Physics-Informed Features for Tuning Predictive Simulations of Battery Remaining Useful Life

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Thanks to
DOE (ARPA-E), U.S. ARMY (GVSC), NSF, NIST, CRC, A123, Amphenol, Daimler, Ford, GE, GM, LG, and Samsung

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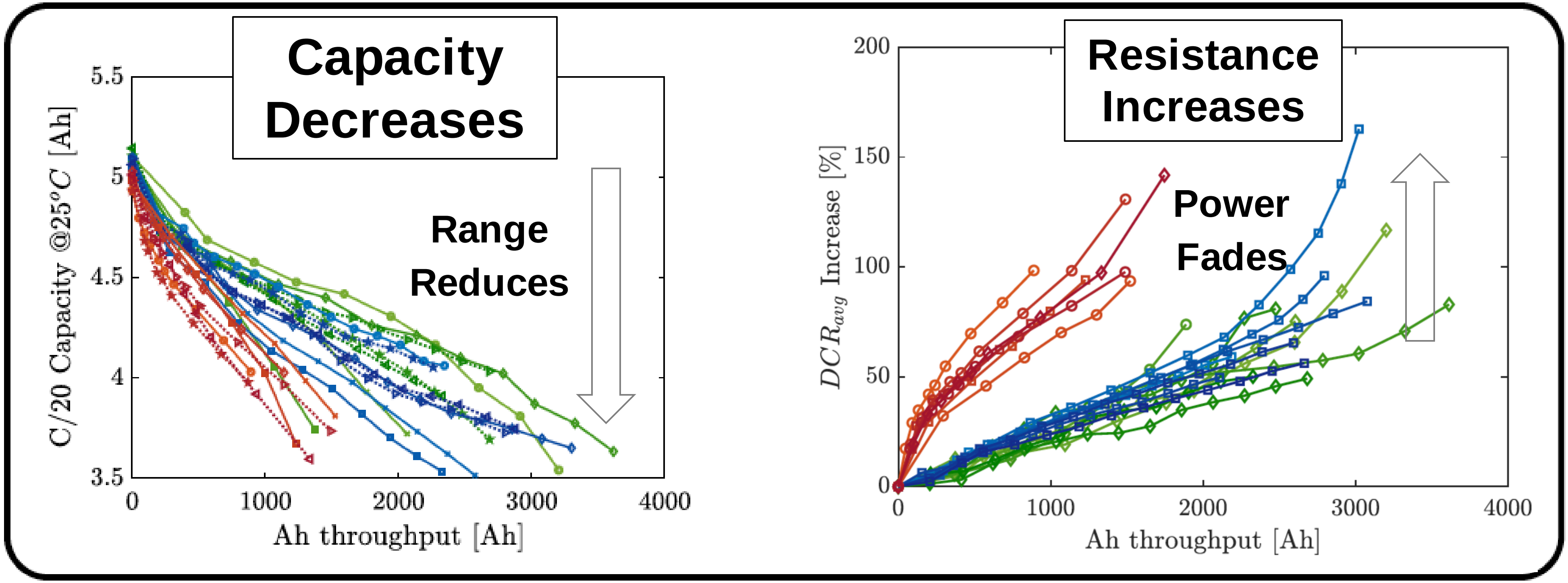
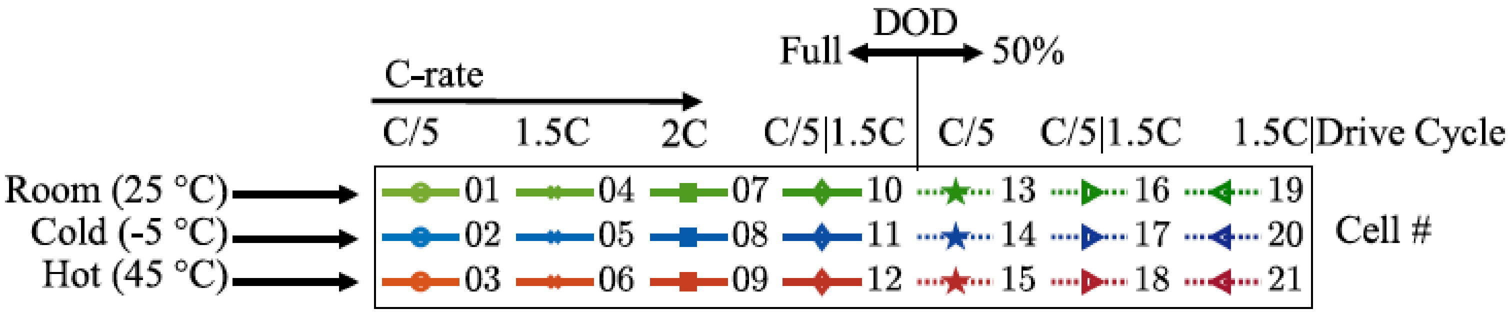
Cycling Conditions and Cell-level Degradation

Knees



Elbows



Mohtat et al, JECS 2021
Mohtat, et al, JPS 2021

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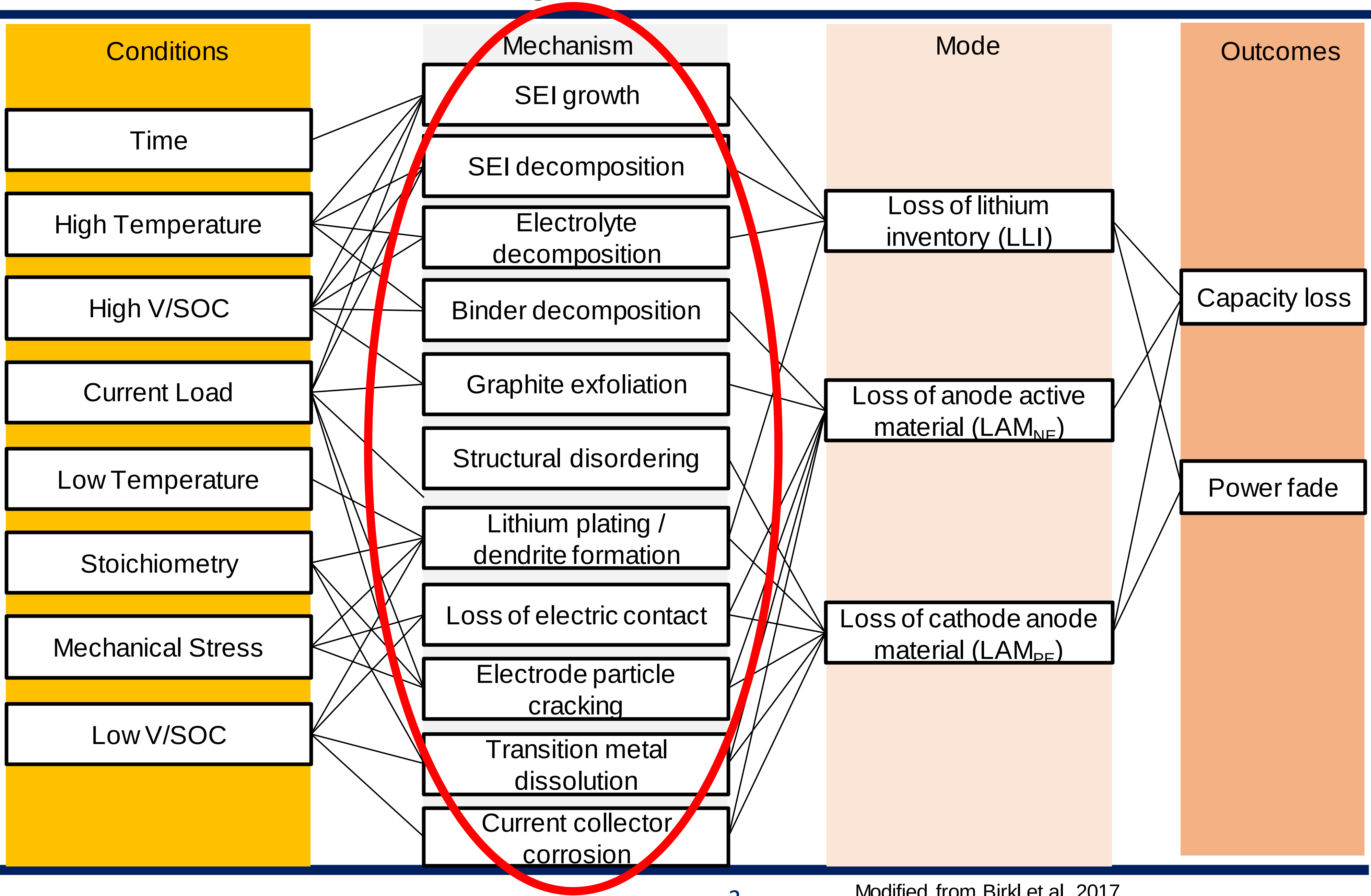
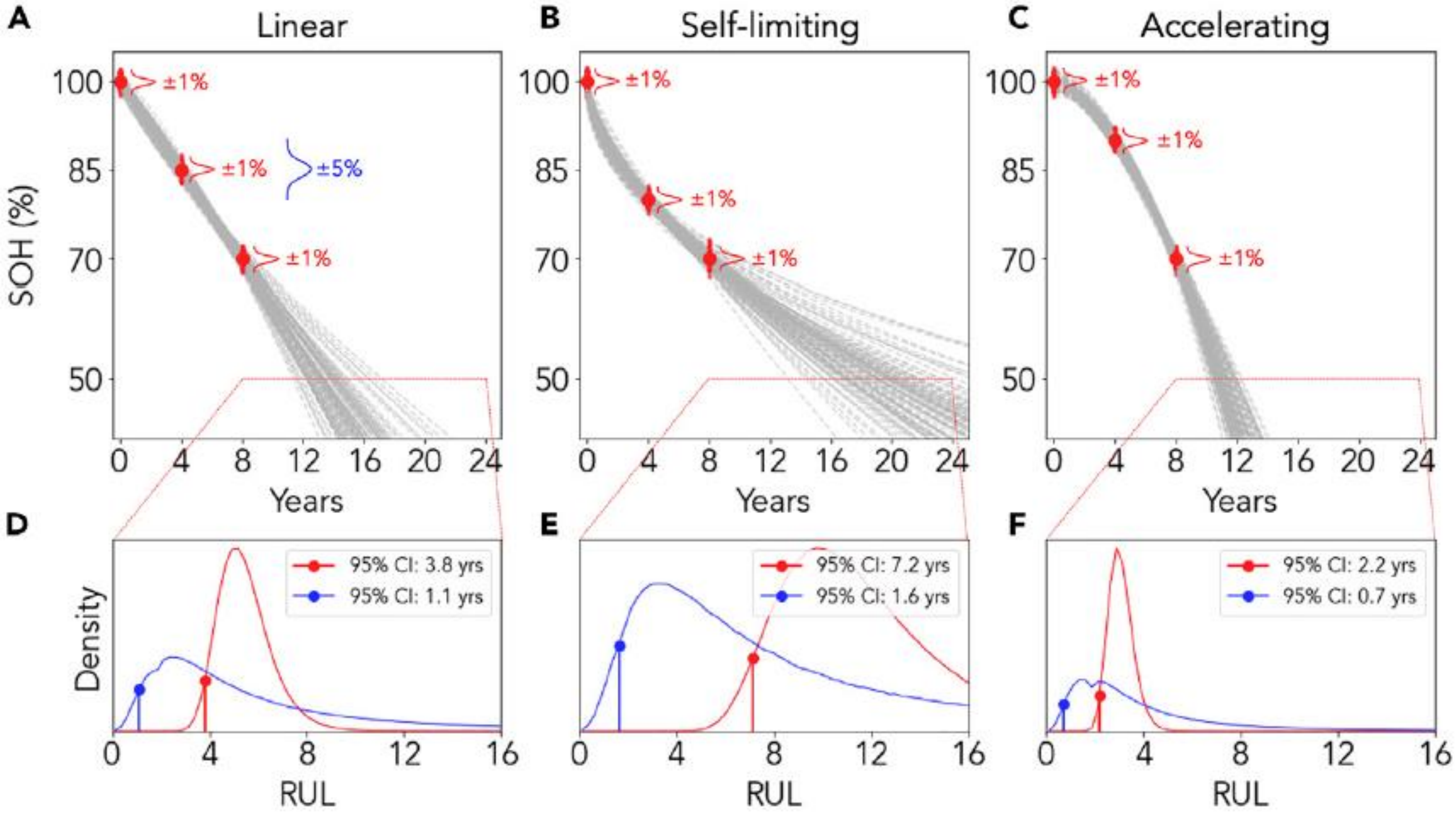
Degradation Mechanisms



