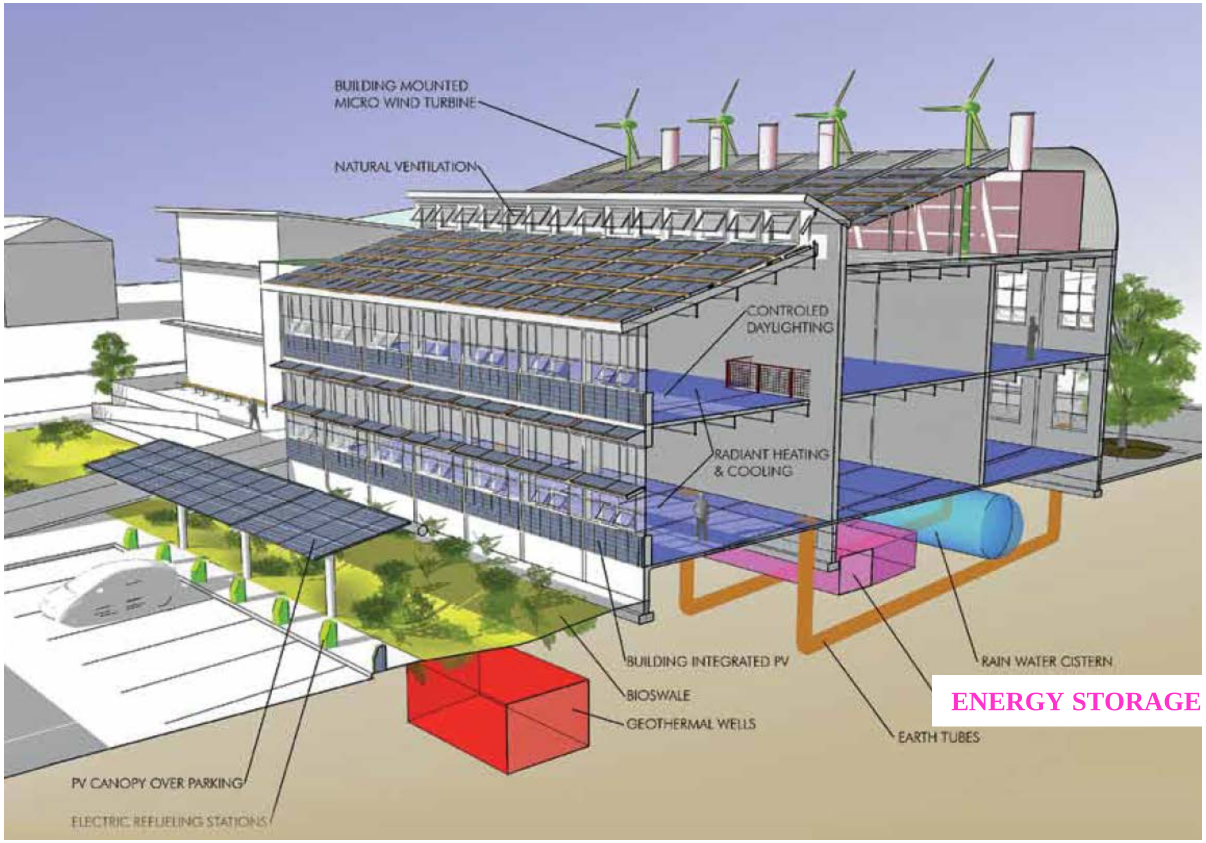
February 03, 2011
President Obama visits Penn State University and speaks about encouraging and investing in innovation and clean energy technologies to create new jobs, grow the economy, and win the future.

Penn State: #1 ranking in alternative energy among universities globally (Elsevier, 2010)

Penn State: #1 ranking in fuel cells among universities worldwide (ScienceWatch, 2009)

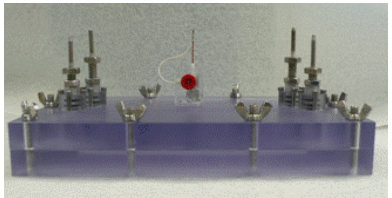
Penn State: one of only 3 Energy Hubs ($129M in Energy Efficient Buildings)

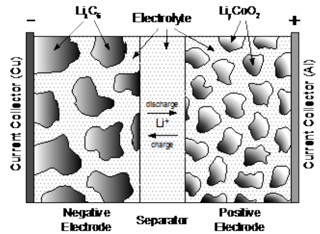
Penn State Energy Efficient Building Hub

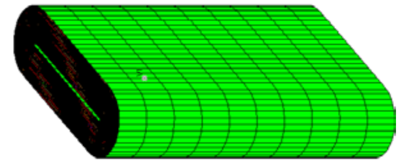


Net-Zero Energy Building

Computer-Aided Engineering of Batteries







Materials Characterization

Physico-chemical Modeling

Computational Algorithms

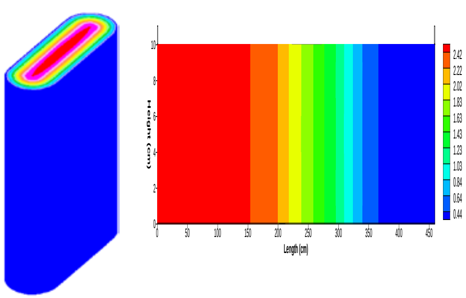
Diagnostics & Validation

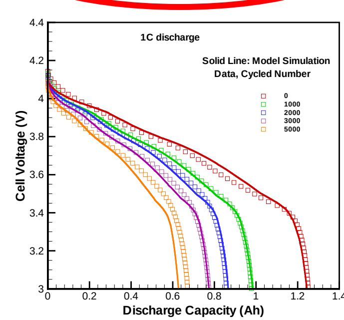
Set **Gold Standard** for Vehicle Battery Engineering

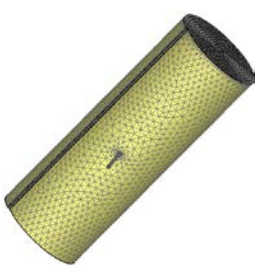
Performance

Cycle Life

Safety







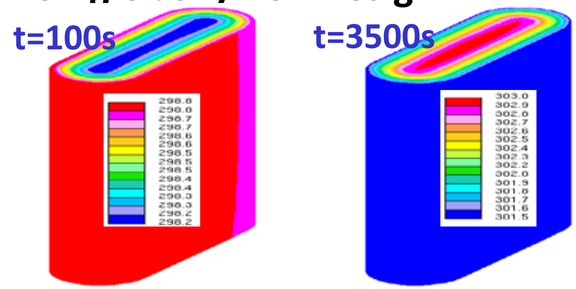
- highest active material utilization
- highest energy density (Wh/kg)
- lowest cost $/kWh

- longest life
- lowest life-cycle cost

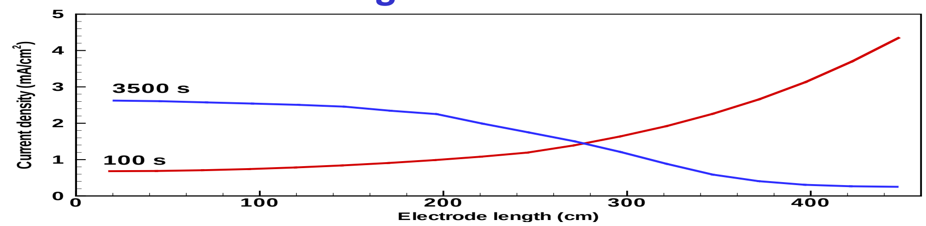
- safest systems by virtual & actual testing

