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Synthetic Training Data for Artificial Intelligence-Based Li-Ion Diagnosis and Prognosis

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Path dependence of battery degradation

Objective/Significance

Traffic

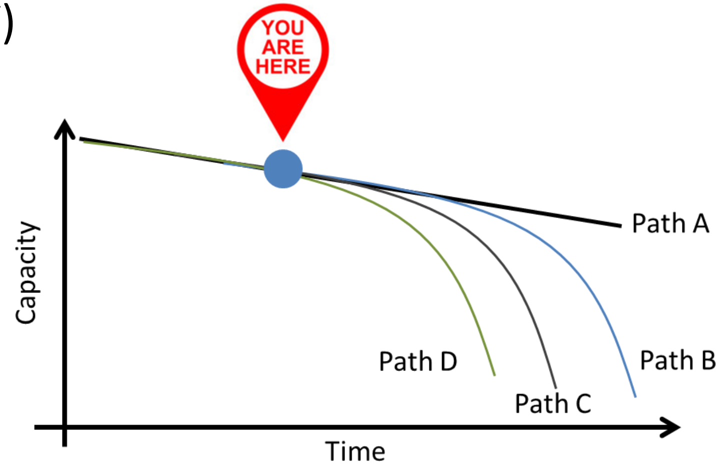
Road type

Driving habits

Charging habits

Temperature

Grid ties (V2G / G2V)



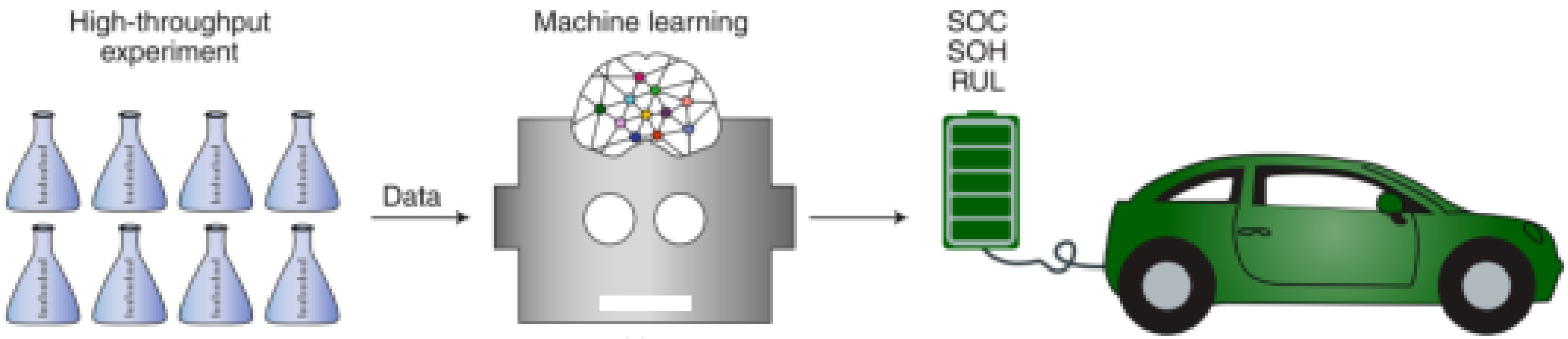
Different paths will lead to different degradation

Every battery is different

Need to test prognosis tools on wide array of scenarios

Artificial Intelligence

Objective/Significance



Little to no effort

Lot of effort

Man-Fai Ng et al., Nature Machine Intelligence, 2(3) p. 161-170 (2020)

Experimental data is costly and time consuming,
Most studies only test a couple batteries,
Biggest dataset we found is 124 batteries with only charge varying

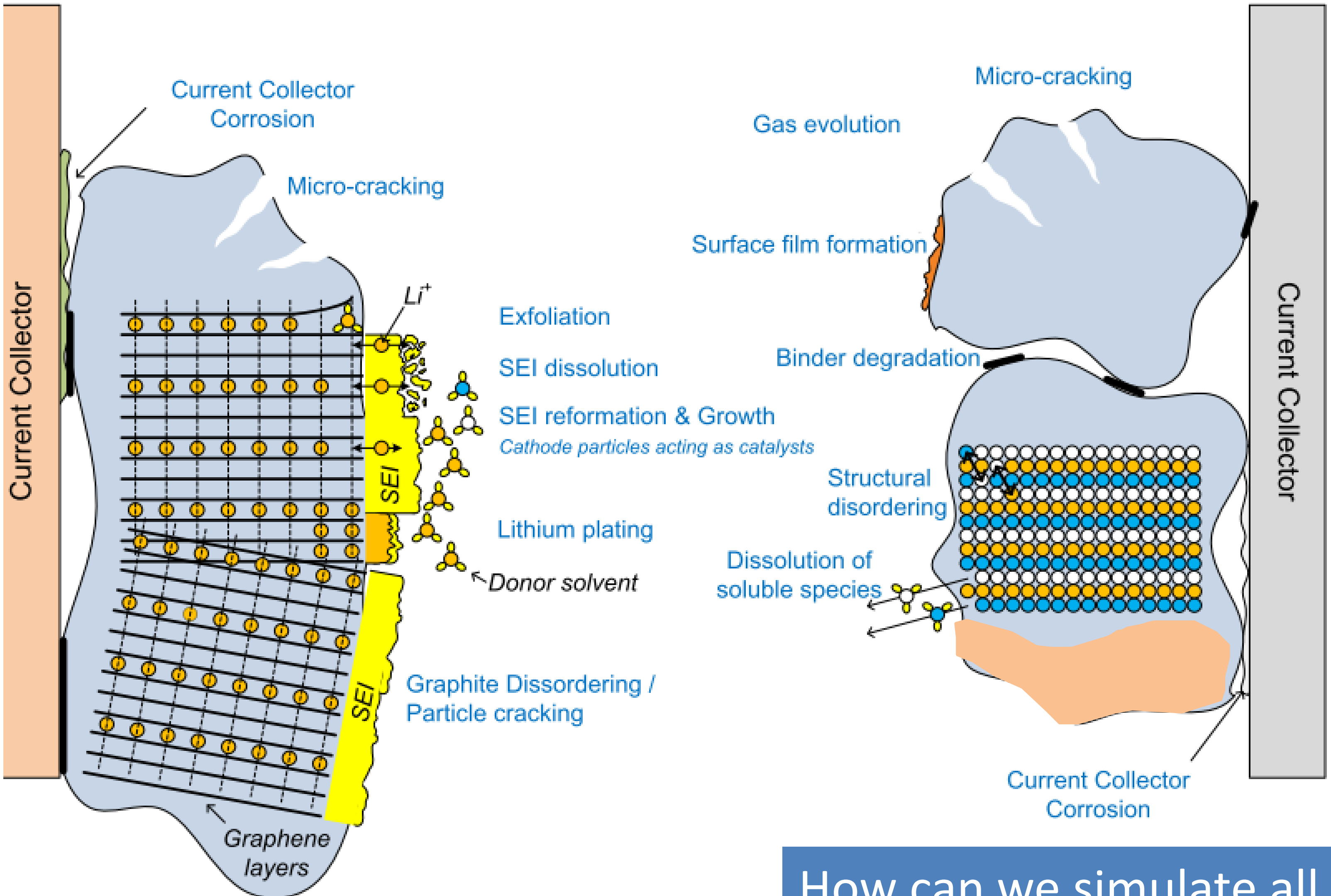
Current state of the art is far from the big data needed to make AI work
Model is at best as good as the training data!