Modified from Birkl et al. 2017

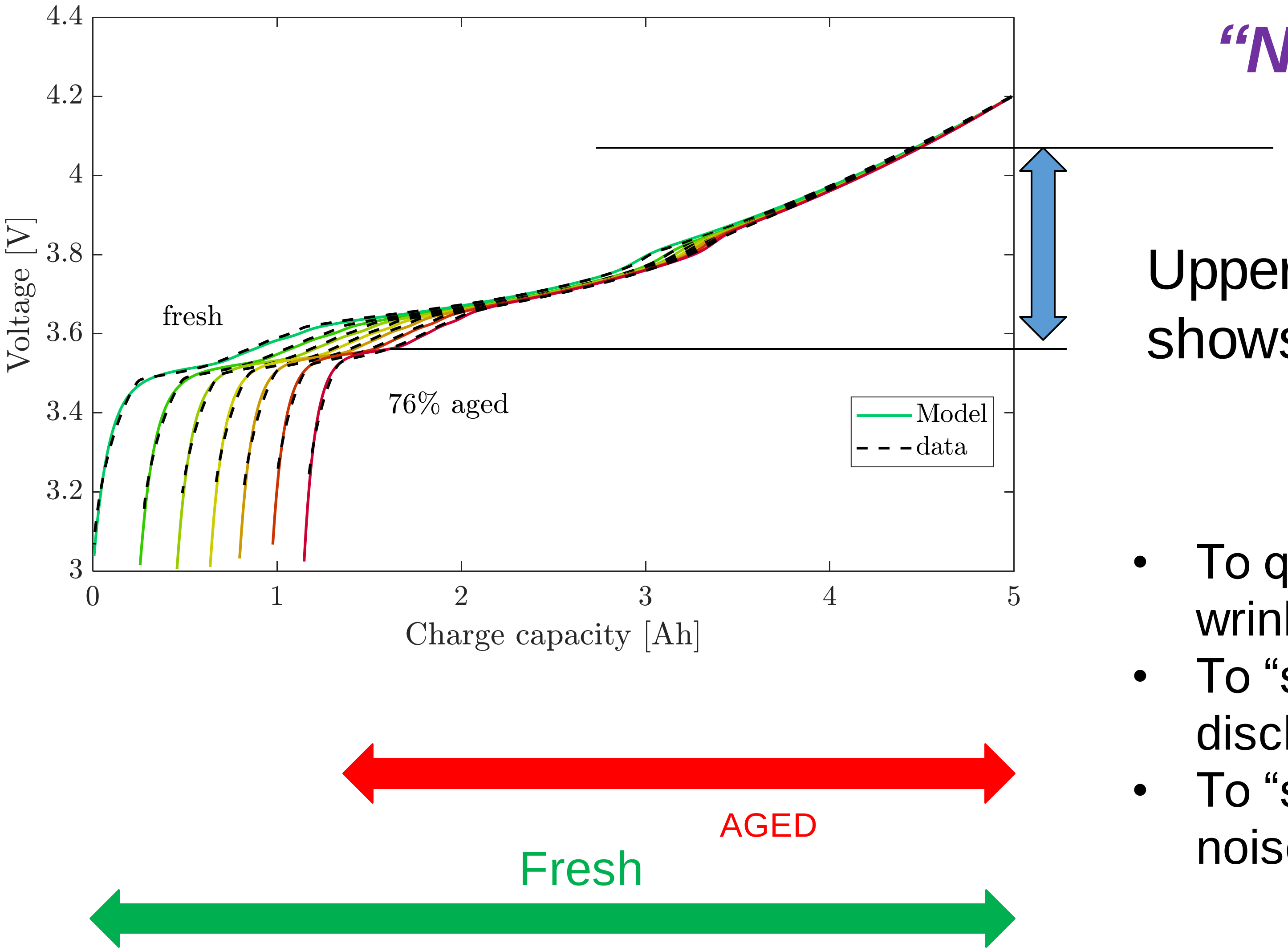
New On-board Diagnostics Regulations

EU Battery Passport and CARB SOH Diagnostics
require <5% accuracy



A. Weng, et al, Battery passports for promoting electric vehicle resale and repurposing, Joule 2023

State of Health (SOH) Estimation for Aged Cells



"Nearly Unobservable until High Depth of Discharges!"

Upper part of voltage range shows little signs of aging

- To quantify capacity fade, you must "see" the wrinkle in V versus accepted charge.
- To "see" them you need high depth of discharge (DOD)
- To "see" them you need low Voltage sensor noise

Estimation error bound of battery electrode parameters with limited data window S Lee, et al IEEE Transactions on Industrial Informatics 16 (5), 3376-3386, 2019

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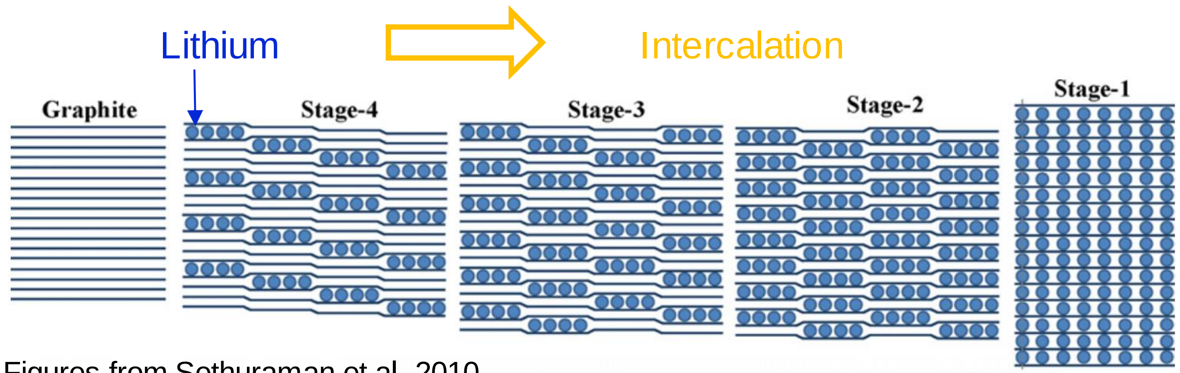
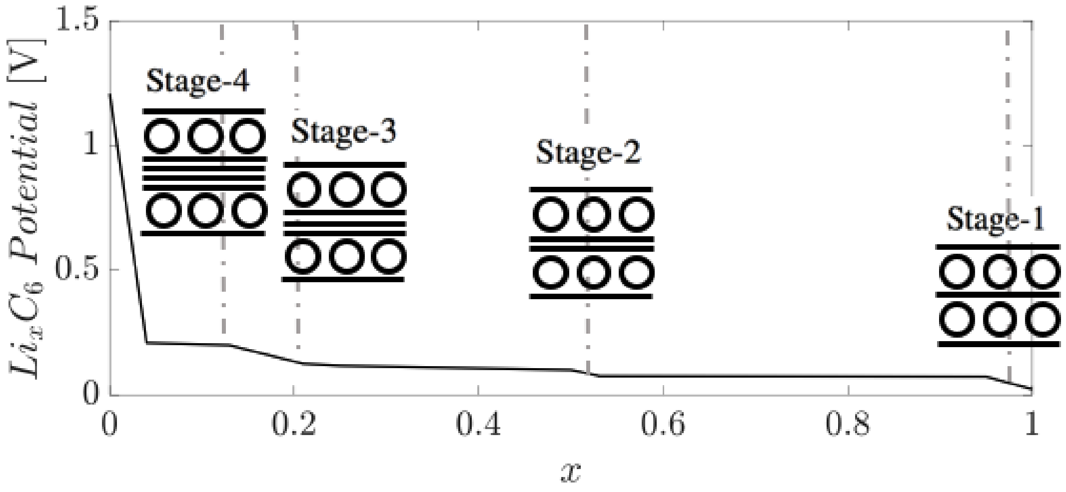
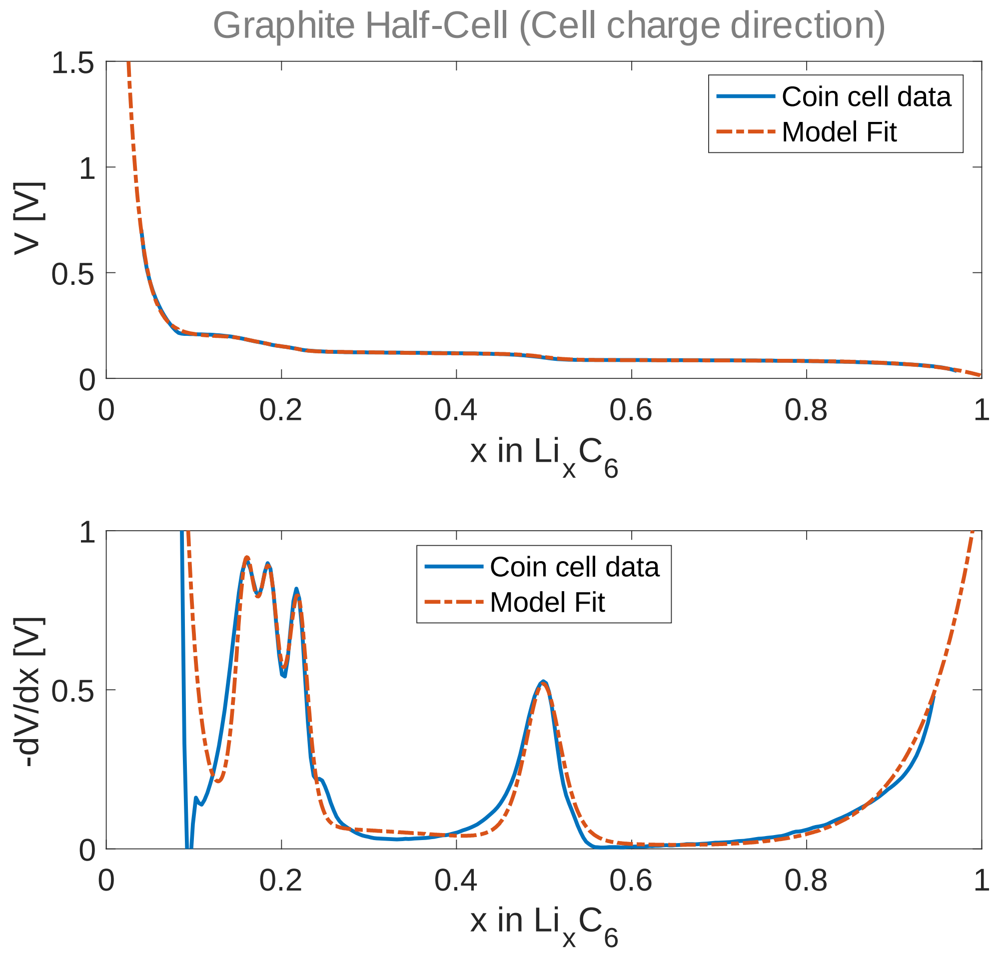
Phase Transition of Graphite Negative Electrode

- Graphite material undergoes phase transitions during lithium intercalation and extraction.
- This electrochemical feature is noticeable as local peaks in the differential voltage (dV/dQ) data.