Evaluating Various Designs

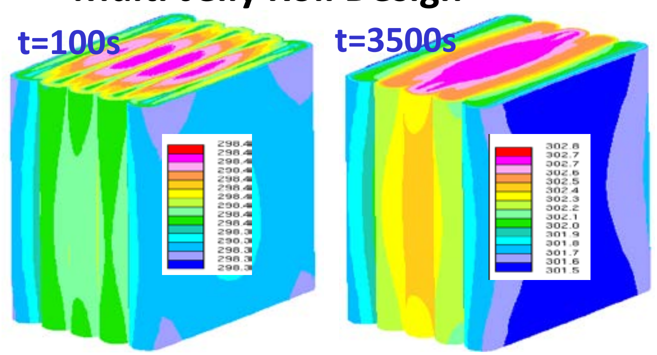
Single-Jelly Roll Design



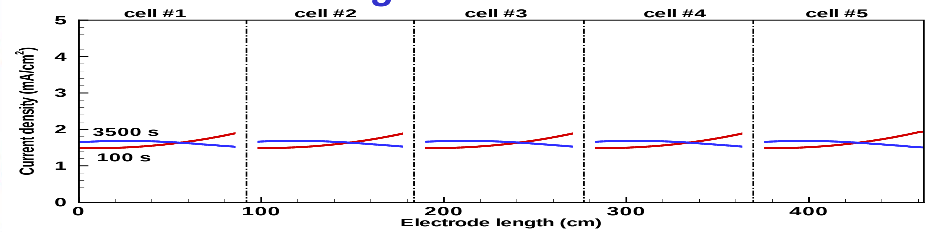
1C discharge current distribution



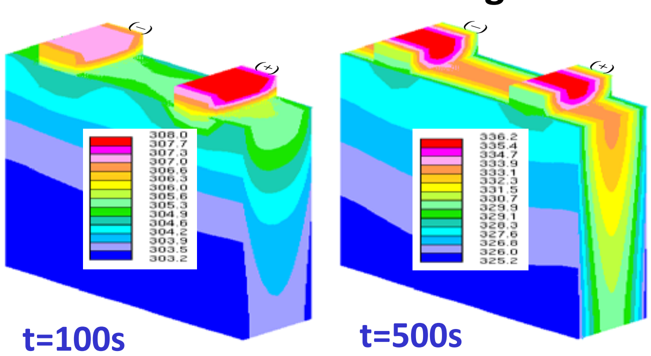
Multi-Jelly Roll Design



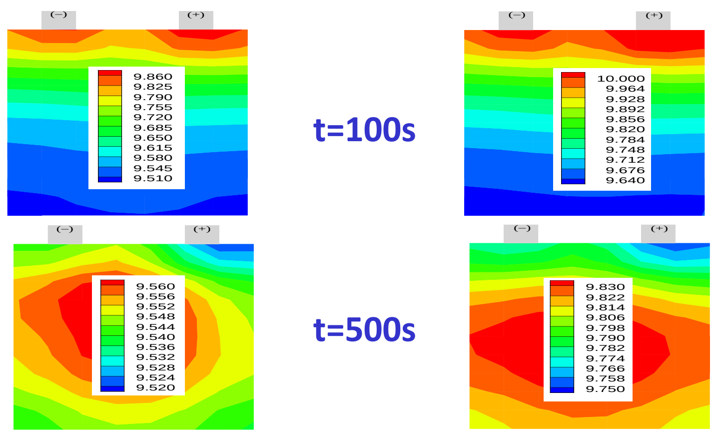
1C discharge current distribution



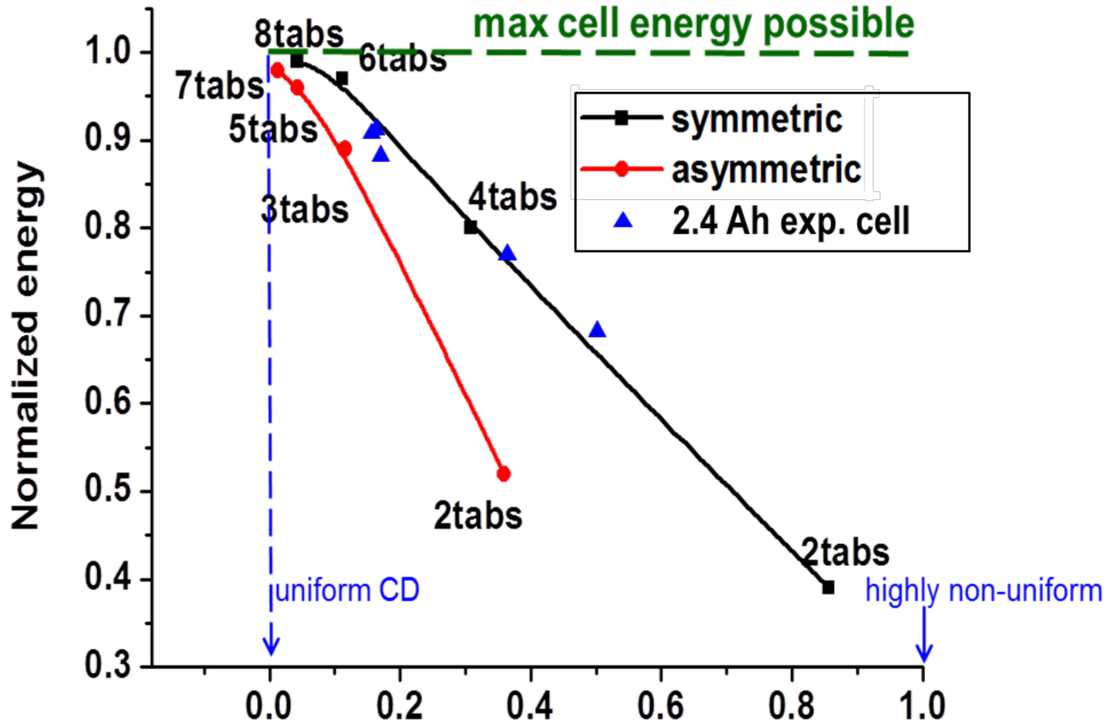
Stacked Electrode Design



6C discharge current distribution

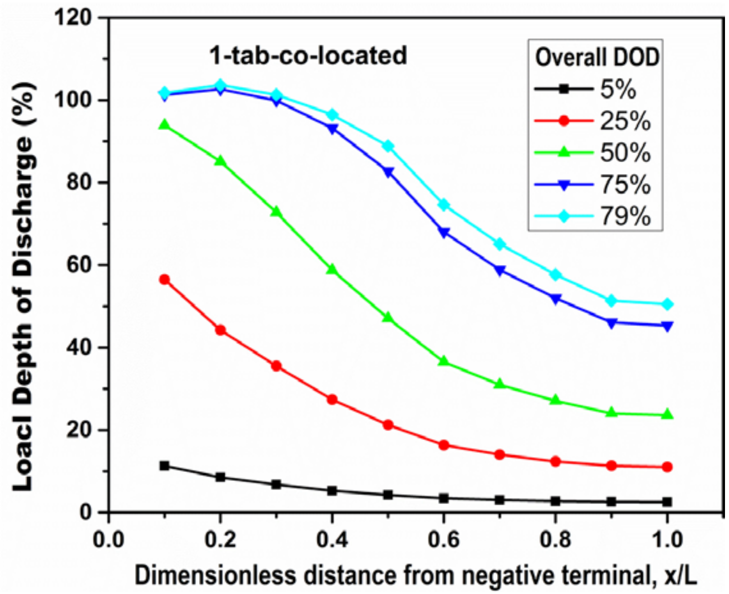


Design Optimization for 50% Gain in Energy Density



Time-averaged CD Non-uniformity Factor (CD standard deviation time-averaged and normalized by average current density)

Measured local DoD profile



- Ensuring current distribution uniformity (and hence uniformly high utilization of active materials) quantitatively impacts the cell's energy density (by as much as 50%)
- It is as significant as developing advanced Li-ion chemistries or going beyond Li-ion! In addition, it makes immediate commercial advances!

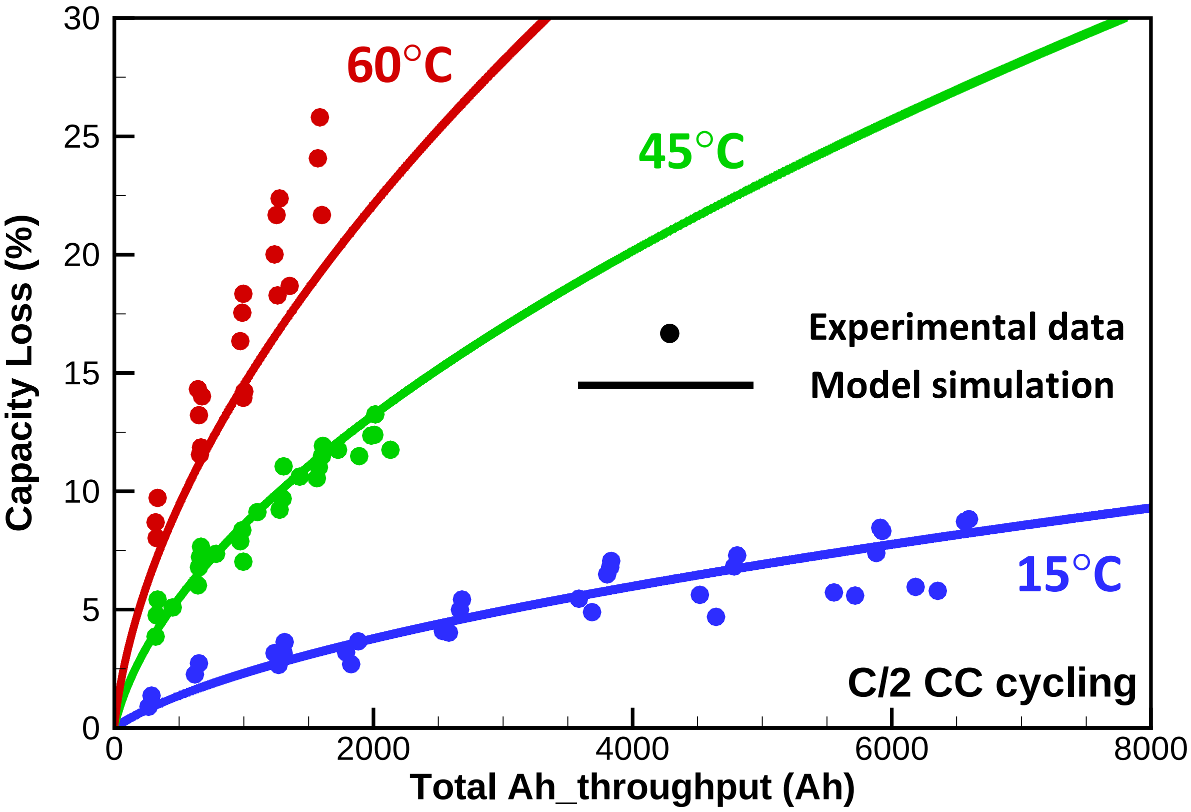
Cycle Life – Key to EV Commercialization

- battery cycle life is a major challenge
- directly impacts warranty and hence cost
- very time-consuming and expensive information
- computer simulation ~500x faster than real testing time, e.g.
  - for 6-min pulsed power cycle, simulation ~ 1 s
  - for 1h charge/discharge, simulation ~ 10 s
  - for 6-12 months cycle life testing, simulation ~ 12-24 hrs