Solution: Create synthetic training datasets

Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms



How can we simulate all of them?

J. Groot, State of Health Estimation of Li-ion batteries cycle life test methods

Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

Model framework considerations

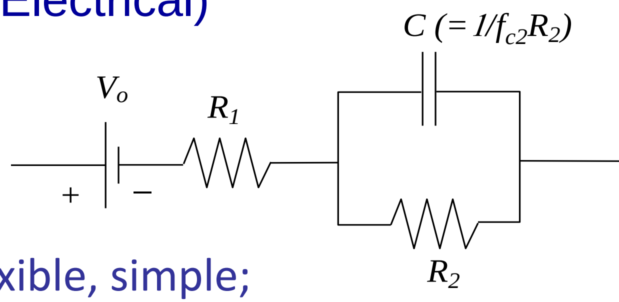
Electrochemical models

“Balance of plant”

$$\frac{\partial i_l}{\partial x} - A_{\max} i_{0,\mathrm{ref}} \left(\frac{c}{c_{\mathrm{ref}}}\right)^{\gamma} SOC^{\zeta} \left(\exp\left(\frac{(1-\alpha)nF}{RT}(\Phi_s - \Phi_l - U)\right) - \exp\left(-\frac{\alpha nF}{RT}(\Phi_s - \Phi_l - U)\right)\right) - A_{\max} C_{\mathrm{dl}} \left(\frac{\partial \Phi_s}{\partial t} - \frac{\partial \Phi_l}{\partial t}\right) = 0$$

Use mechanistic descriptions with system topology for analysis

Equivalent circuit models (Electrical)



Universal, flexible, simple; mechanistic for diagnosis
Difficult for path dependence

Use conservation principles to solve kinetic and mass transport equations

Different flavors with “forward looking” approach

Empirical models

Need a large amount of training data to derive fitting parameters and algorithms

Computation intensive; very challenging with path dependence; difficult for diagnosis

What about a backward looking model?

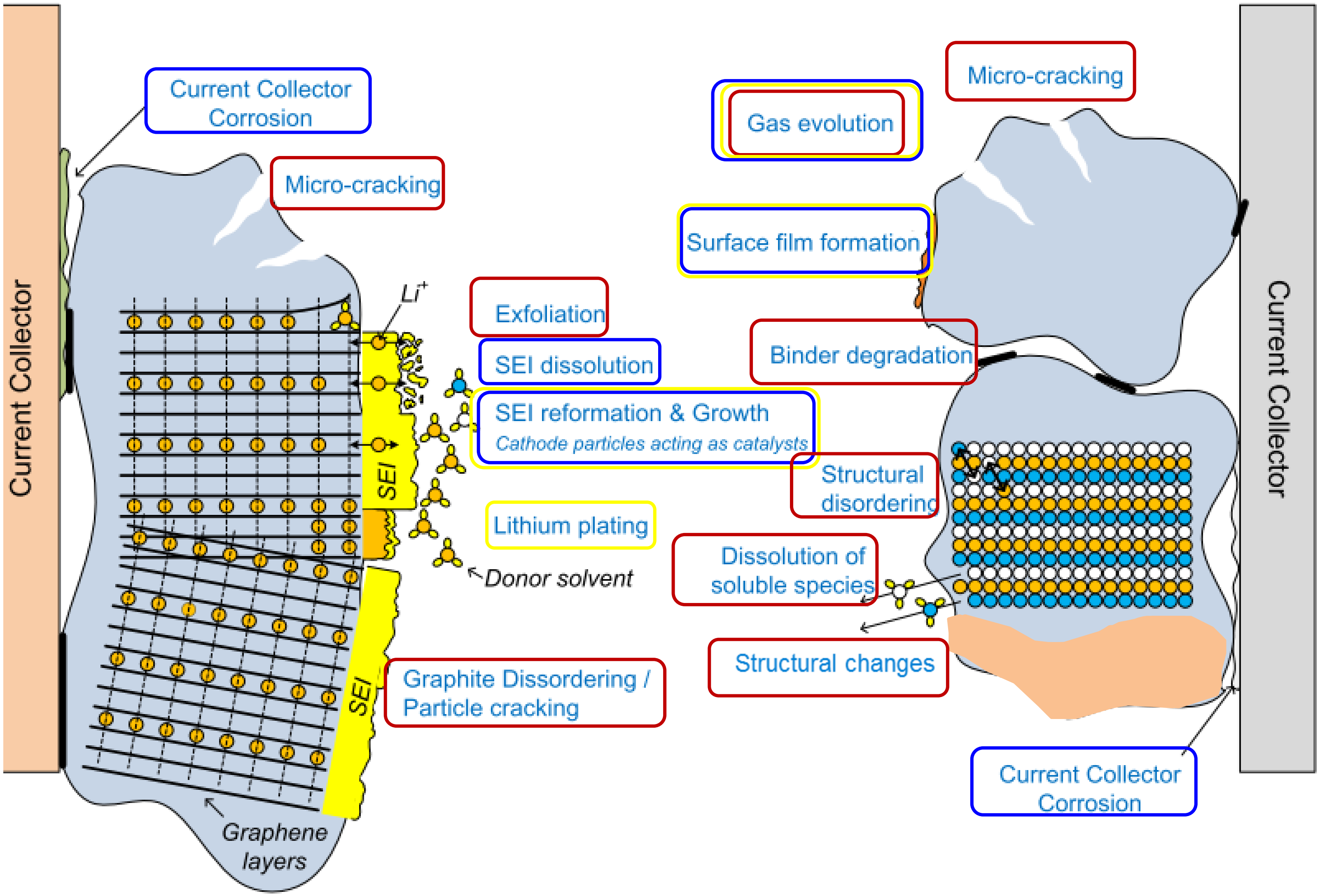
…bstantial resources to develop; limited applicability & less practical