Figures from Sethuraman et al. 2010





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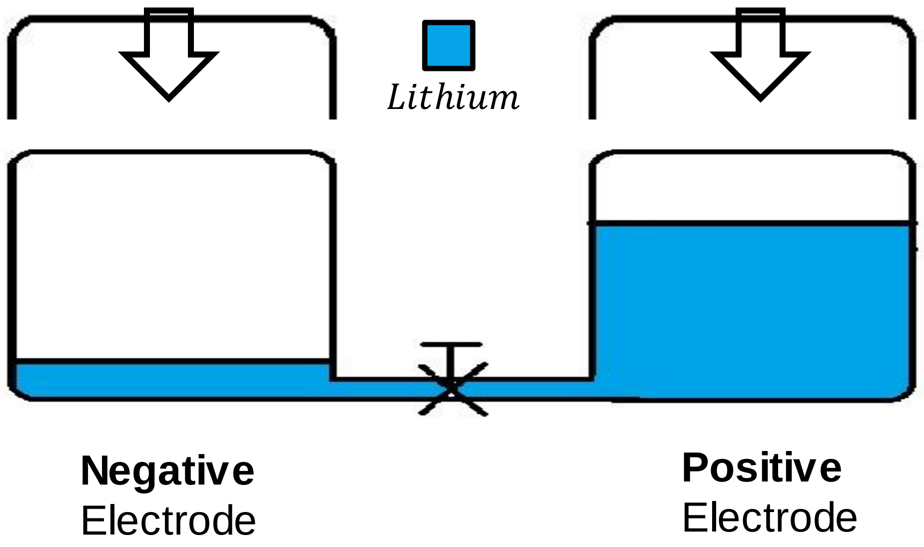
Li-ion Battery Degradation Mode and Water Tank Analogy

- Battery has two Electrodes (two tanks)
- Electrode-specific degradation modes are: LLI, LAM_{NE}, LAM_{PE}

Water Tank Analogy:

✓ LLI: amount of water decreases

✓ LAM: size of the water tank reduces



Identify Tank Capacities and Utilization (electrode State of Health – eSOH)

Electrode SOH Parameters

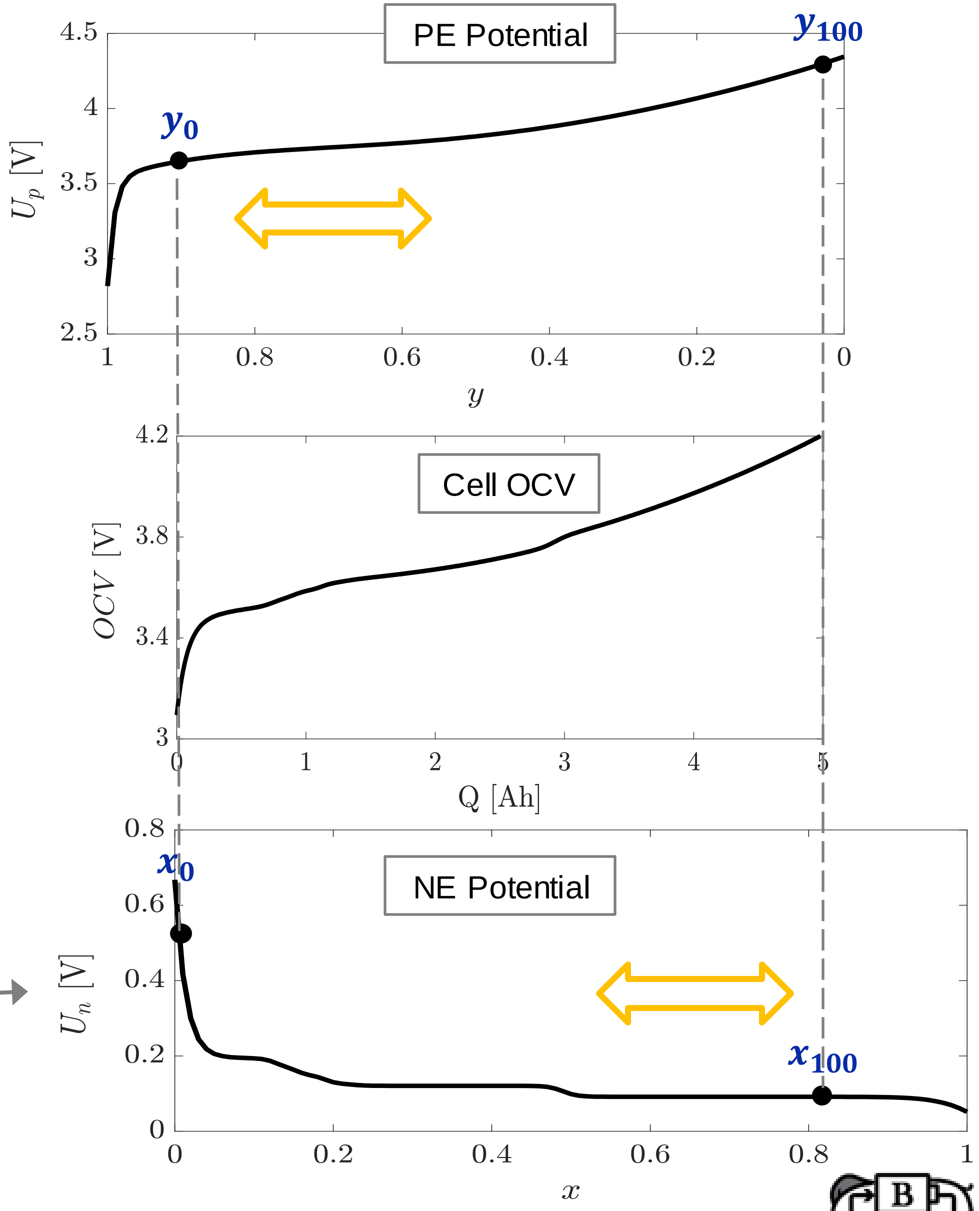
- Utilization window of PE: $[y_0, y_{100}]$
- Utilization window of NE: $[x_0, x_{100}]$

Slide

- Capacity of PE: C_p [Ah]
- Capacity of NE: C_n [Ah]

Scale

$$V_{oc}(Q;\theta) = U_p\left(y_0 - \frac{Q}{C_p}\right) - U_n\left(x_0 + \frac{Q}{C_n}\right).$$



Chemistry: NMC/graphite

Identify Tank Capacities and Utilization (electrode State of Health – eSOH)

Electrode SOH Parameters

- Utilization window of PE: $[y_0, y_{100}]$ — Slide
- Utilization window of NE: $[x_0, x_{100}]$ — Slide
- Capacity of PE: C_p [Ah] — Scale
- Capacity of NE: C_n [Ah] — Scale

OCV Model w/ Electrode SOH Parameters

- OCV is the difference between the two half-cell potentials

$$V_{oc}(z) = U_p(y) - U_n(x), \quad \text{Eq. (1)}$$

- Relating cell SOC (z) to the electrode's utilization window

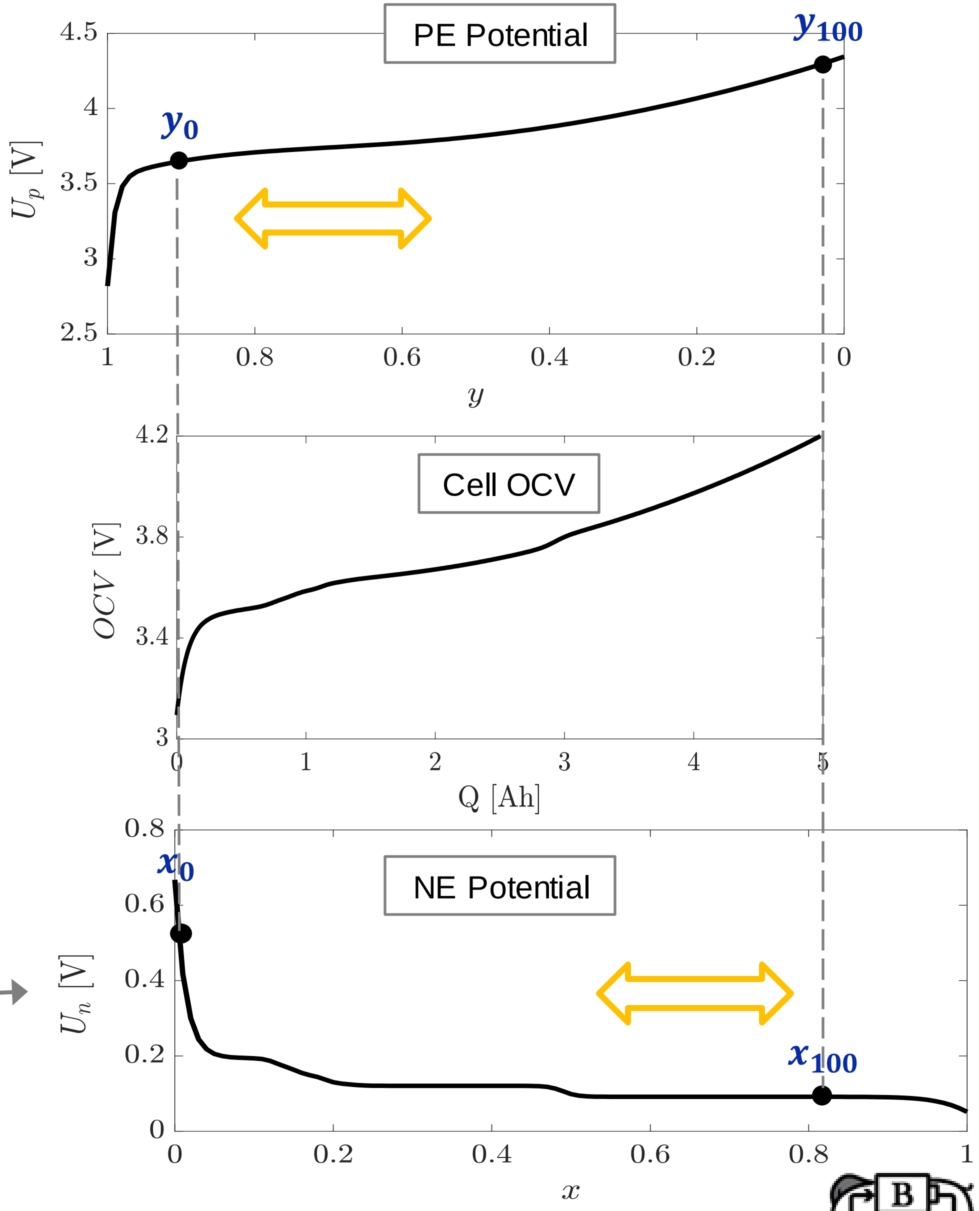
$$z = \frac{Q}{C} = \frac{y_0 - y}{y_0 - y_{100}} = \frac{x - x_0}{x_{100} - x_0}, \quad \text{Eq. (2)}$$

- Relating cell capacity, C, to the electrode capacity

$$C = C_p(y_0 - y_{100}) = C_n(x_{100} - x_0). \quad \text{Eq. (3)}$$

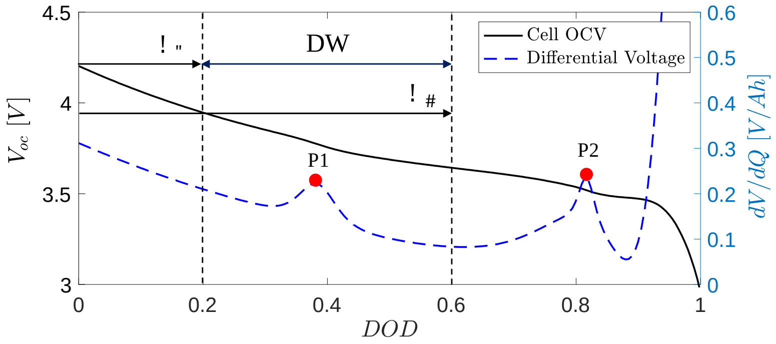
- We can parameterize Eq. (1) for $\theta = [C_p, C_n, y_0, x_0]$

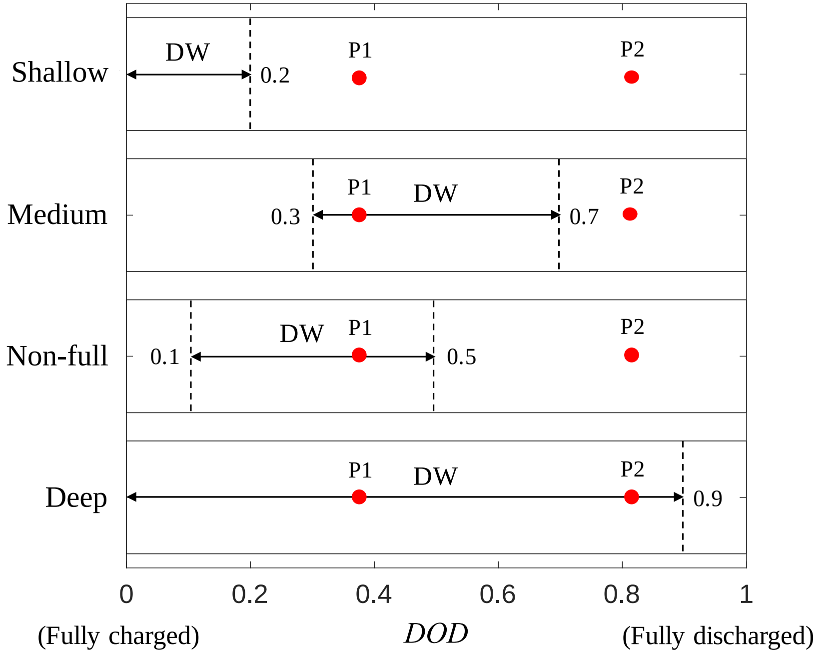
$$\boxed{V_{oc}(Q;\theta) = U_p\left(y_0 - \frac{Q}{C_p}\right) - U_n\left(x_0 + \frac{Q}{C_n}\right).} \quad \text{Eq. (4)}$$



Data Window (DW) in Limited Field Use

- DW represents the partial availability of OCV data for the electrode SOH parameter estimation.