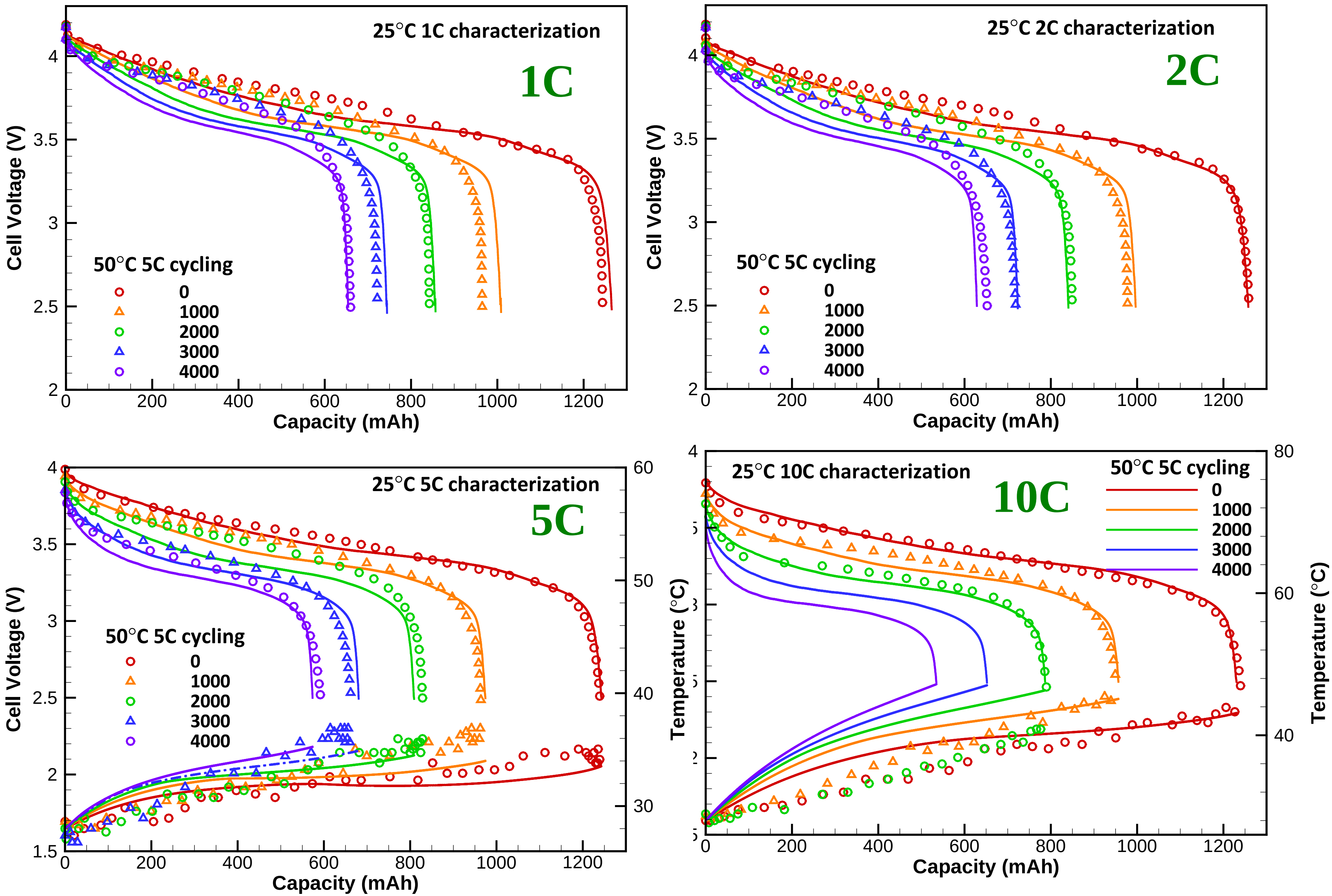
10% error in life prediction results in 50% cell failure before expiration of warranty.

Cycle Life Prediction – Key to EV Commercial Viability

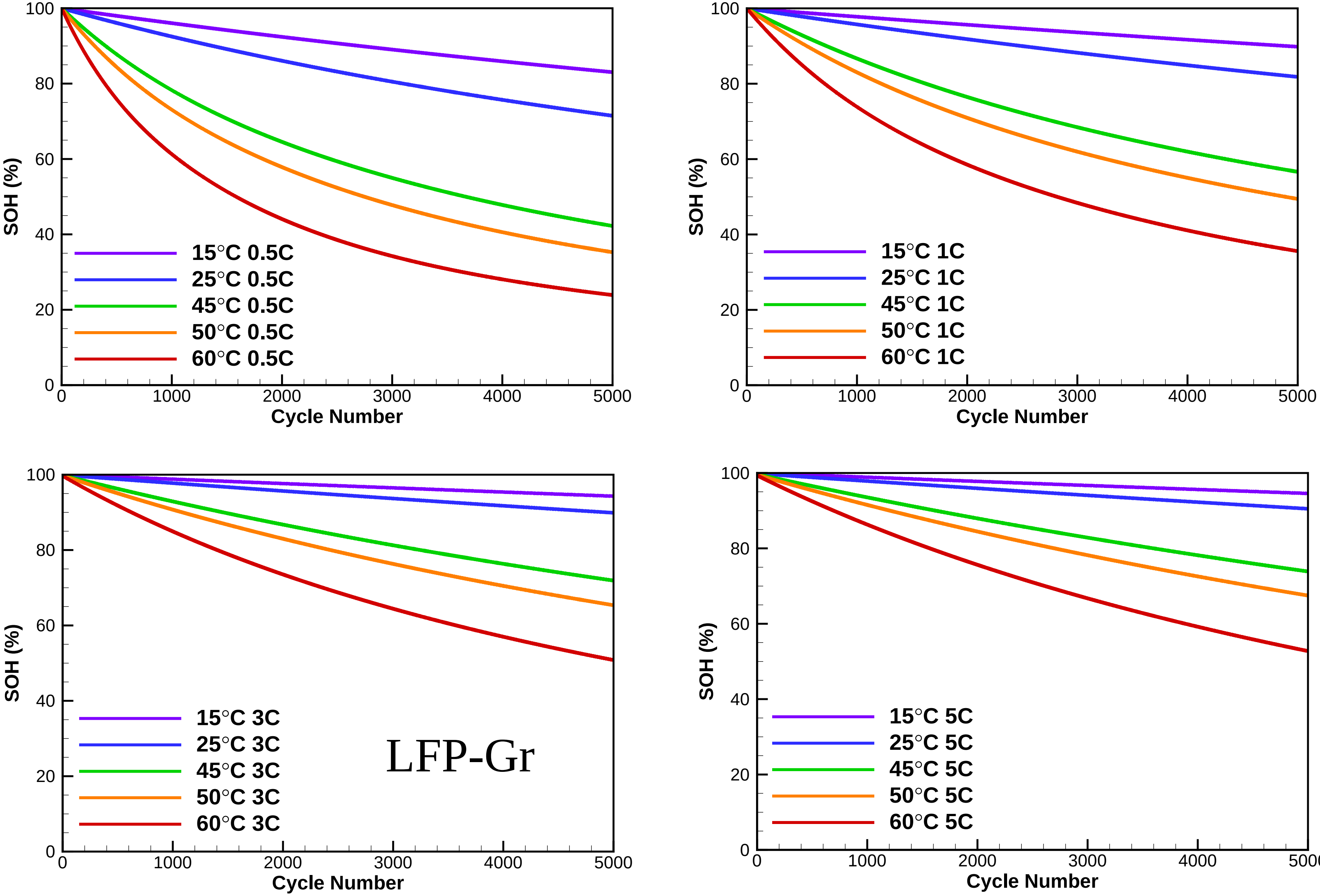
LFP cell cycled @ C/2 between 2.0-3.6V



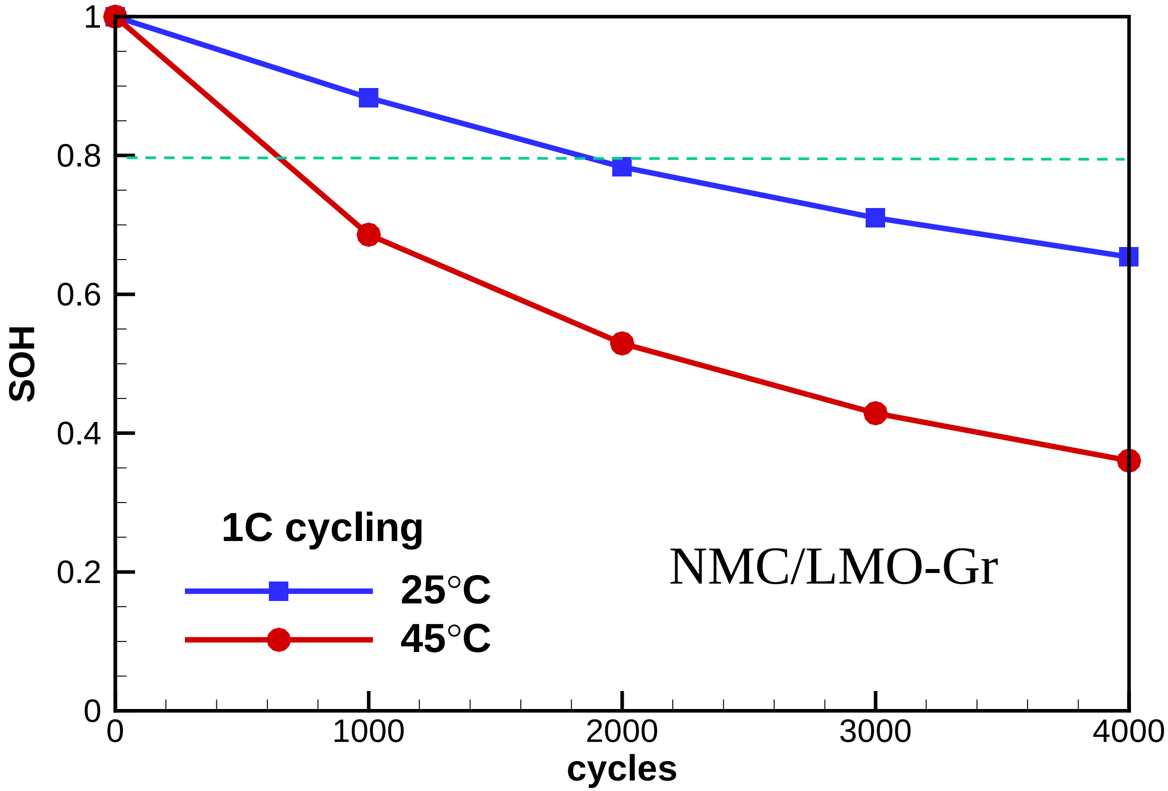
Cycle Life Prediction & Exp. Validation – NMC-Gr Chemistry