Dubarry, M., et al. (2012). Journal of Power Sources **219**: 204-216.

Li-ion batteries are complex systems

Lithium ion battery degradation mechanisms

Useful categorization for diagnostics



Thermodynamics

Change in active material

Change in lithium inventory

Kinetics

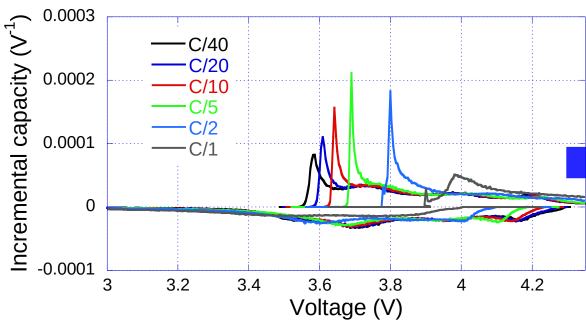
Change in ohmic and faradic resistances

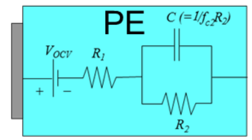
J. Groot, State of Health Estimation of Li-ion batteries cycle life test methods

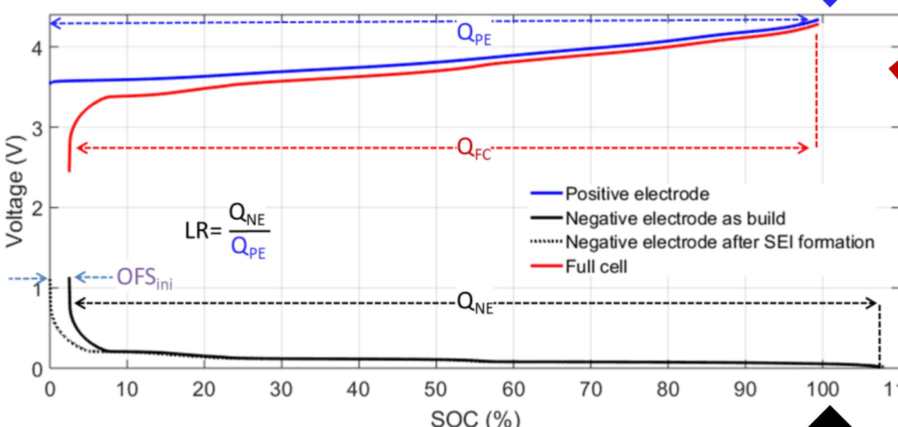
Mechanistic diagnosis and prognosis

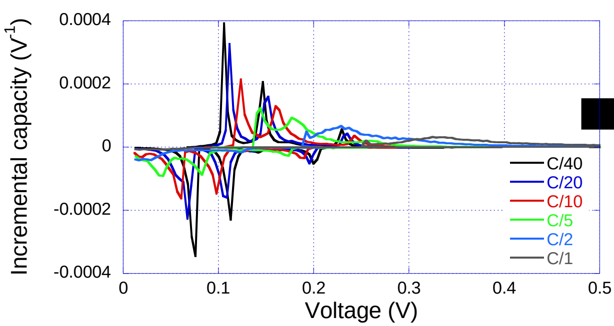
Cell emulation: the ‘alawa toolbox

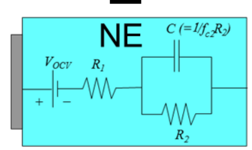
Mechanistic modeling

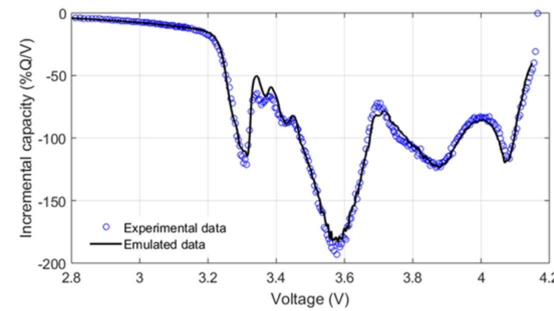


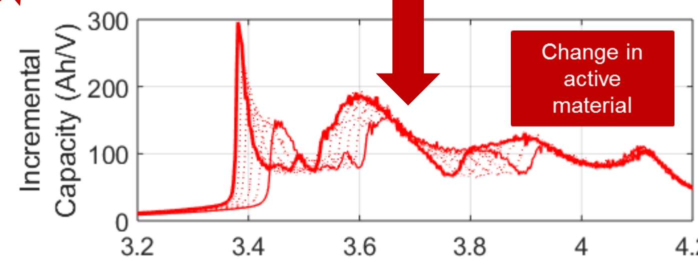


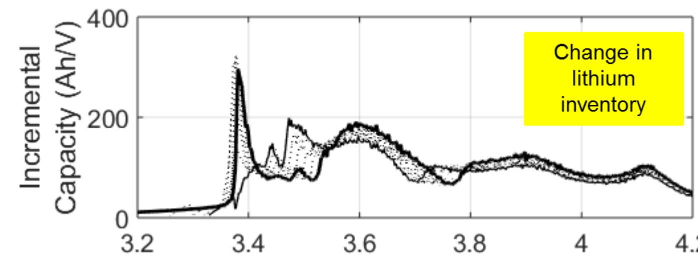


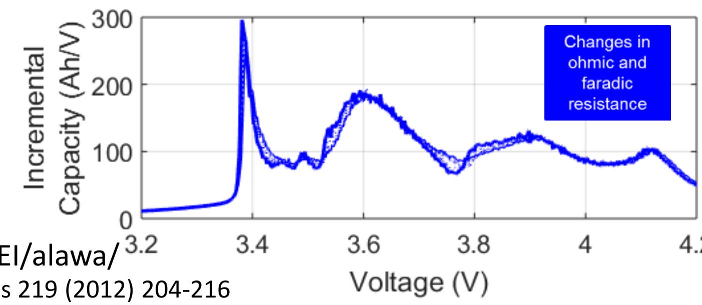












https://www.soest.hawaii.edu/HNEI/alawa/

M. Dubarry et al. Journal of Power Sources 219 (2012) 204-216

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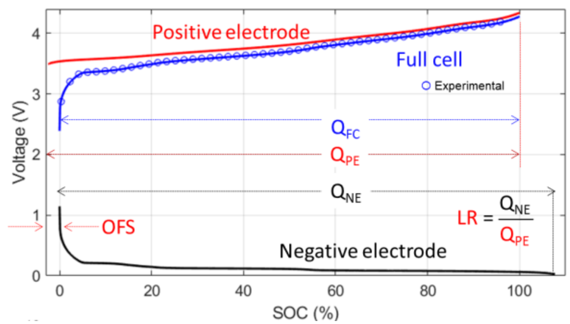
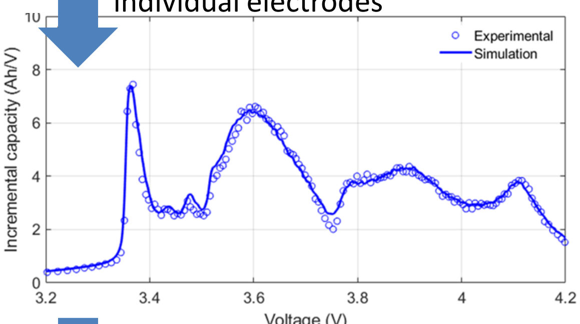
Mechanistic modeling

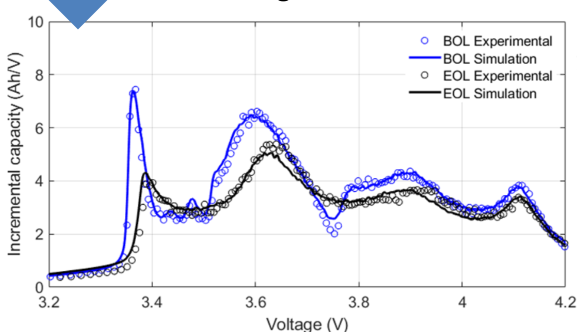
Simulation of individual degradation modes