Different size and location of DWs

- For a partial DW, likely not including all peak information, hence use Voltage Fitting method.

$$\underset{\theta}{\text{minimize}} \quad \sum_{i=1}^{n} \left\| V_{oc}(Q_i;\theta) - V_{oc,i}^{data} \right\|^2$$

Partial DW

$$\text{subject to} \quad V_{max} = U_p(y_{100}) - U_n(x_{100}).$$

Equality constraint

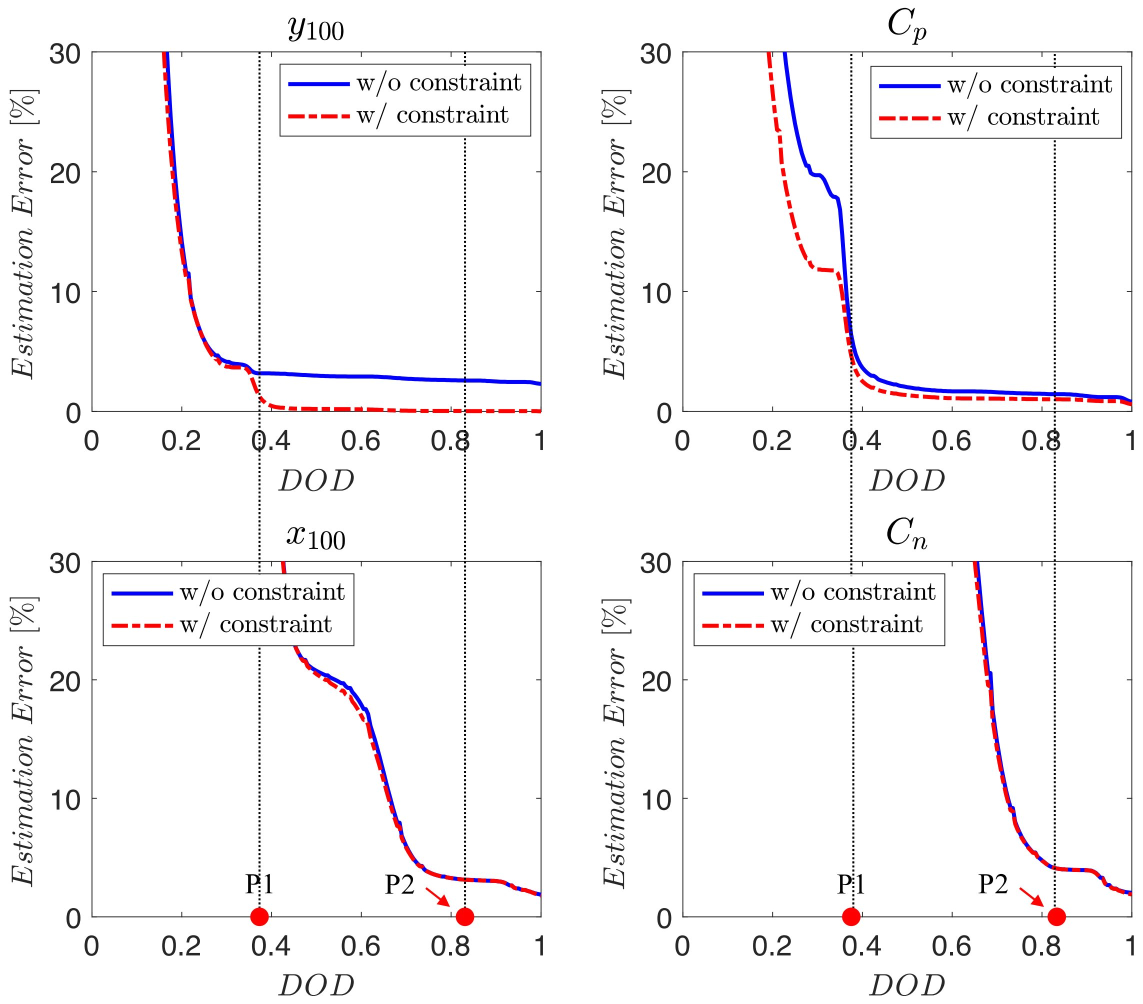
- Quantifying estimation accuracy based on nominal parameters for 5 Ah NMC/graphite pouch cell.

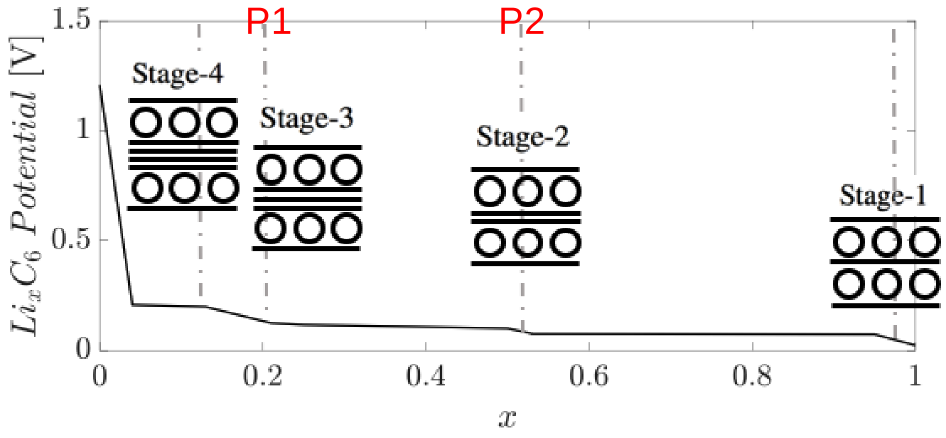
	Parameters	Values
Full-Cell	C	4.95 Ah
	V_{max}	4.2 V
	V_{min}	3.0 V
Positive Electrode	C_p	5.78 Ah
	$[y_{100}, y_0]$	[0.10, 0.95]
Negative Electrode	C_n	6.24 Ah
	$[x_{100}, x_0]$	[0.81, 0.02]

Analysis Results – Impact of Phase Transition

- Phase transition of electrode material is associated with half-cell potential slope changes, providing information on the corresponding electrode.
- Error bound becomes much narrow (i.e. improving estimation accuracy) when the DW include phase transition area.

Analytic error bound w.r.t depth of discharge (DOD). The error bound decreases with transitions around the peaks (P1 and P2).





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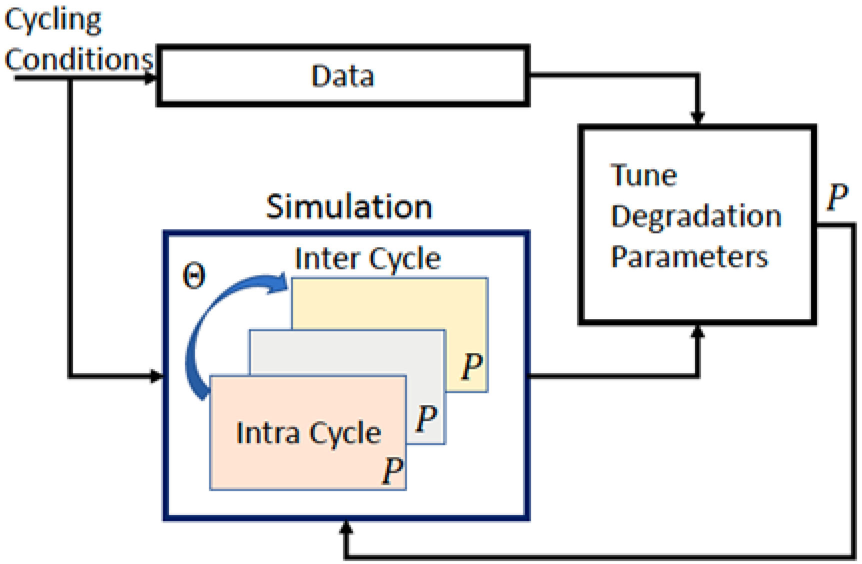
Digital Twin: Calibration from Lab Data



Automatically tune degradation model parameters until a good fit with experimental data is found.

Electrode Utilization (Y output matching)

$$n_{Li} = \frac{3600}{F}(x_{100}C_n + y_{100}C_p)$$

$$C_n(x_{100} - x_0) = C_p(y_0 - y_{100})$$

$$V_{max} = U_p(y_{100}) - U_n(x_{100})$$

Intra-cycle states

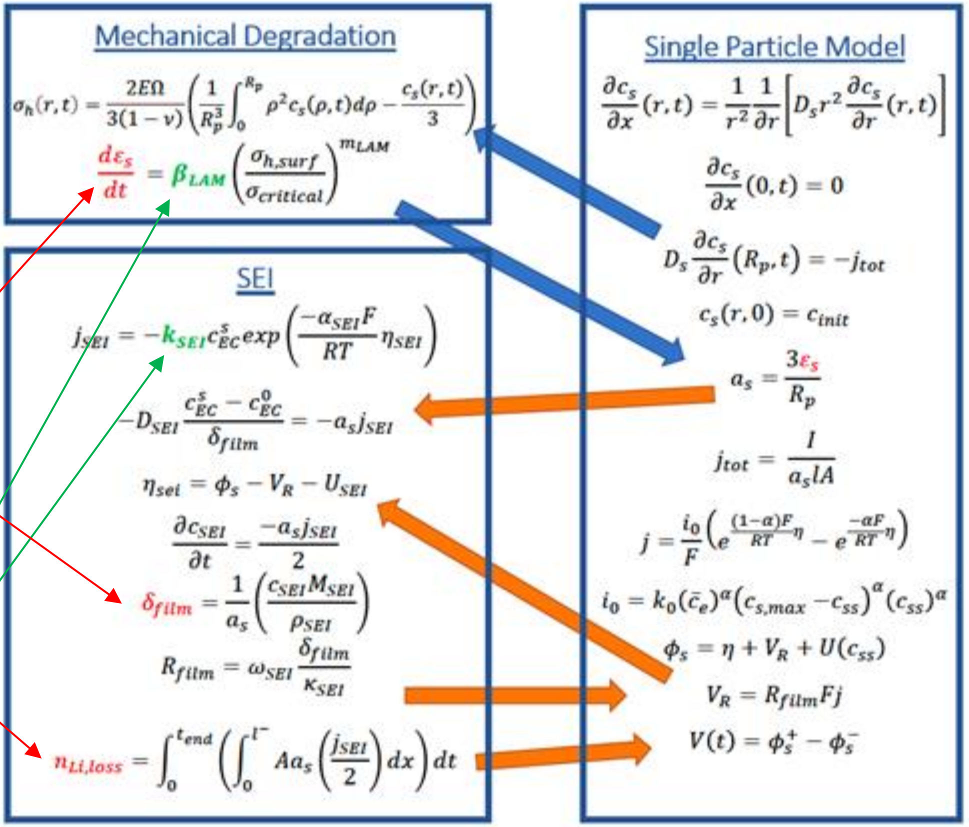
$$\boldsymbol{x} = \begin{bmatrix} c_s^+ \\ c_s^- \end{bmatrix}$$

Inter-cycle states

$$\boldsymbol{\Theta} = \begin{bmatrix} \delta_{\mathrm{SEI}} \\ \varepsilon_{\mathrm{s}}^- \\ \varepsilon_{\mathrm{s}}^+ \\ n_{\mathrm{Li,s}} \end{bmatrix}$$

Parameters

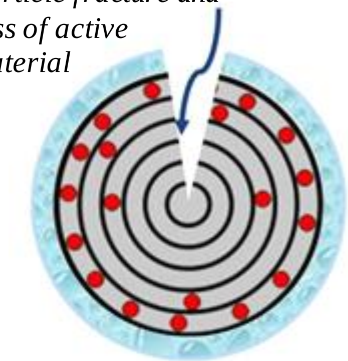
$$\boldsymbol{P} = \begin{bmatrix} k_{\mathrm{SEI}} \\ \beta_{\mathrm{LAM}}^- \\ \beta_{\mathrm{LAM}}^- \end{bmatrix}$$



Pannala S. et al, "Methodology for Accelerated Inter-Cycle Simulations of Li-ion Battery Degradation with Intra-Cycle Resolved Degradation Mechanisms"' ACC 2022

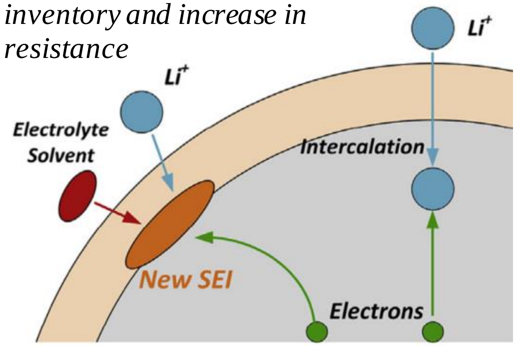
Battery Digital Twin (Learning Degradation Mechanisms)

Particle fracture and loss of active material



Laresgoiti, Izaro, et al. "Modeling mechanical degradation in lithium ion batteries during cycling: Solid electrolyte interphase fracture." *Journal of Power Sources* 300 (2015): 112-122.