Predicting Battery SOH at Various T and C-rate



Predicting Battery SOH for Different Chemistry



SOH = capacity of aged cell/initial capacity (nominal)

- Cycle life is significantly shortened by elevated temperature: ~2,000 cycles at RT but <1,000 cycles at 45^{o}C. This indicates the paramount importance of thermal management for battery pack life extension.

Lithium Battery Safety


Peter Cohan, Contributor
I write from near Boston about startups and political economy
+ Follow (263)

Forbes

TECH | 2/06/2013 @ 5:49AM | 13,234 views

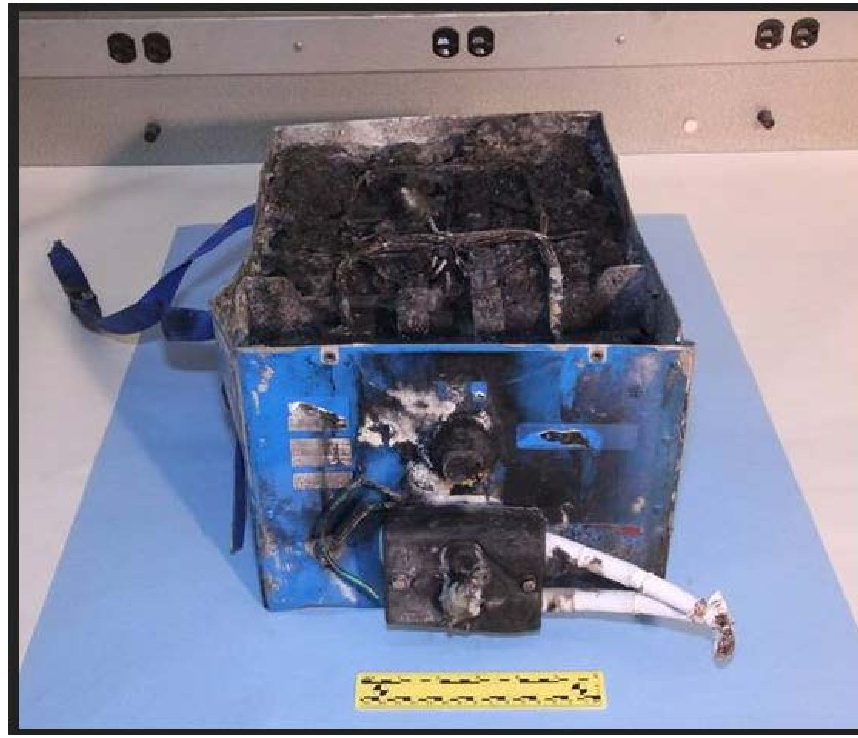
'Thermal Runaway' in 787 Dreamliner Batteries Must Be Stopped

+ Comment Now + Follow Comments

Boeing (BA) is certainly eager to get its 787 Dreamliner back into service. Unfortunately, all 50 of the over 500,000 pound, $207 million aircraft that it's shipped – years late after at least seven missed delivery deadlines – have been grounded.

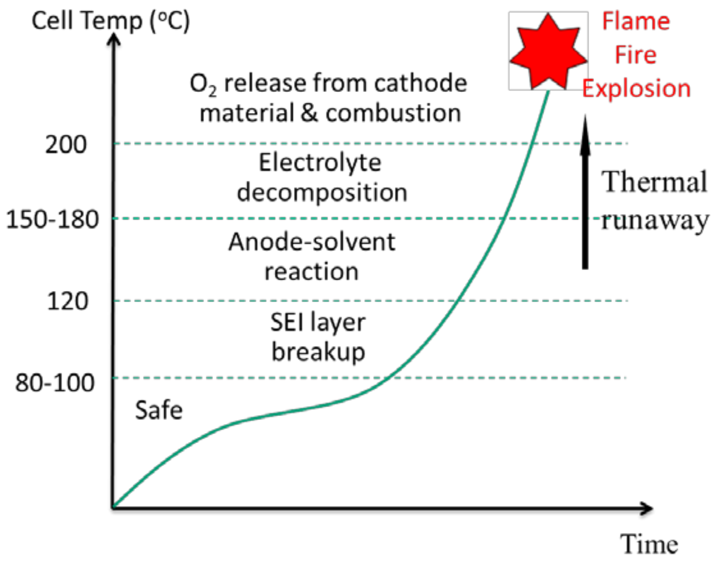
My photos that I took at today's First Flight of the Boeing 787 Dreamliner. (Photo credit: Wikipedia)

And in a test of how much

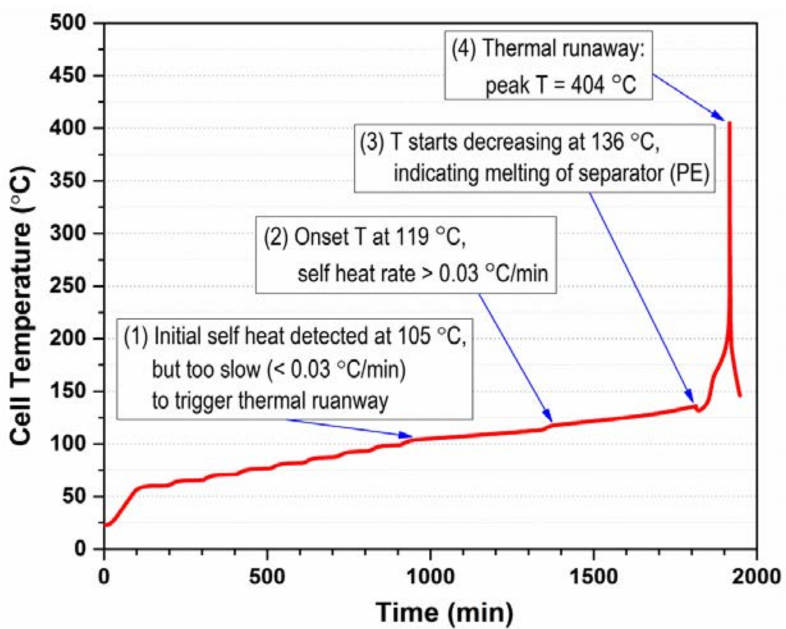


- Cost to Boeing of reimbursing airlines for the lost revenue due to Li-ion safety-related grounding of 787 was $550M*
- As Li-ion batteries become more energy dense (smaller), potential for catastrophic safety incident increases

Fundamentals of Battery Safety

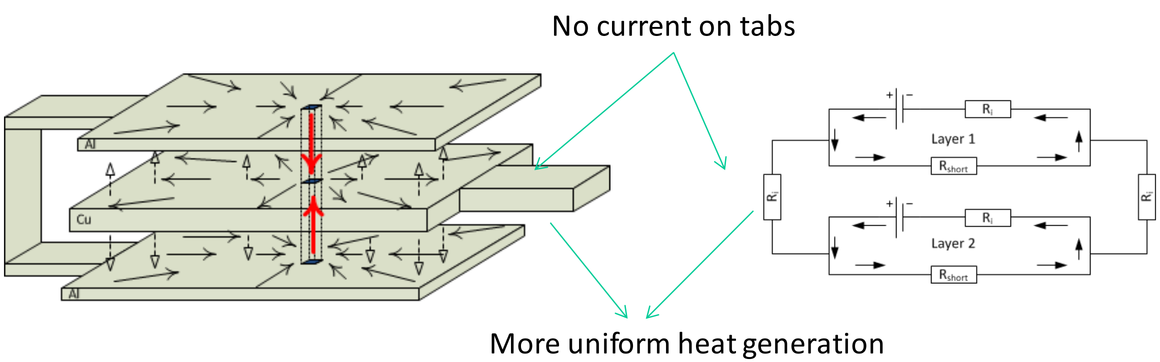


<u>Active material thermal stability is NOT equal to battery safety. The latter is an integrated result of SEI layer stability, electrolyte stability, & anode/cathode material stability, as well as cell structure.</u>