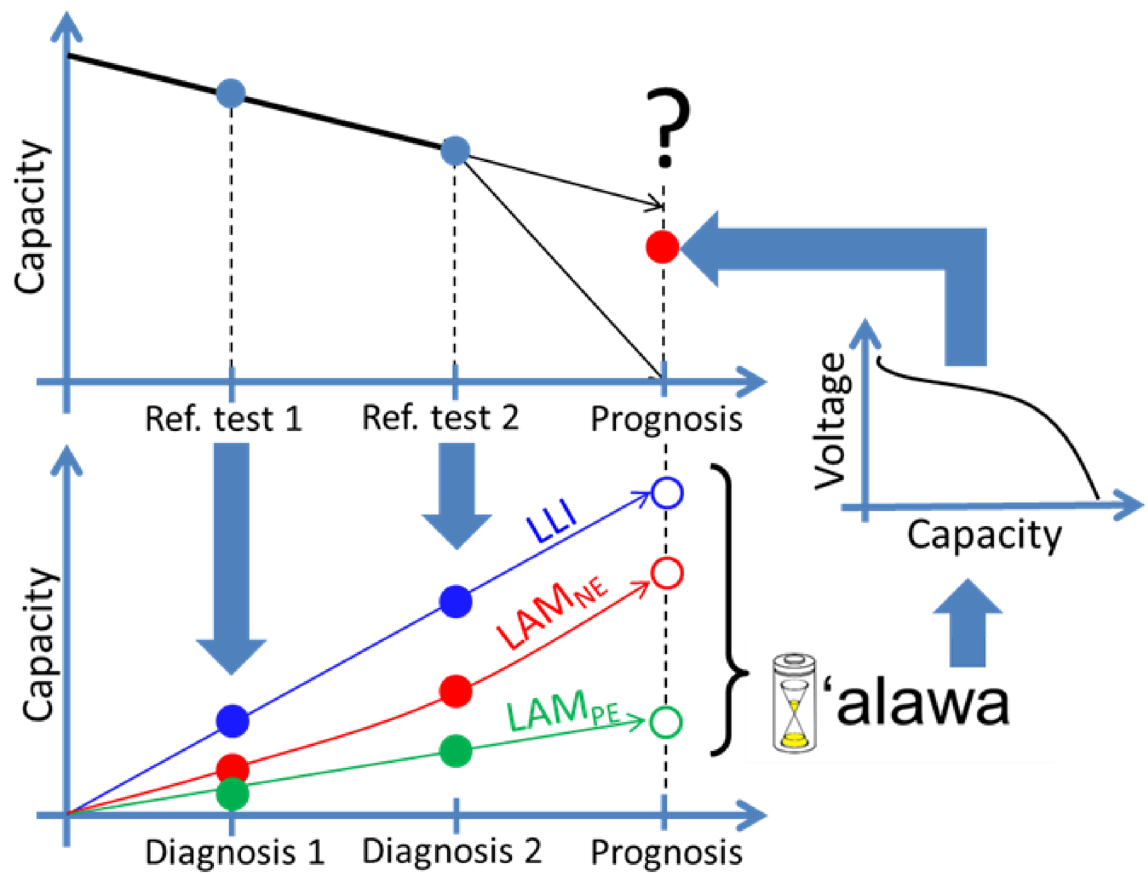


Match experimental cell based on individual electrodes



Vary matching parameters to emulate degradation





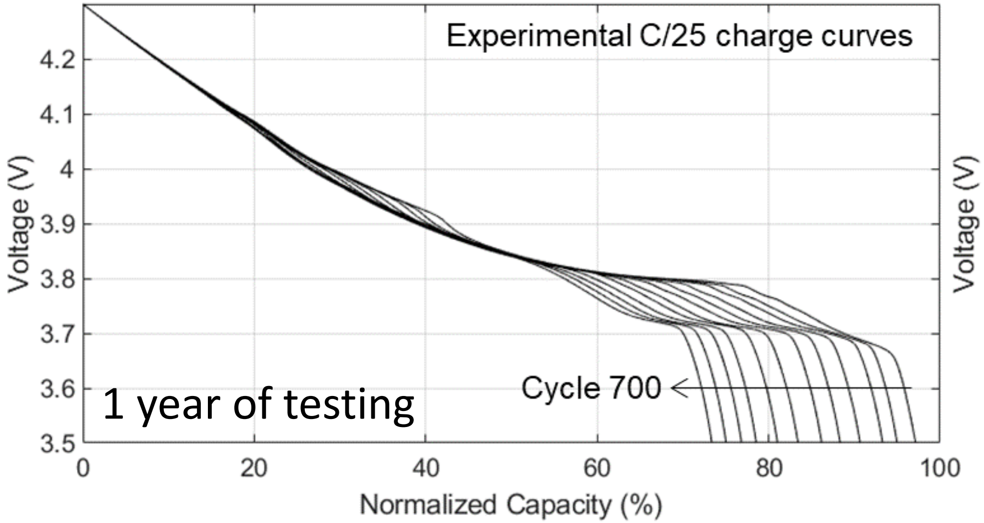
M. Dubarry et al. / Journal of Energy Storage, 29, 101391 (2020); doi: 10.1016/j.est.2020.101391

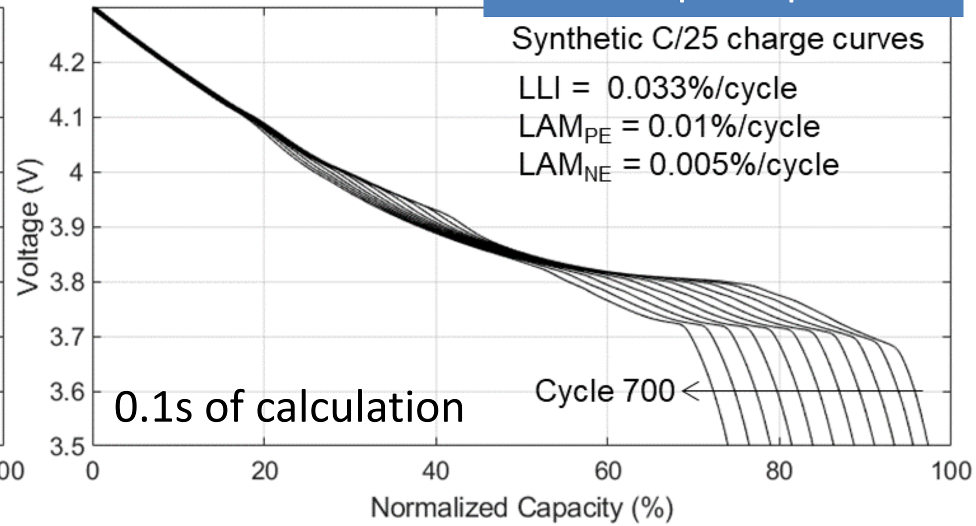
Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