Film growth with loss of lithium inventory and increase in resistance



Yang, Xiao-Guang, et al. "Modeling of lithium plating induced aging of lithium-ion batteries: Transition from linear to nonlinear aging." *Journal of Power Sources* (2017)

Mechanical Degradation

$$\sigma_h(r,t) = \frac{2E\Omega}{3(1-\nu)}\left(\frac{1}{R_p^3}\int_0^{R_p}\rho^2 c_s(\rho,t)d\rho - \frac{c_s(r,t)}{3}\right)$$

$$\frac{d\varepsilon_s}{dt} = \beta_{LAM}\left(\frac{\sigma_{h,surf}}{\sigma_{critical}}\right)^{m_{LAM}}$$

SEI

$$j_{SEI} = -k_{SEI}c_{EC}^{s}exp\left(\frac{-\alpha_{SEI}F}{RT}\eta_{SEI}\right)$$

$$-D_{SEI}\frac{c_{EC}^{s}-c_{EC}^{0}}{\delta_{film}} = -a_s j_{SEI}$$

$$\eta_{sei} = \phi_s - V_R - U_{SEI}$$

$$\frac{\partial c_{SEI}}{\partial t} = \frac{-a_s j_{SEI}}{2}$$

$$\delta_{film} = \frac{1}{a_s}\left(\frac{c_{SEI}M_{SEI}}{\rho_{SEI}}\right)$$

$$R_{film} = \omega_{SEI}\frac{\delta_{film}}{\kappa_{SEI}}$$

$$n_{Li,loss} = \int_0^{t_{end}}\left(\int_0^{l^-} Aa_s\left(\frac{j_{SEI}}{2}\right)dx\right)dt$$

Single Particle Model

$$\frac{\partial c_s}{\partial x}(r,t) = \frac{1}{r^2}\frac{1}{\partial r}\left[D_s r^2\frac{\partial c_s}{\partial r}(r,t)\right]$$

$$\frac{\partial c_s}{\partial x}(0,t) = 0$$

$$D_s\frac{\partial c_s}{\partial r}(R_p,t) = -j_{tot}$$

$$c_s(r,0) = c_{init}$$

$$a_s = \frac{3\varepsilon_s}{R_p}$$

$$j_{tot} = \frac{I}{a_s lA}$$

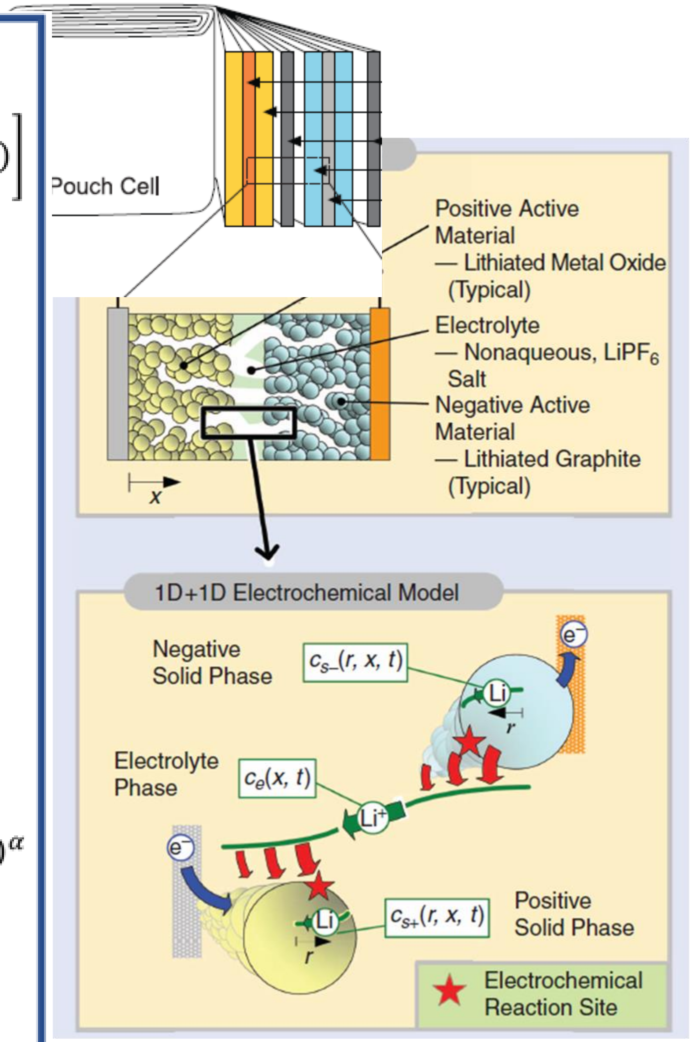
$$j = \frac{i_0}{F}\left(e^{\frac{(1-\alpha)F}{RT}\eta} - e^{\frac{-\alpha F}{RT}\eta}\right)$$

$$i_0 = k_0(\bar{c}_e)^{\alpha}(c_{s,max} - c_{ss})^{\alpha}(c_{ss})^{\alpha}$$

$$\phi_s = \eta + V_R + U(c_{ss})$$

$$V_R = R_{film}Fj$$

$$V(t) = \phi_s^+ - \phi_s^-$$



K.Smith, CSM 2010

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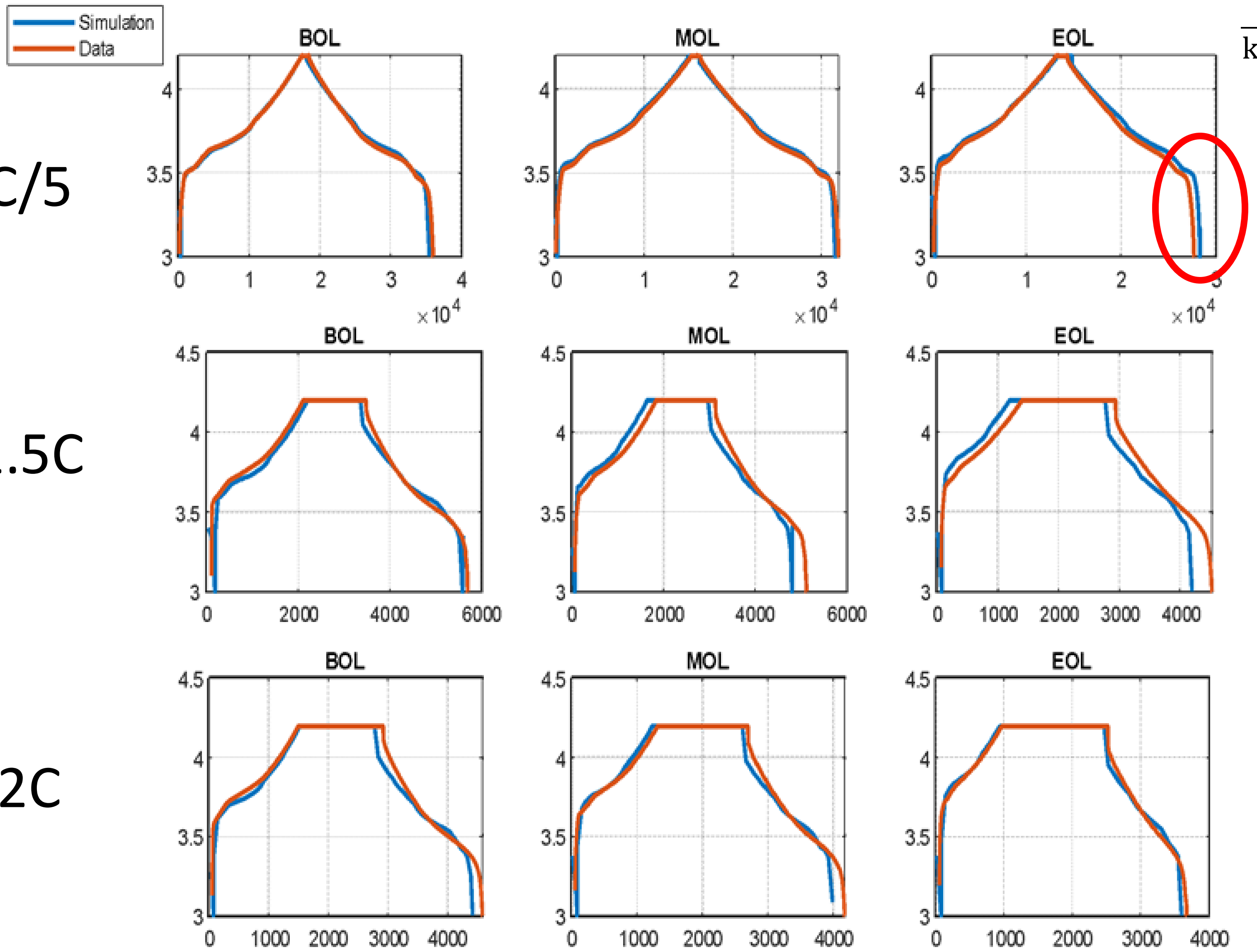
SPM with Learned Degradation Mechanisms: NMC111

$$\frac{1}{k_{SEI}} = 3e4\ \Omega m$$

- C/5
- 1.5C
- 2C



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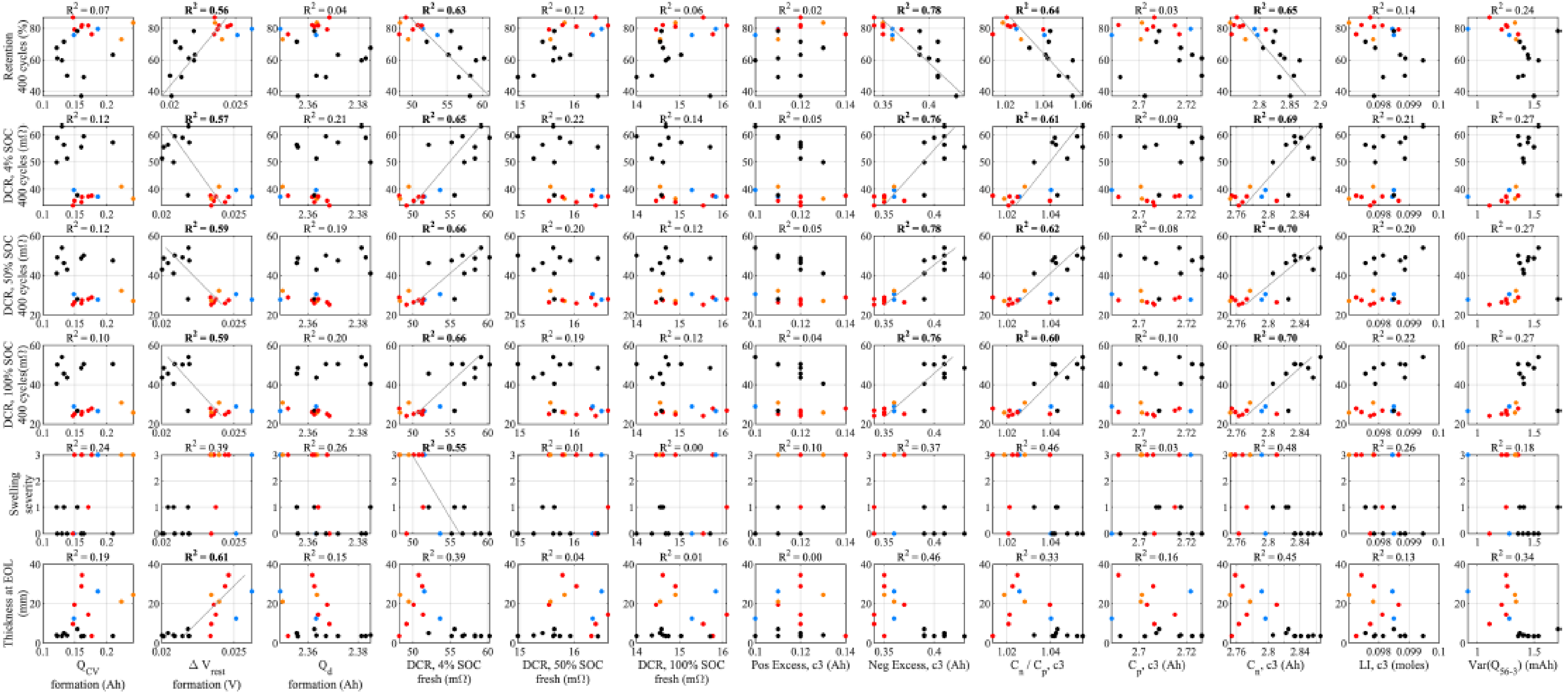
Looking for Aging Wrinkles → Useful Lifetime Features