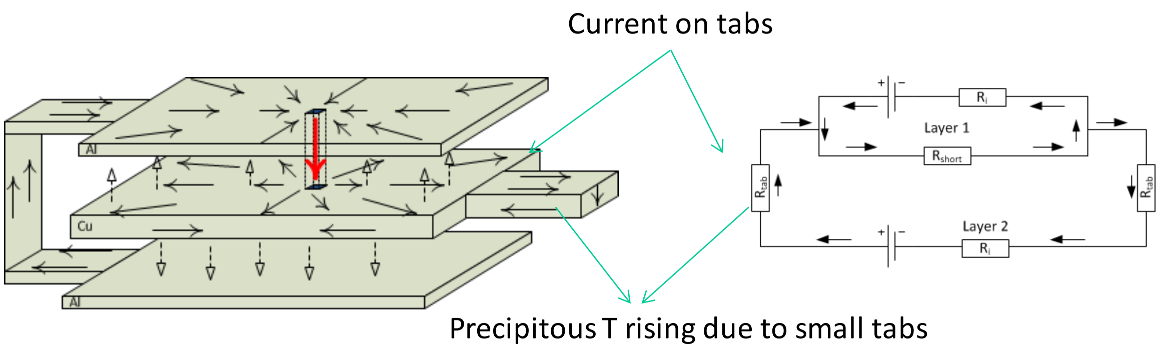


<u>Thermal runaway experiment</u>

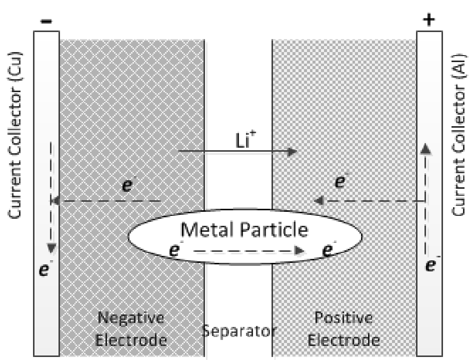
Nail Penetration & Internal Short

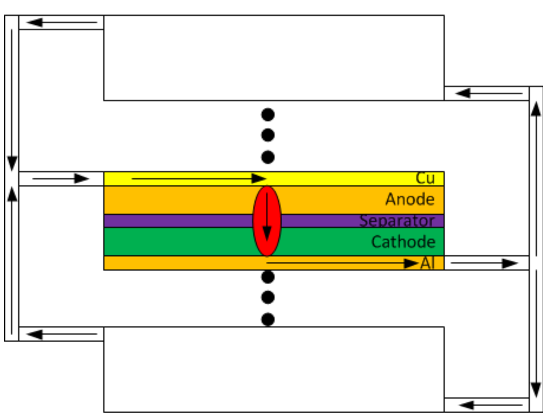


Full Nail Penetration



Partial Nail Penetration

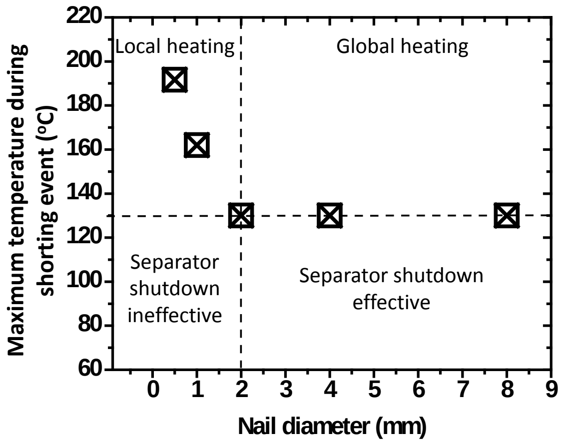


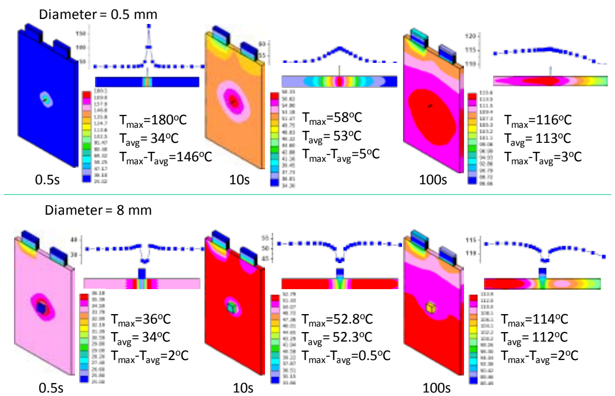


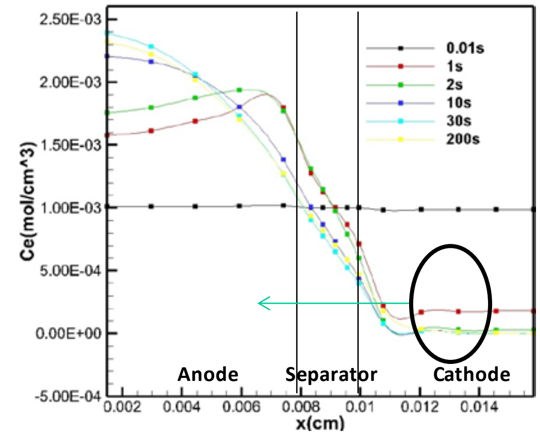
Internal Short

Full and partial penetration

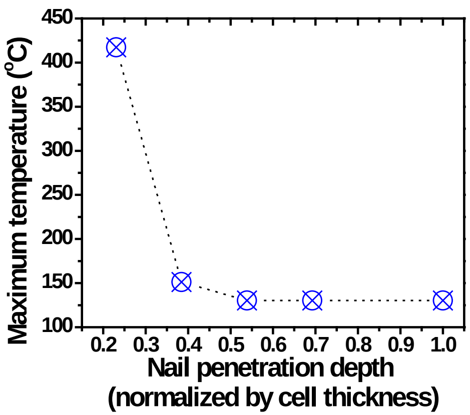
Full Penetration

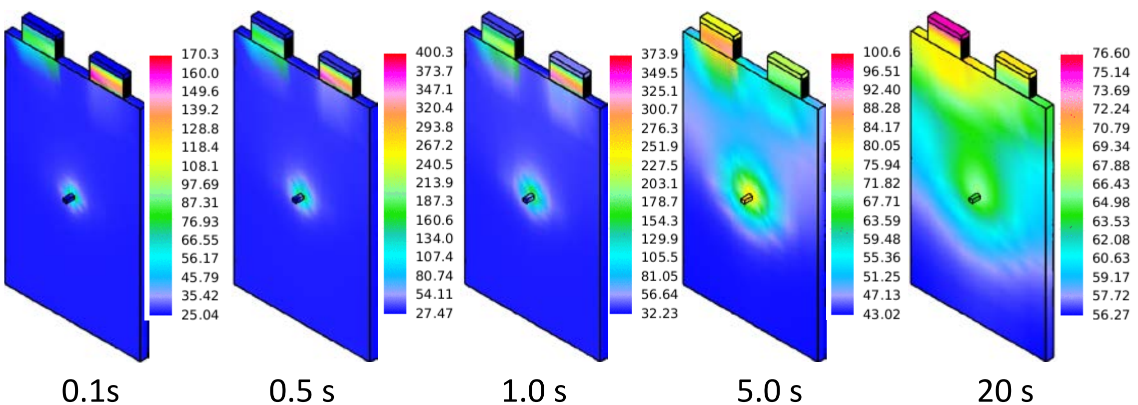






Partial Penetration

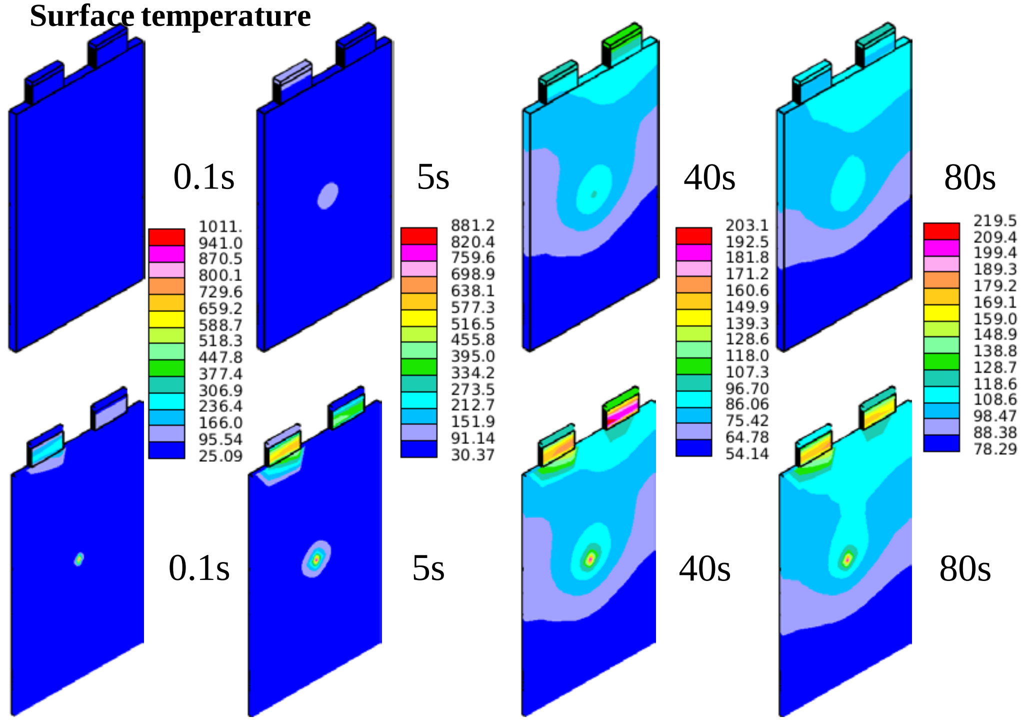




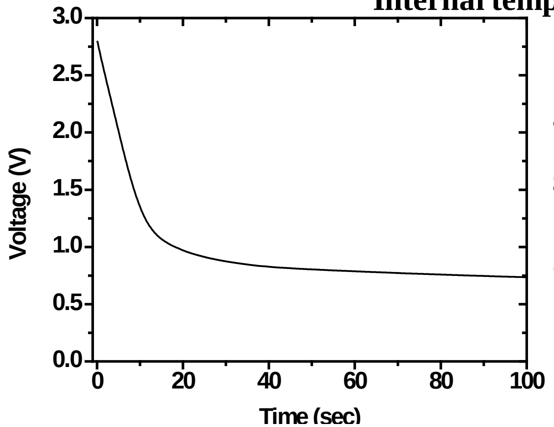
Internal short

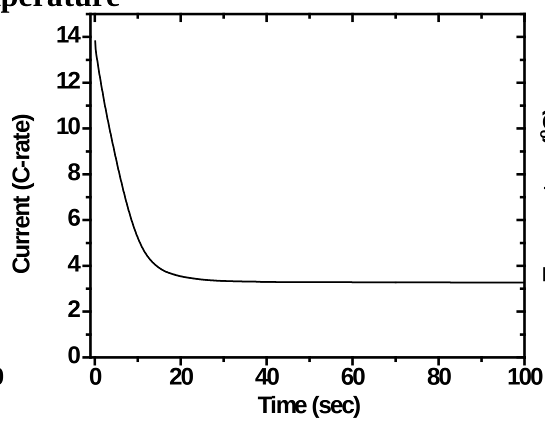
Internal Short (R_{short} = 10 milliohms)