Use the mechanistic modeling approach

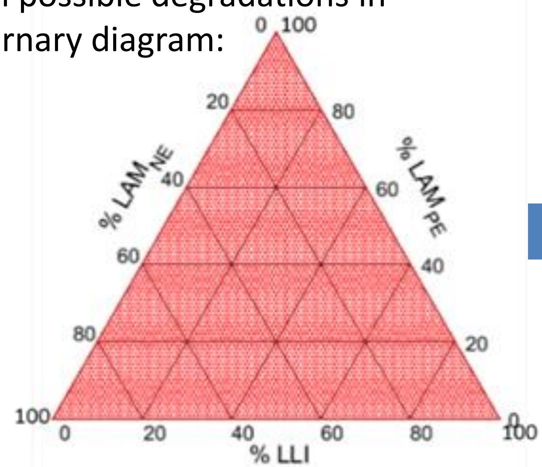
Emulation of battery electrochemical response

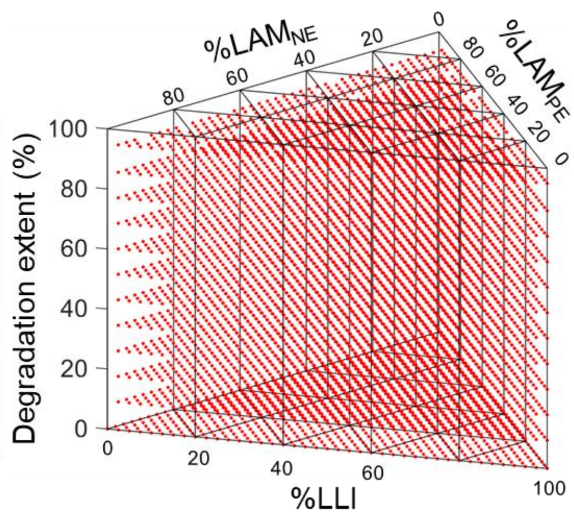
Aging reconstructed from simple equations





All possible degradations in ternary diagram:





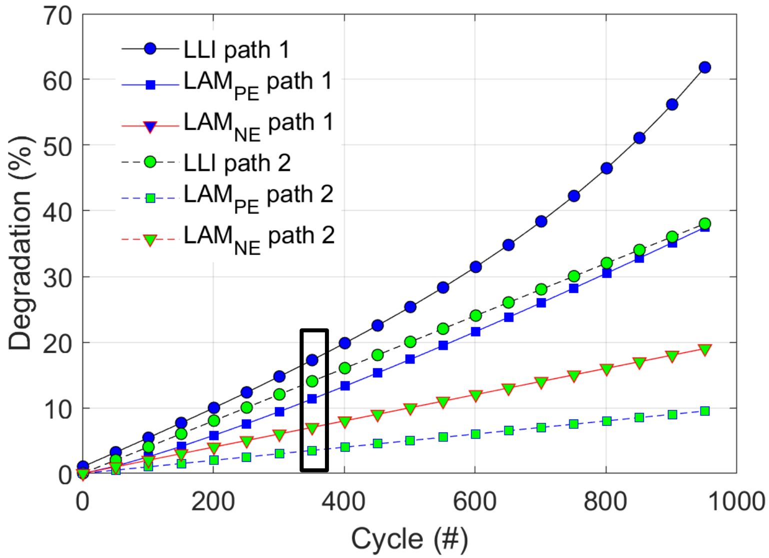
Infinite training data for diagnosis AI algorithms