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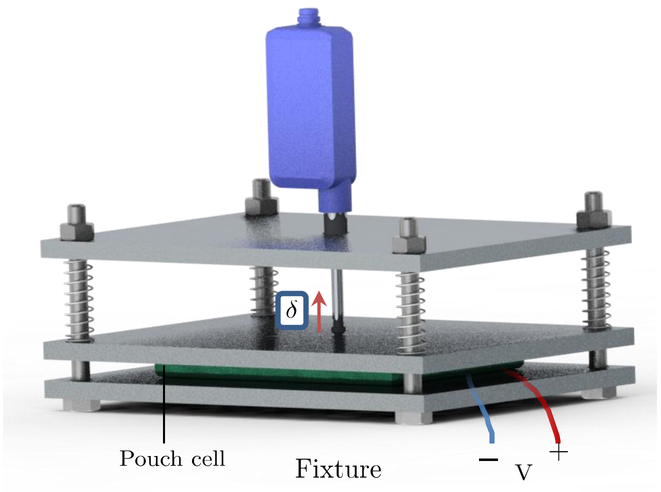
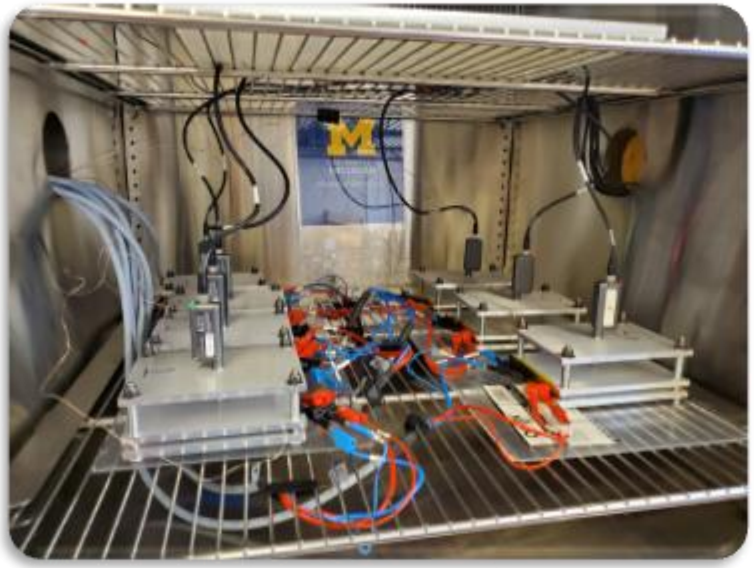
Other Features for Accurate eSOH Estimation?

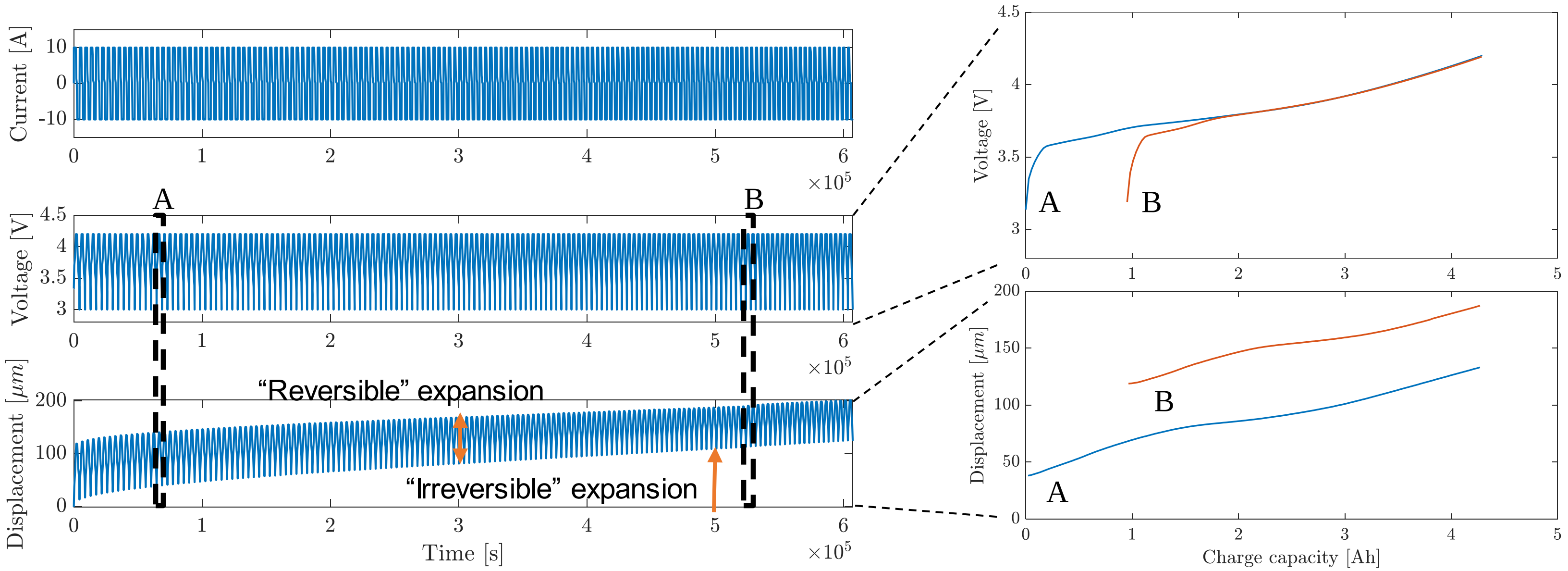




Current

Voltage

Expansion



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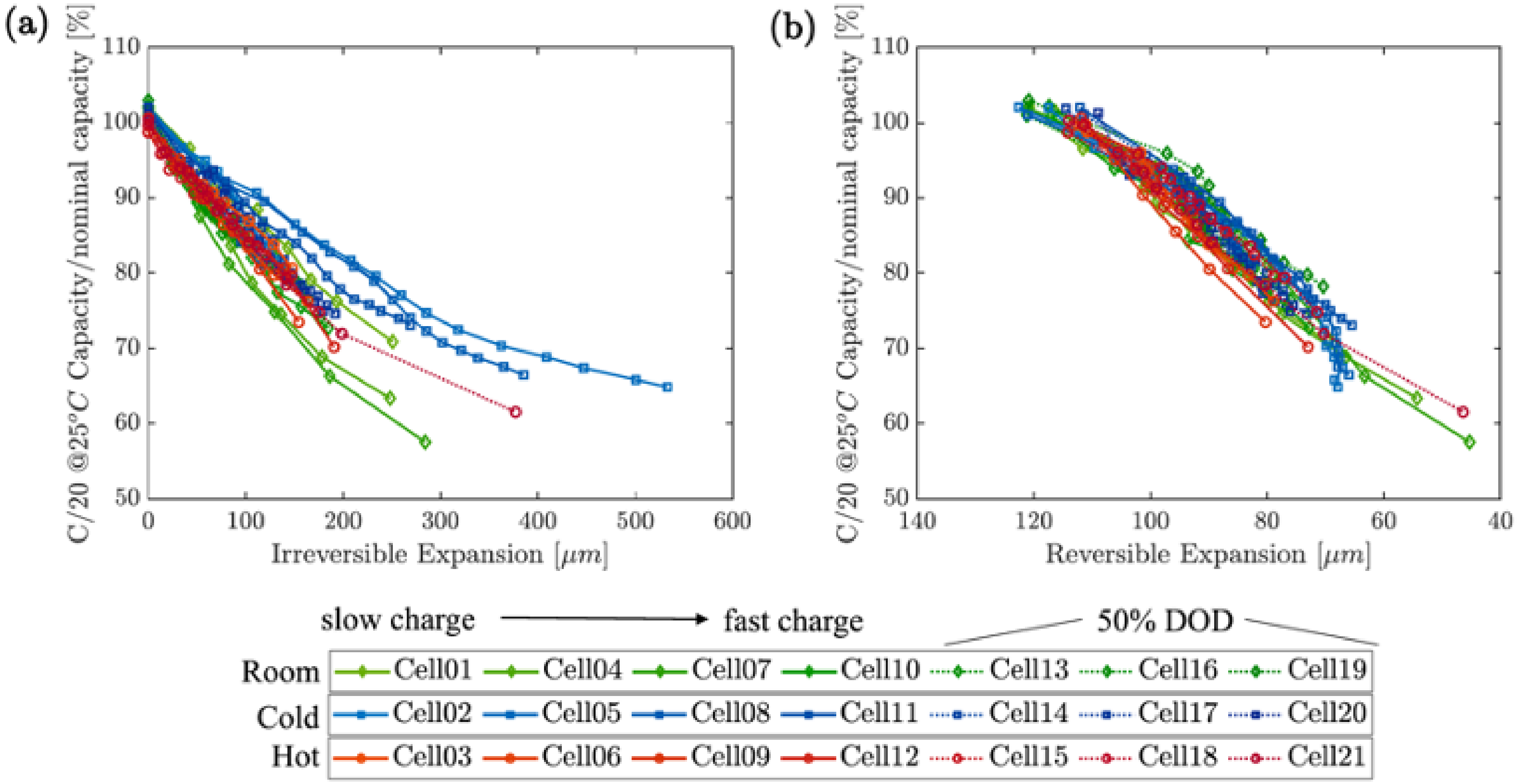
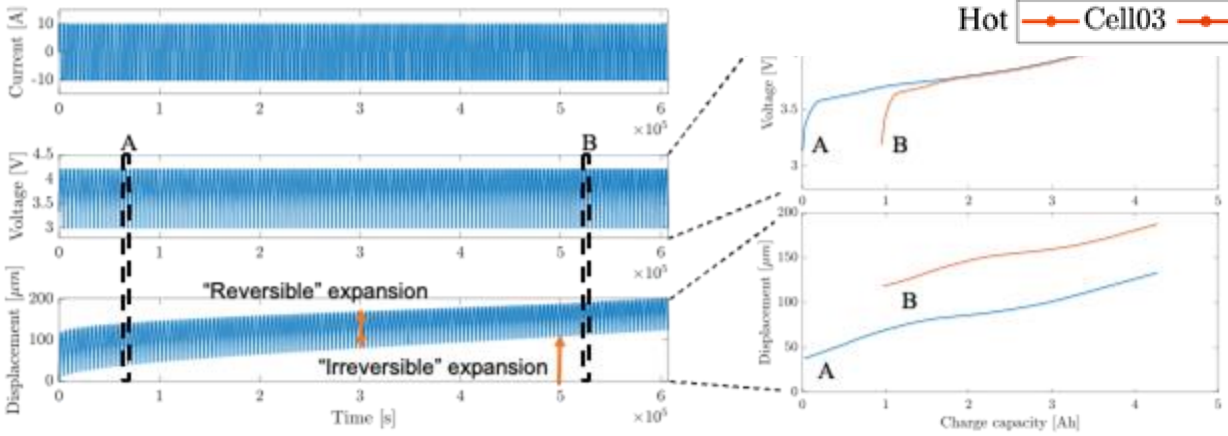
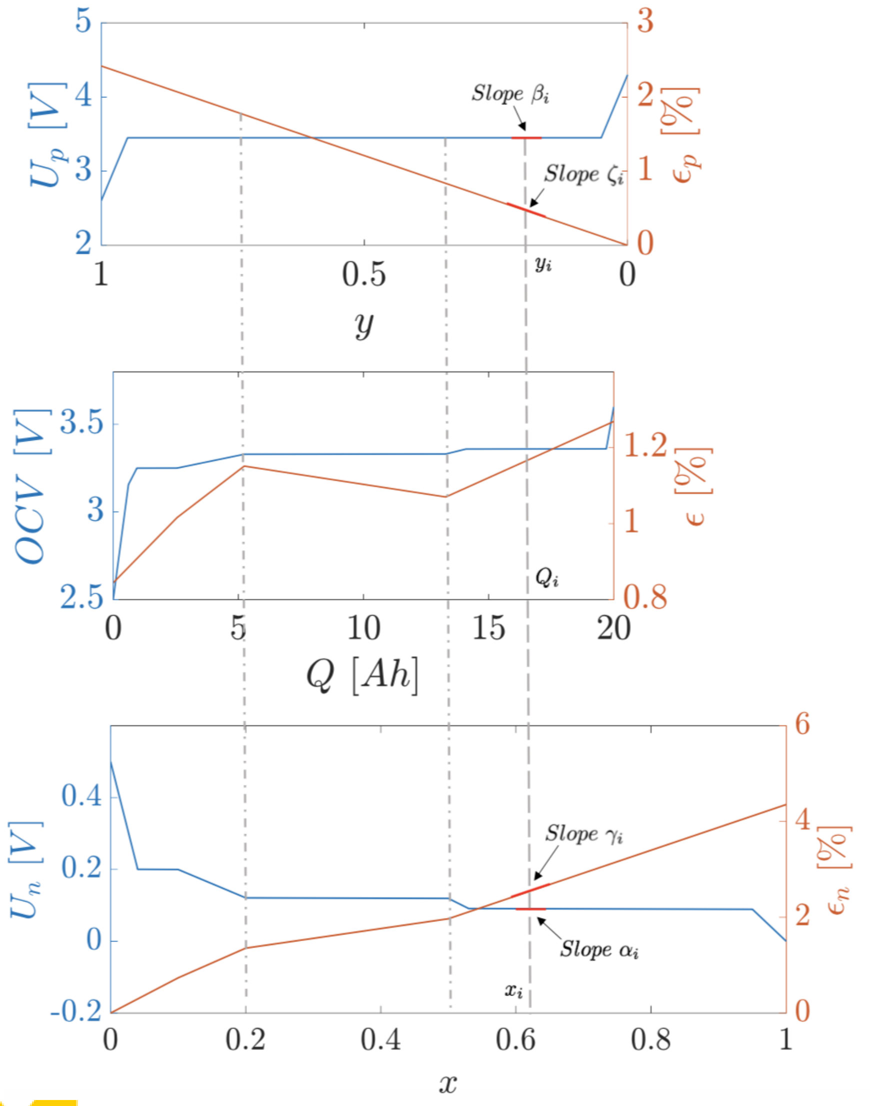
Reversible Expansion→ Universal Linearly Correlated Feature for all Cycling Conditions