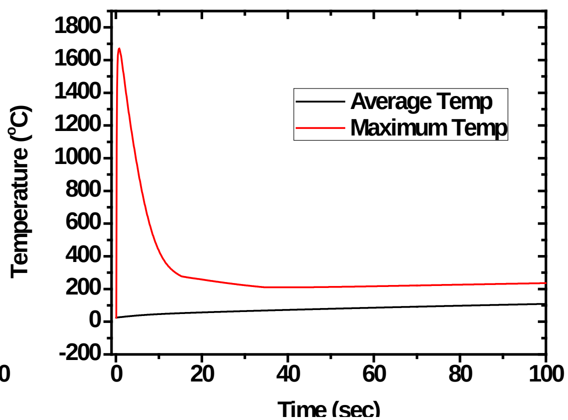
Surface temperature



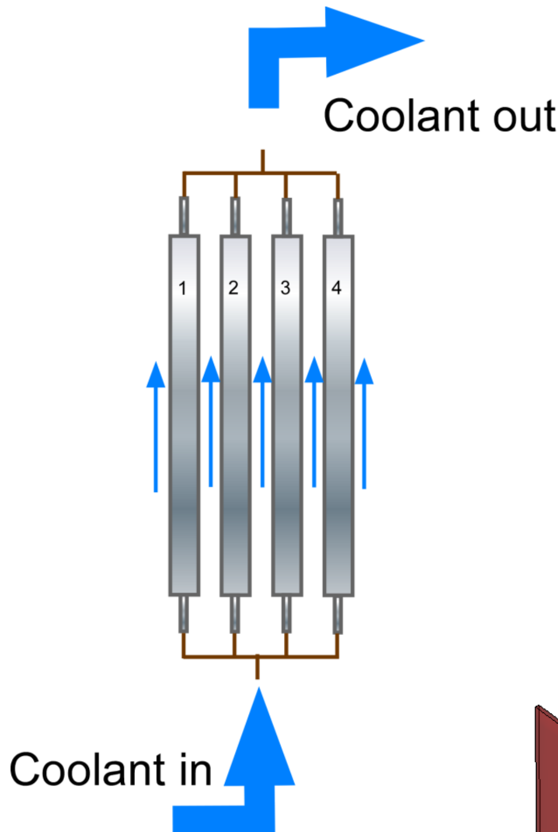
Internal temperature

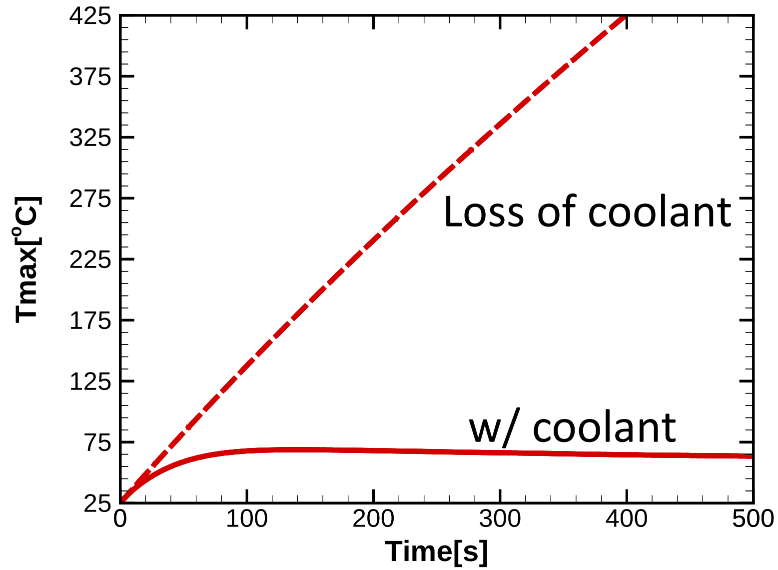






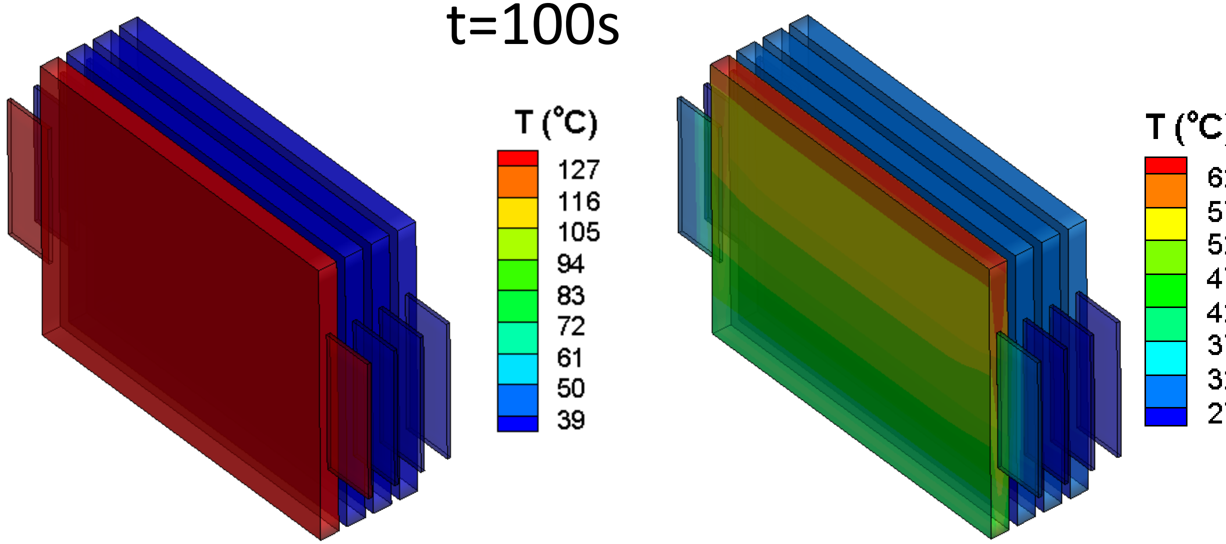
Enhanced Module/Pack Safety





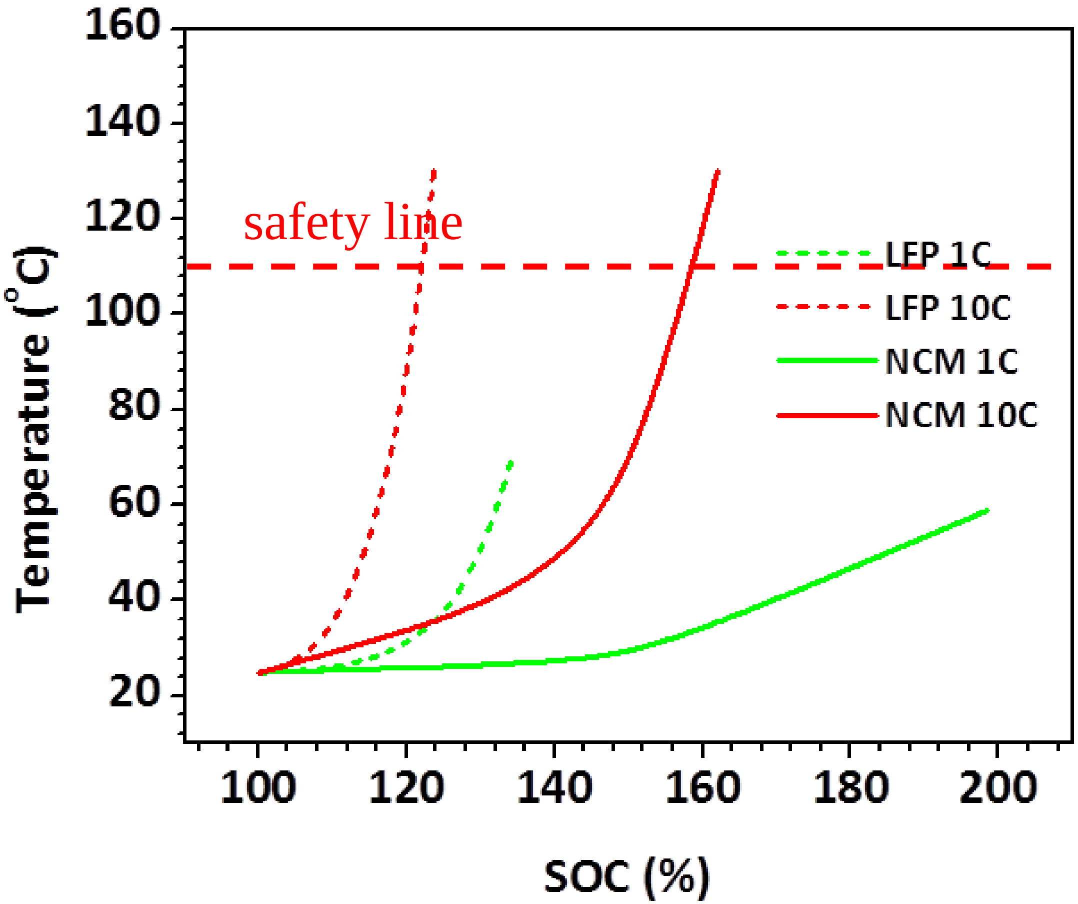
Cells: 35Ah, 4P
AM: Graphite/NMC
Cooling: Liquid
Cell 1 nail-penetrated