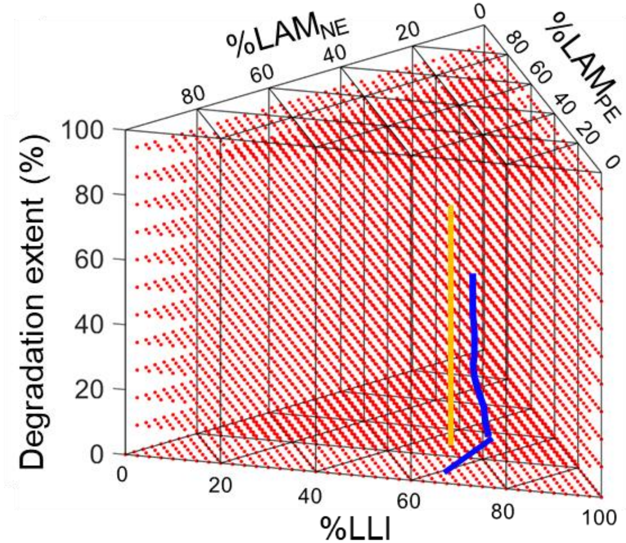
Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

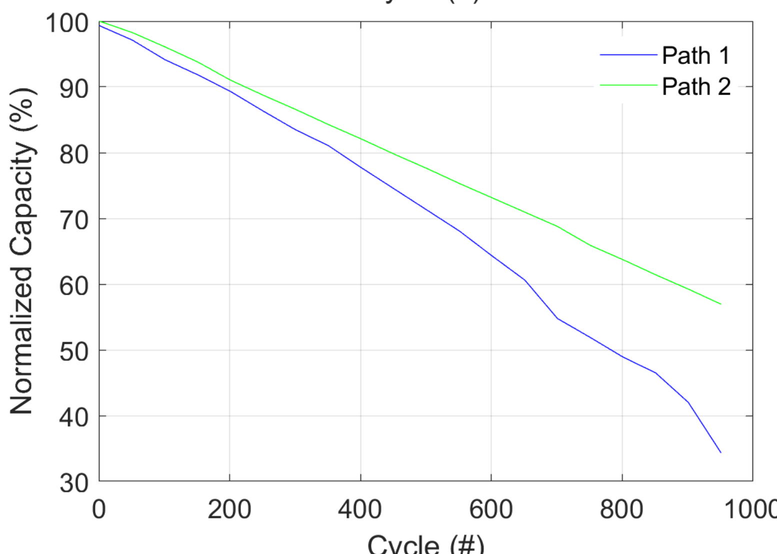
Dubarry, M., et al. (2017). "State of health battery estimator enabling degradation diagnosis: Model and algorithm description." Journal of Power Sources **360**: 59-69.