P. Mohtat, et al. JPS, 2019

- The unknown parameters are defined as $\theta = [x_{100}, y_{100}, C_n, C_p]$
- The estimation problem is defined as follows:

$$\min_{\theta} \sum_{i=1}^{n} \left\| Y(\theta, Q_i) - \hat{Y}_i \right\|^2$$
$$s.t. \quad U_p(y_{100}) - U_n(x_{100}) = V_{max}$$

where $Y(\theta, Q_i) = \begin{bmatrix} OCV(\theta, Q_i) \\ \epsilon(\theta, Q_i) \end{bmatrix}$, and the vector of measurements is $\hat{Y}_i = \begin{bmatrix} OCV_i \\ \epsilon_i \end{bmatrix}$.

- Finally the voltage and strain functions are defined as below:

$$OCV(\theta, Q) = U_p\left(y_{100} + \frac{Q}{C_p}\right) - U_n\left(x_{100} - \frac{Q}{C_n}\right)$$
$$\epsilon(\theta, Q) = \epsilon_p\left(y_{100} + \frac{Q}{C_p}\right) + \epsilon_n\left(x_{100} - \frac{Q}{C_n}\right)$$

$$\boxed{LAM_{pe} = \left(1 - \frac{C_p^a}{C_p^f}\right) \times 100}$$

$$\boxed{LLI = \left(1 - \frac{x_{100}^a C_n^a + y_{100}^a C_p^a}{x_{100}^f C_n^f + y_{100}^f C_p^f}\right) \times 100}$$

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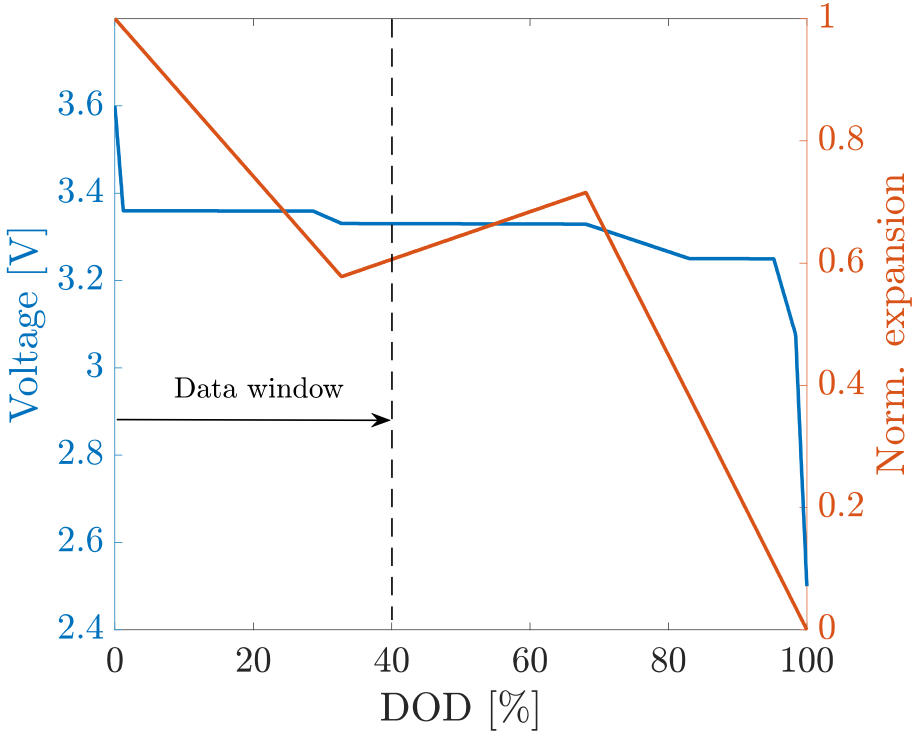
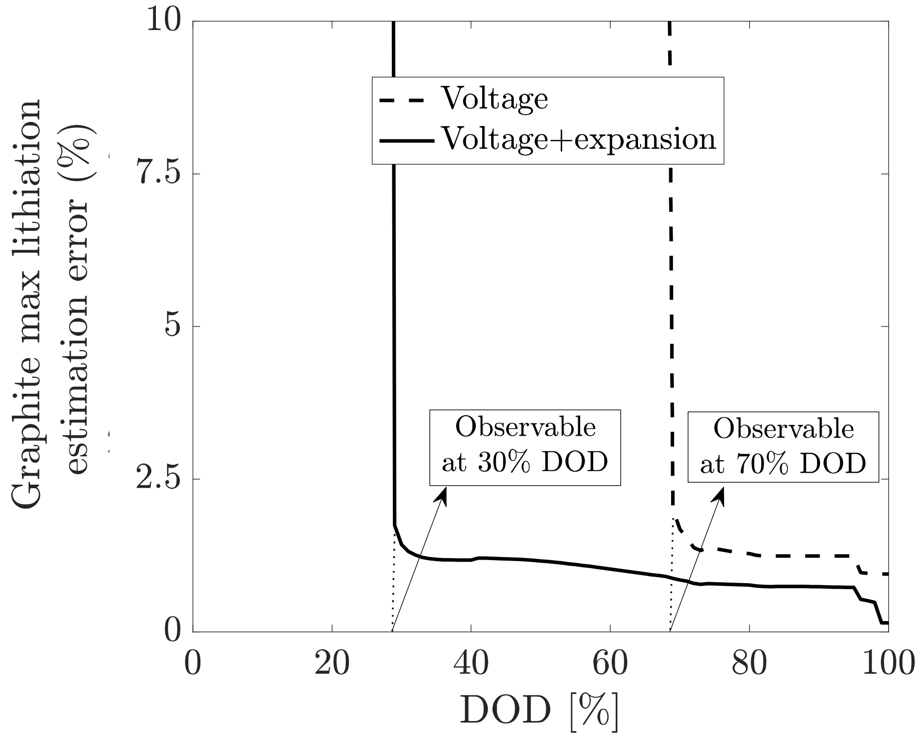
Expansion Feature appears at Low DOD

- Monitoring individual electrode health is essential for protecting the battery
- Expansion improves the identifiability
- DOD required for observability is reduced to 30% from 75%





S. Lee, et al. "Electrode-Specific State of Health Diagnostics for Lithium Ion Batteries Using Cell Voltage and Expansion. IIT, 2019.

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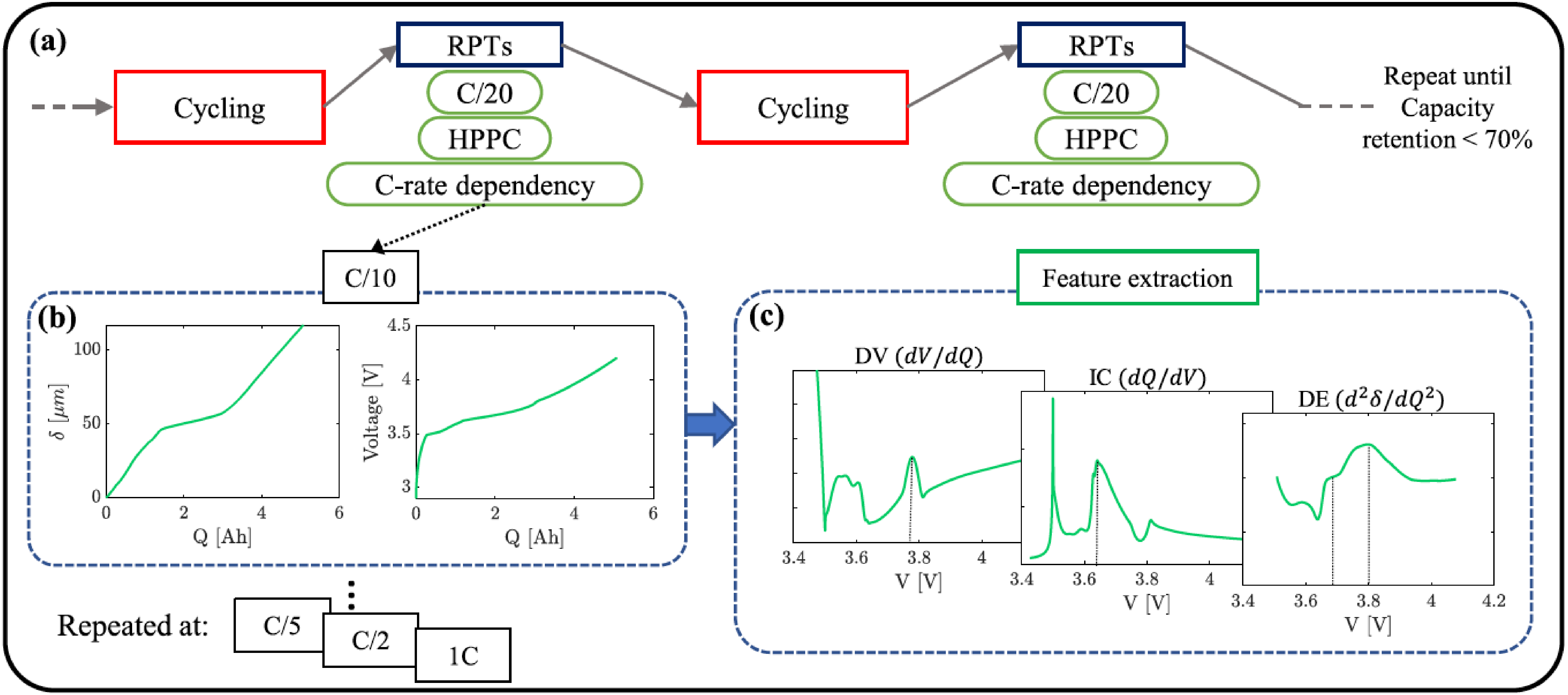
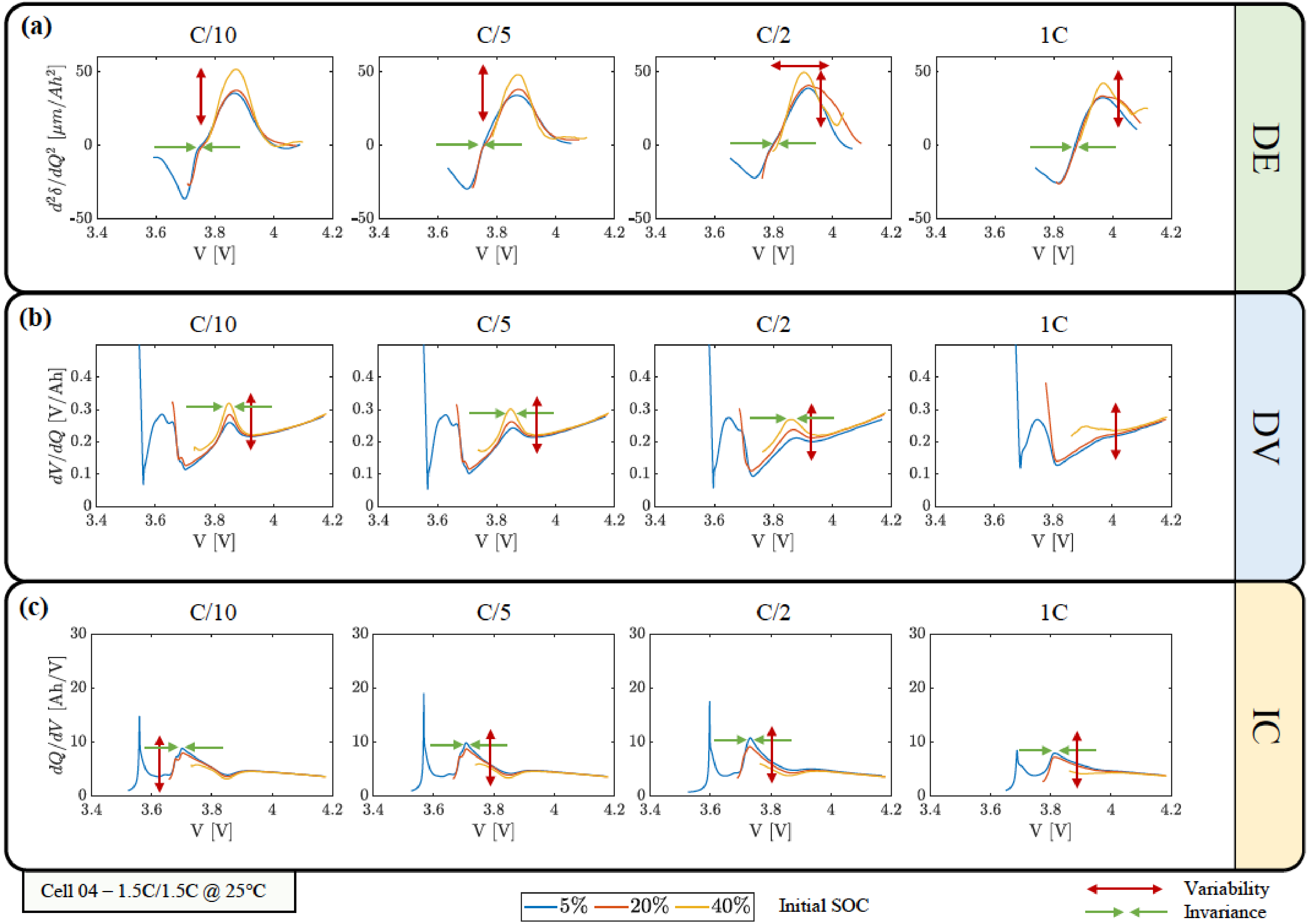
Testing Procedure