t=100s



w/o coolant w/ coolant

Overcharge: Effect of Cathode Material



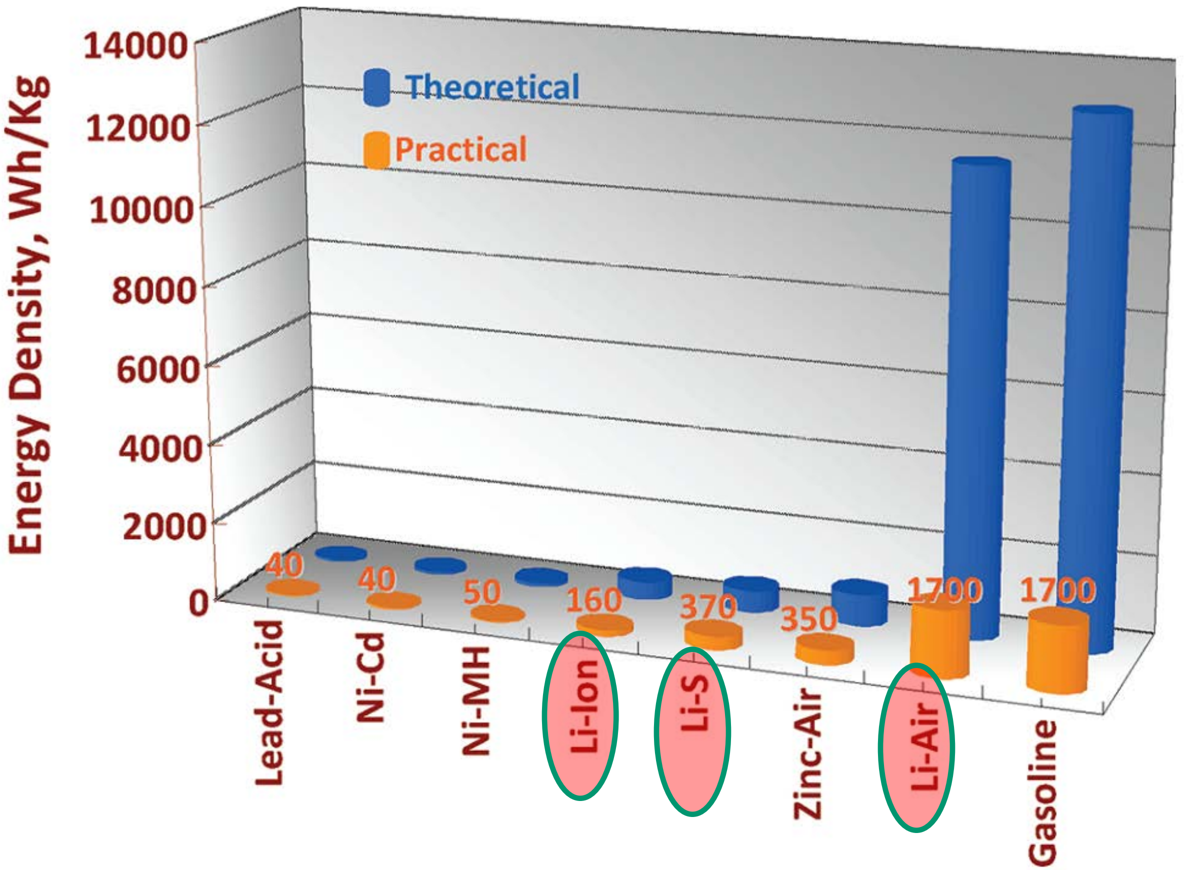
- Cell : NCM 20 Ah, LFP 20 Ah
- Thermal condition: Adiabatic
- Charge current : 1C, 10C

BYD e6 taxi (powered by LFP batteries) caught fire on 6/20/2013 at charging station in Hong Kong.

- Cathode material has dramatic effect on overcharge behavior. LFP is less tolerant to overcharge.
- Significant overcharge of LFP battery even at 1C leads to thermal runaway.

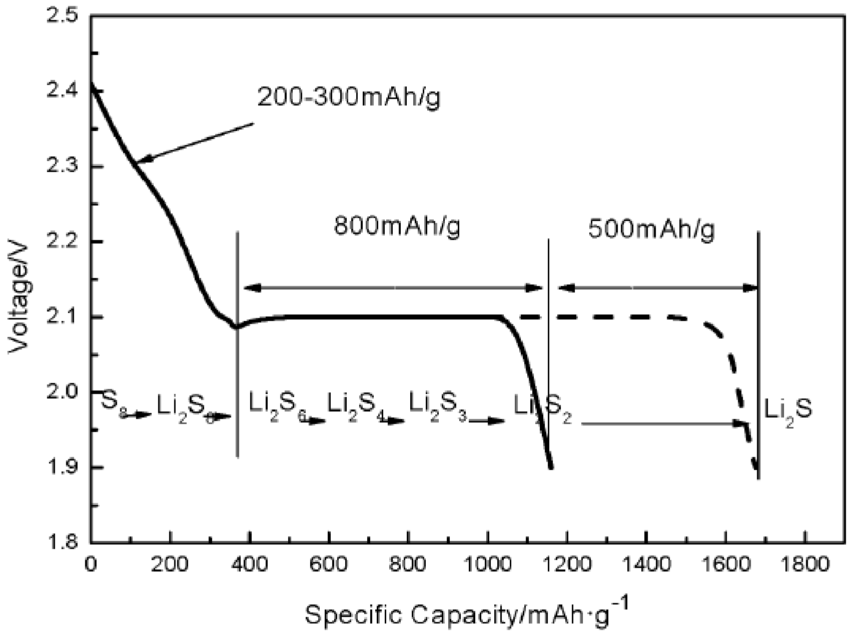
Li-S Battery for Transportation Energy Storage

• Driving range per charge solely depends on energy density of batteries; 300-mile batteries are desirable.