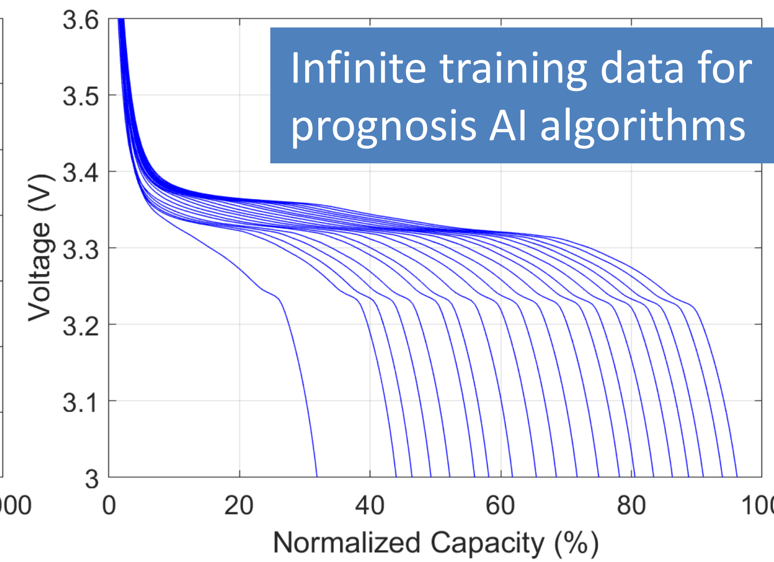
From diagnosis to prognosis

Prognosis: Needs to build full life-cycles









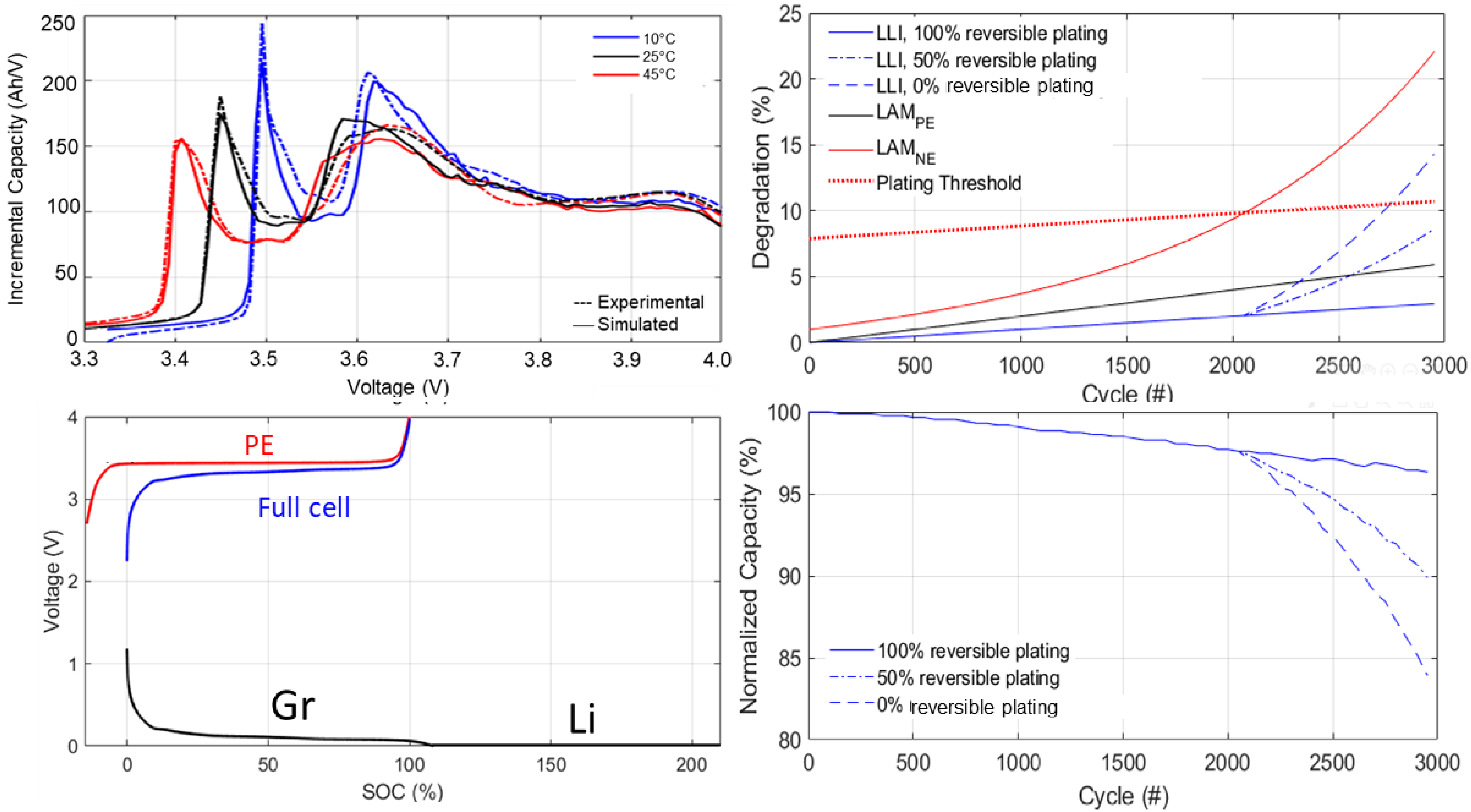
Infinite training data for prognosis AI algorithms

Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Synthetic Training Data for AI Li-Ion Diagnosis and Prognosis

More complexity for real scenarios

More than LLI and LAMs… Kinetics, blends and plating



Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Baure, G. and M. Dubarry (2019). "Synthetic vs. Real Driving Cycles: A Comparison of Electric Vehicle Battery Degradation." Batteries **5**(2).

Dubarry, M., et al. (2020). "Perspective on State-of-Health Determination in Lithium-Ion Batteries." Journal of Electrochemical Energy Conversion and Storage **17**(4): 1-25.

Schindler, S., et al. (2019). "Kinetics accommodation in Li-ion mechanistic modeling." Journal of Power Sources **440**: 227117.