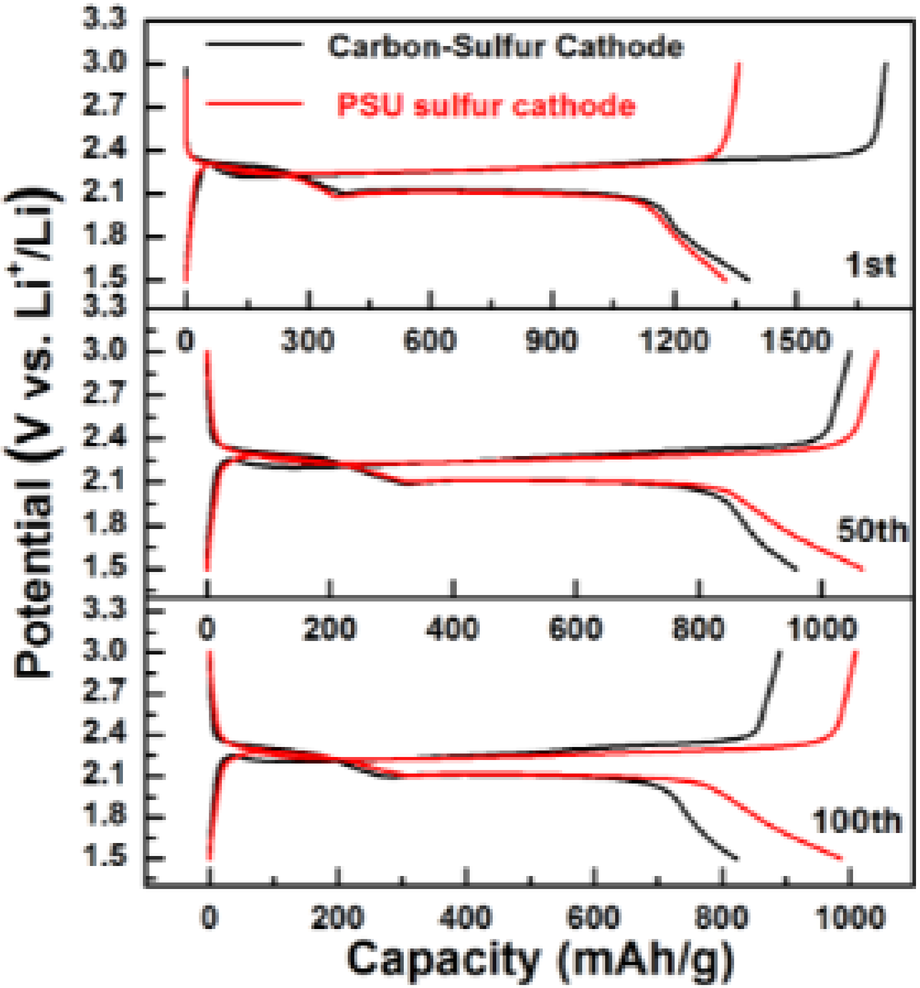
Li-S Battery

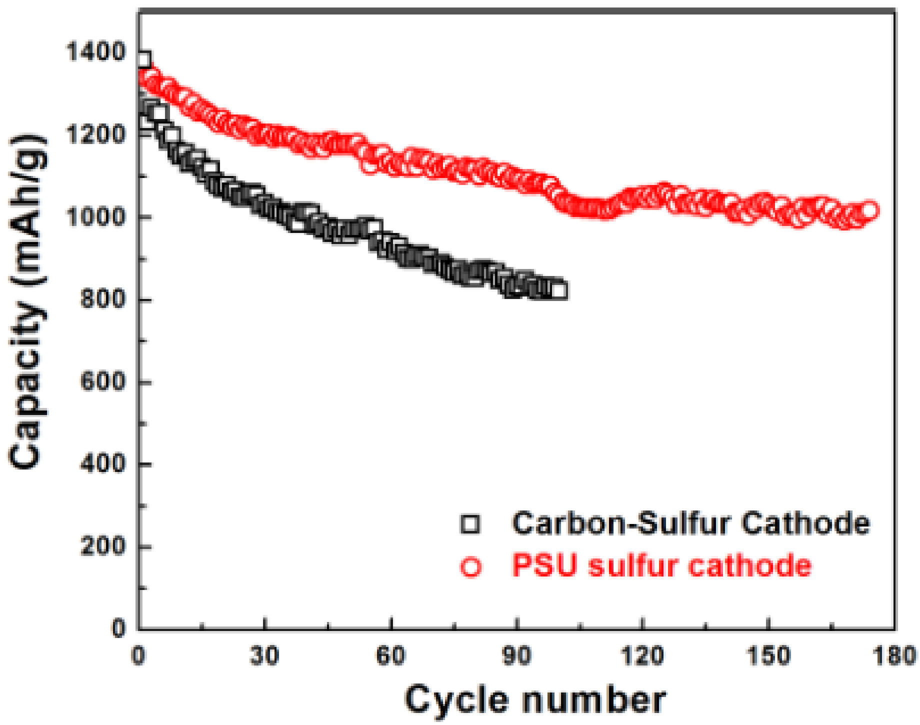
cathode	theoretical capacity (mAh/g)	electrode voltage	actual capacity (mAh/g)	estimated price ($)
$LiCoO_2$	275	3.7	130-140	1
$LiNiO_2$	274	3.4	170-180	0.86
$LiMn_2O_4$	148	3.8	100-120	0.17
V_2O_5	400	2.5	120-200	
S_8	1672	2.1	>1000	0.017



- Issues: polysulfide shuttle effect after dissolution, resulting in low efficiency, low active material utilization; low electronic conductivity
- Solutions: absorbents, electrolyte additives, graphene fillers, etc.

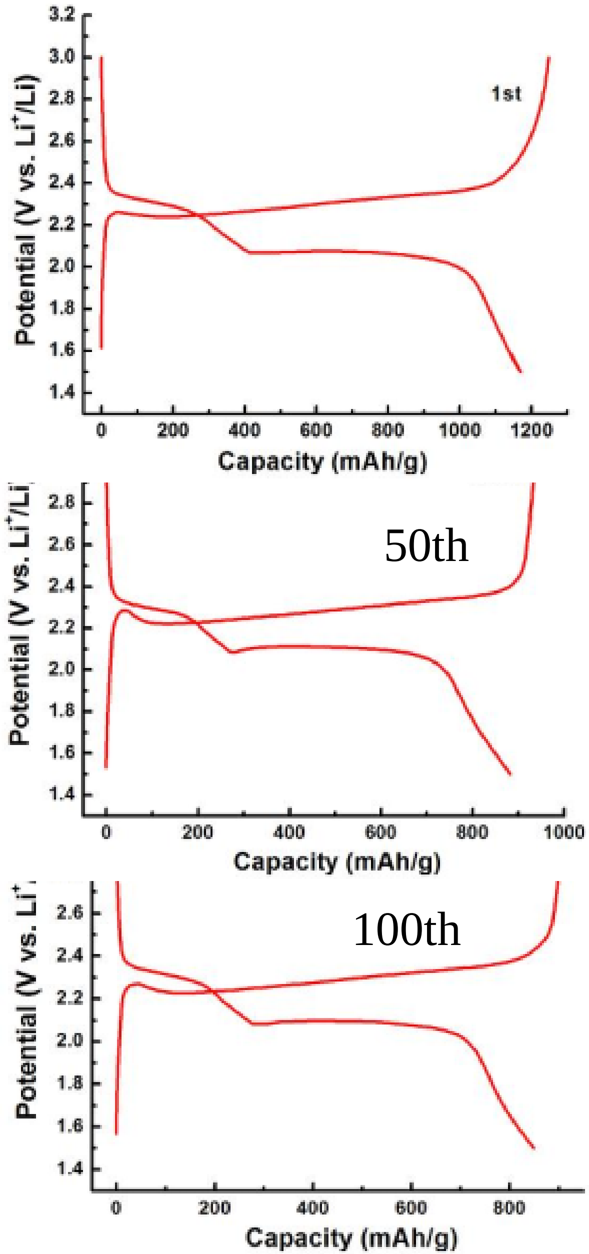
Li-S Cell Performance @ C/10 Rate

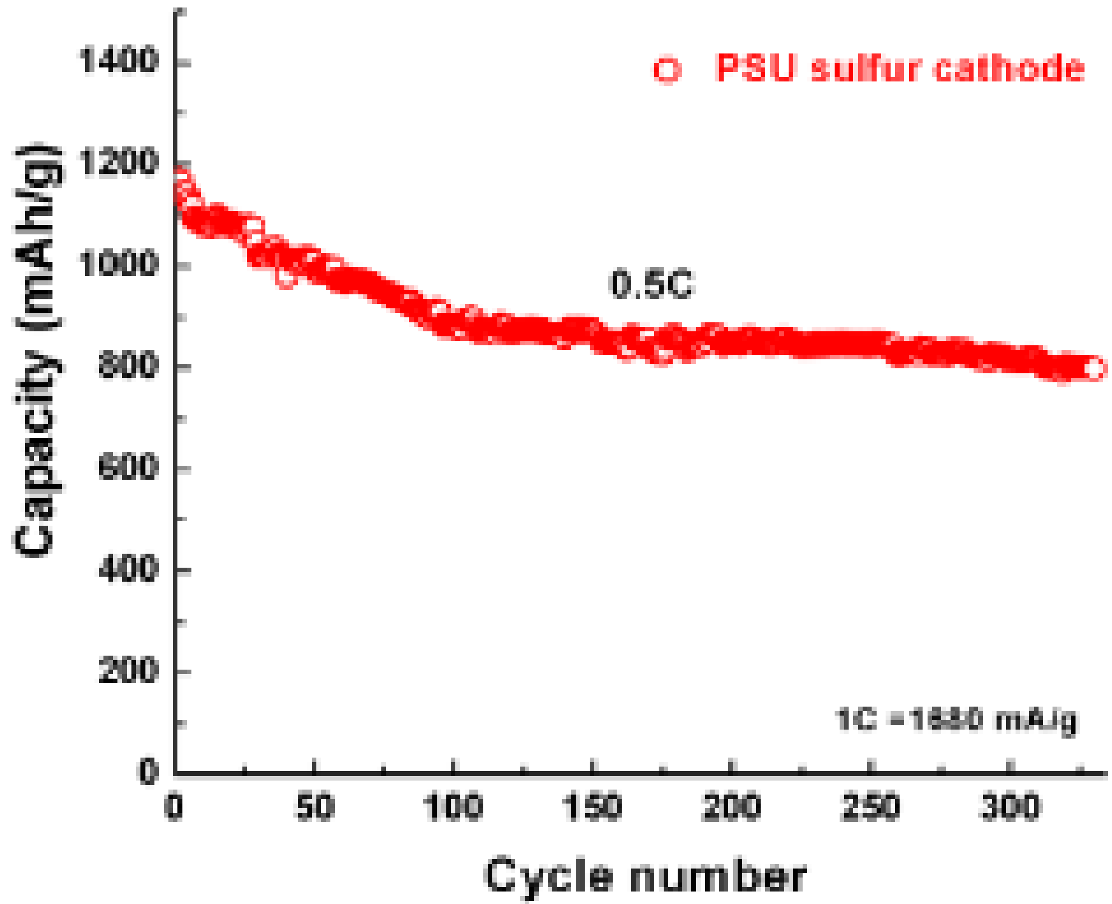




80% capacity retained in 100 cycles
77% capacity retained in 170 cycles

Li-S Cell Performance @ C/2 Rate





75% capacity retained in 100 cycles

70% capacity retained in 300 cycles

Summary

- Current Generation Li-ion Battery for Vehicle Electrification:
  - Specific Energy or Energy Density： 200 Wh/kg or 400 Wh/L
  - Cycle Life： >5000
  - Cost (@ Cell Level)： <$150/kWh
  - High Safety： ~60Ah Cells and large packs still safe
  - CAE of vehicle batteries is a main tool to achieve all above.
- Beyond Li-ion:
  - Li-S battery for 300+ mile range
  - 2x or 3x energy density of current LiB
  - potentially low-cost
  - has achieved 1,000 mAh/g after 200 cycles in coin cells
  - prototyping in 1-10Ah being pursued.

Acknowledgements