Computed datasets

Open access synthetic datasets : LFP vs. Graphite

Diagnosis

>5,000 {LLI,LAM_{PE},LAM_{NE}}

0.85% resolution

> 500,000 V vs. Q curves

Prognosis

> 100,000 duty cycles

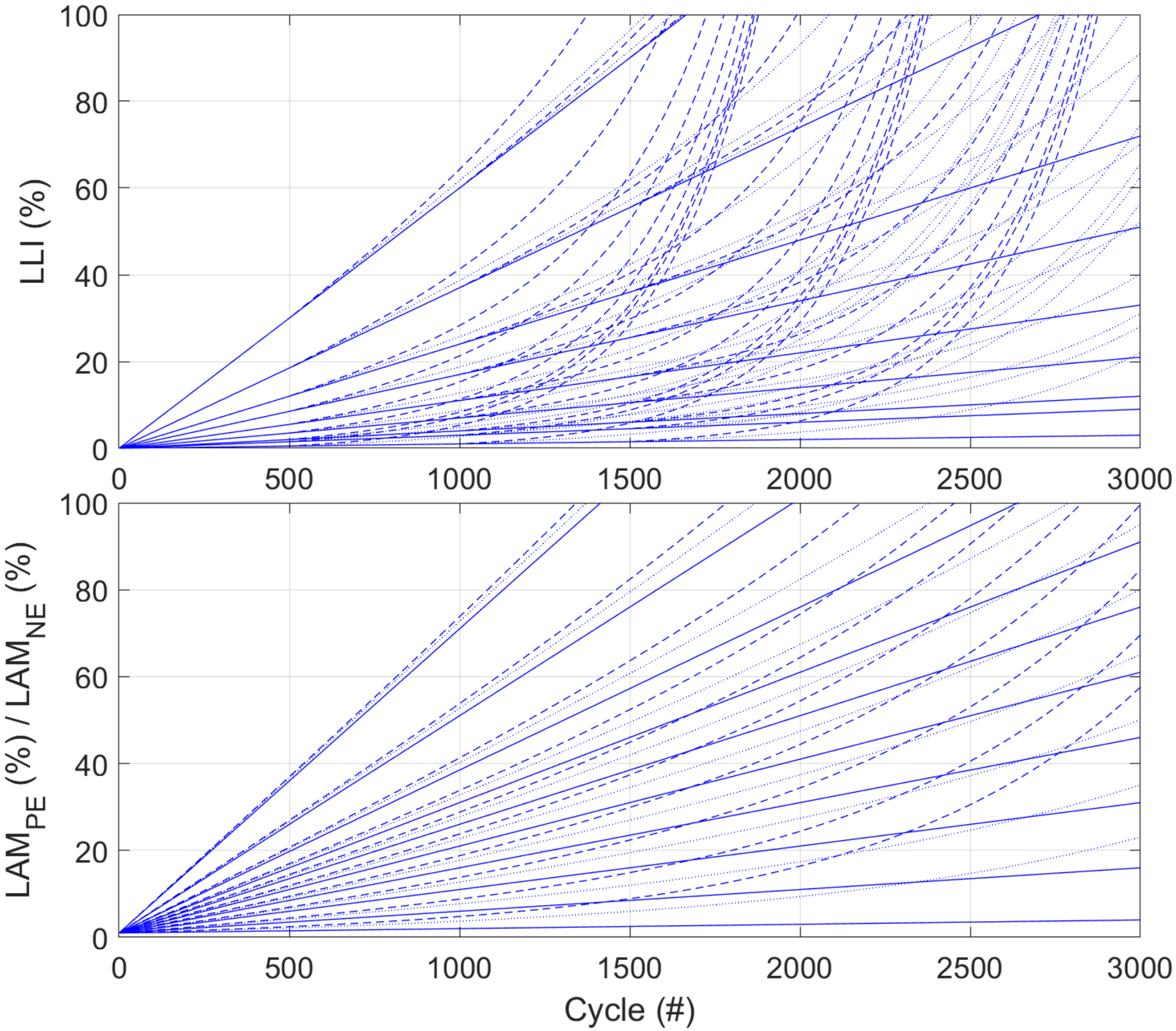
> 3,000,000 V vs. Q curves

8 parameters varied

$\%deg = a \times cycle + e^{(b \times cycle)-1)}$

For LLI, LAM_{NE}, & LAM_{PE}

Plus delay and plating rev.

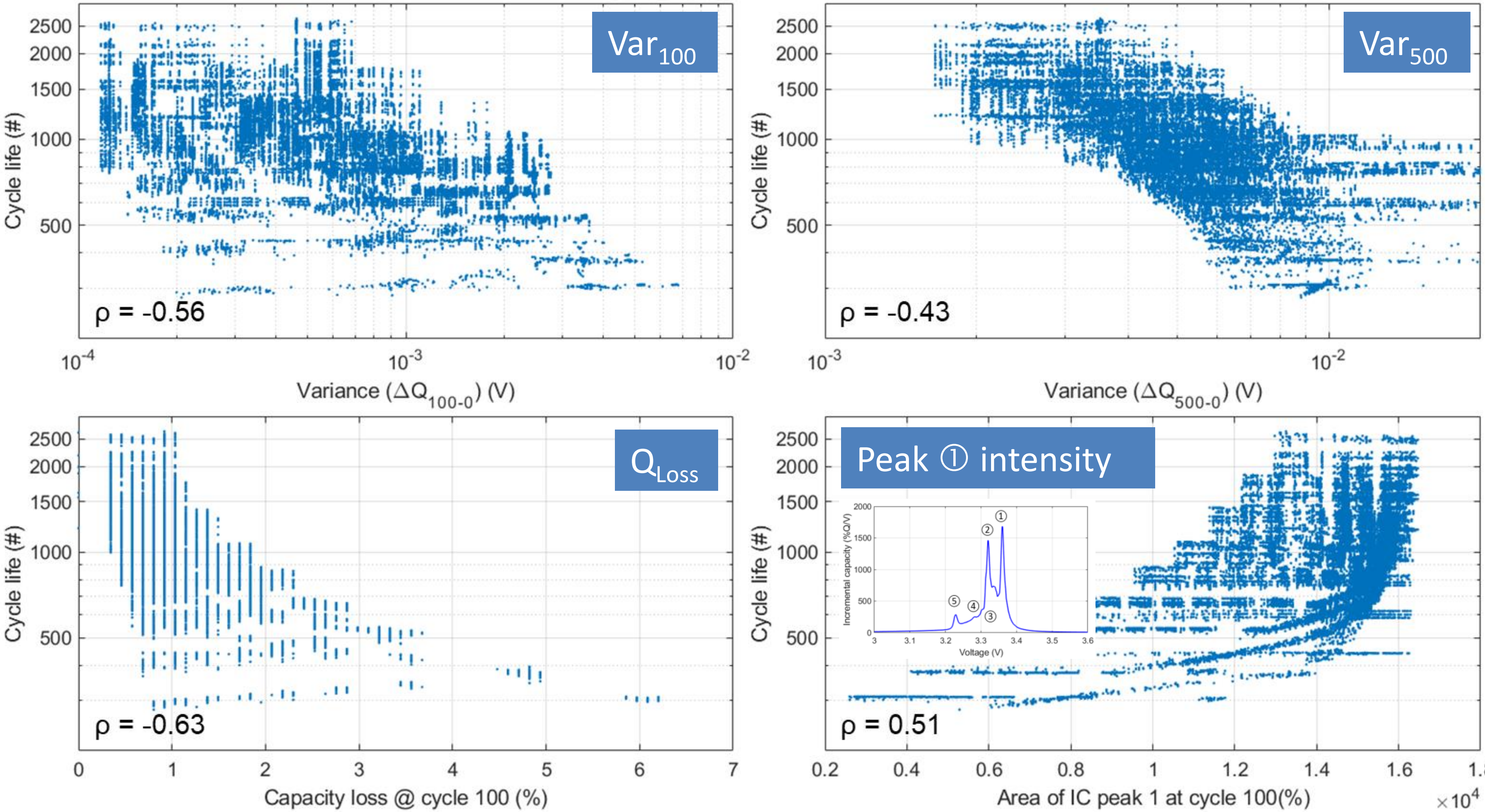


Graphite//LFP synthetic training diagnosis dataset, https://data.mendeley.com/datasets/bs2j56pn7y/1,
Graphite//LFP synthetic training prognosis dataset, https://data.mendeley.com/datasets/6s6ph9n8zg/1

Sensibility analyses

Datasets can be used for training or for sensibility analysis.

What parameters can be used for early prognosis?



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Conclusions

Proof-of-concept methodology to generate big data training datasets

Universal tool for creation of data indistinguishable from real one

Broad applicability: cell chemistries, designs, and operating modes

Methodology could be applied to different conditions such as rate and temperature

Can handle lithium plating with adjustable reversibility

The approach do not remove the need for experimental testing

It is still essential, and the only way, to decipher which conditions cater to specific degradation.

More details: M. Dubarry et al., Journal of Power Sources 479 (2020) 228806

Acknowledgments

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Thank you for tuning in!

Other presentations at PRIME: A01-0046 & A06-1063

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