Aging Wrinkles: Independent 1C-rate and Initial SOC



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Features during Manufacturing for Quality Control and Lifetime Prediction!

Battery Manufacturing

Aging

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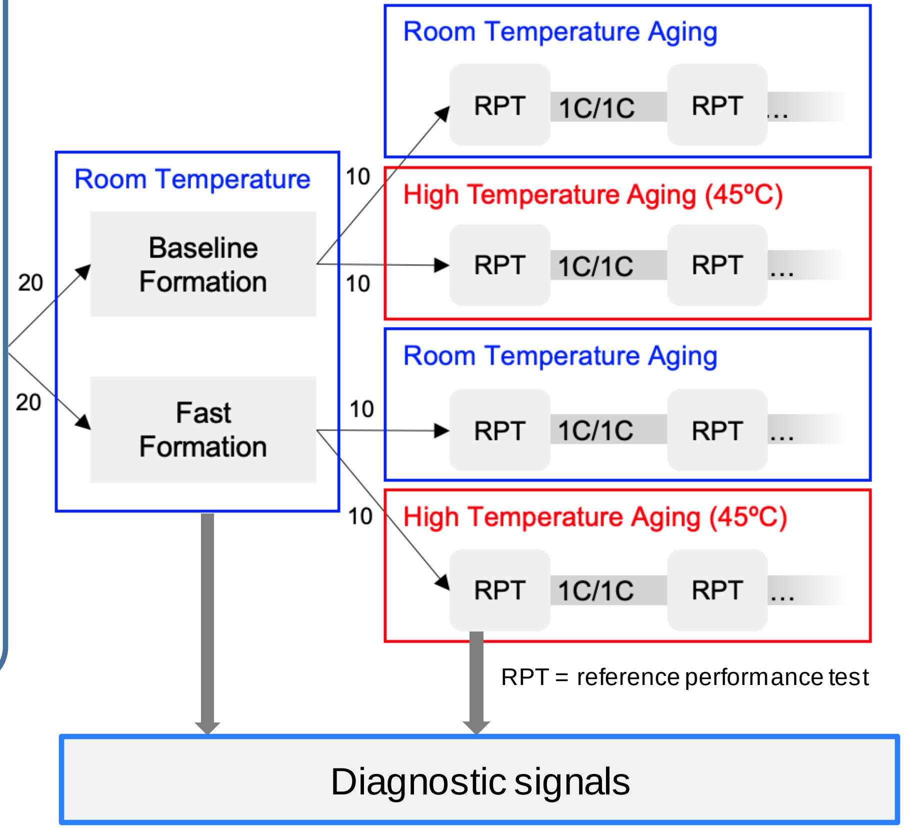
NMC111 / Gr cells (x40)



40 NMC / Graphite pouch cells were built at the University of Michigan Battery Lab.

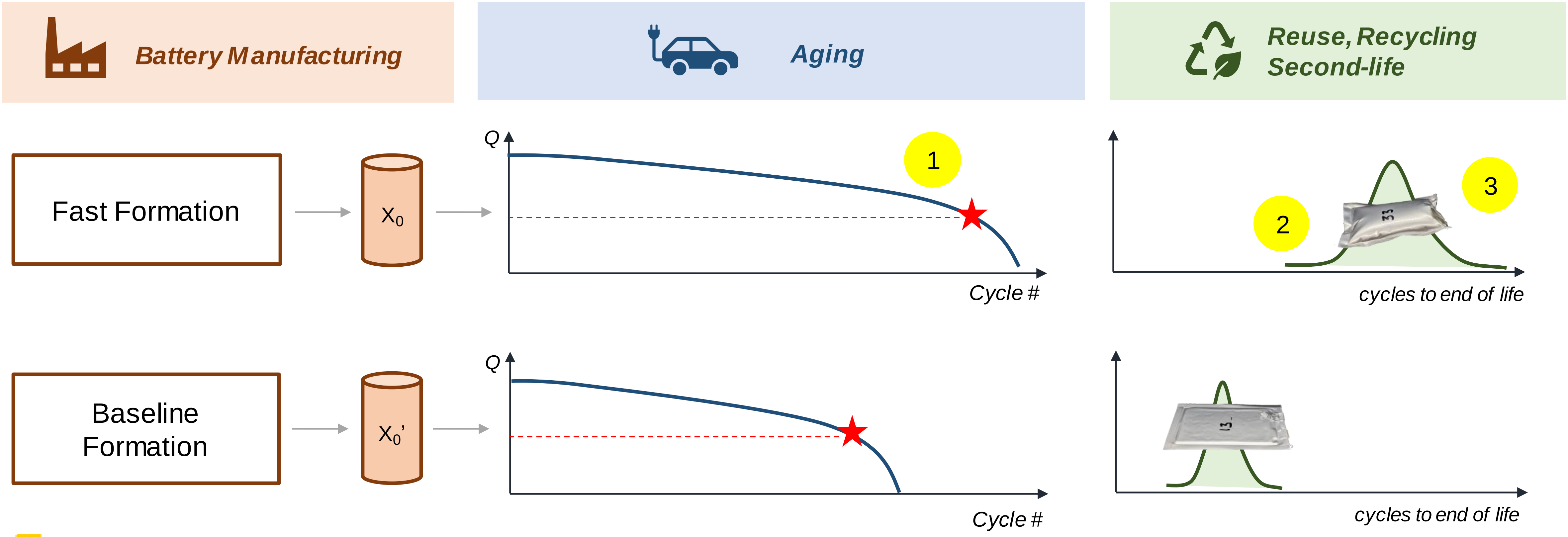
Cells were formed and cycled until <50% capacity retention.

Current-voltage signals were collected along the way and analyzed.

Looking for Early Features (during or immediately after manufacturing)

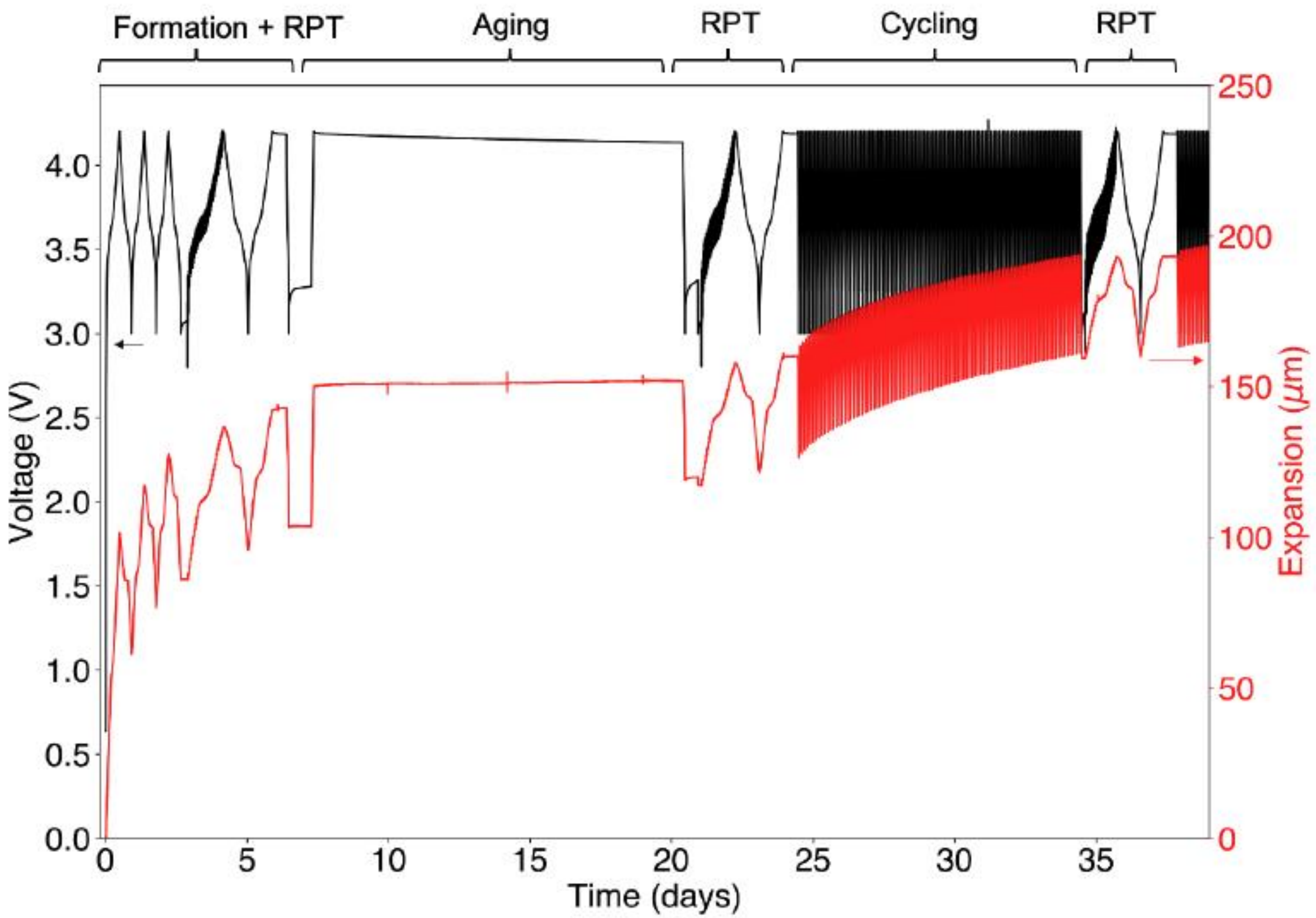
Fast formation:

1. ↑ Cycle life
2. ↑ Cell-to-cell variability
3. ↑ Pouch swelling



A. Weng, et al "Predicting the impact of formation protocols on battery lifetime immediately after manufacturing" *Joule* 5, 1-22, November 17, 2021,

Expansion During Formation for SEI Quality → Life



A. Weng, presented to ECS (last week)!! Submitted to J-ECS

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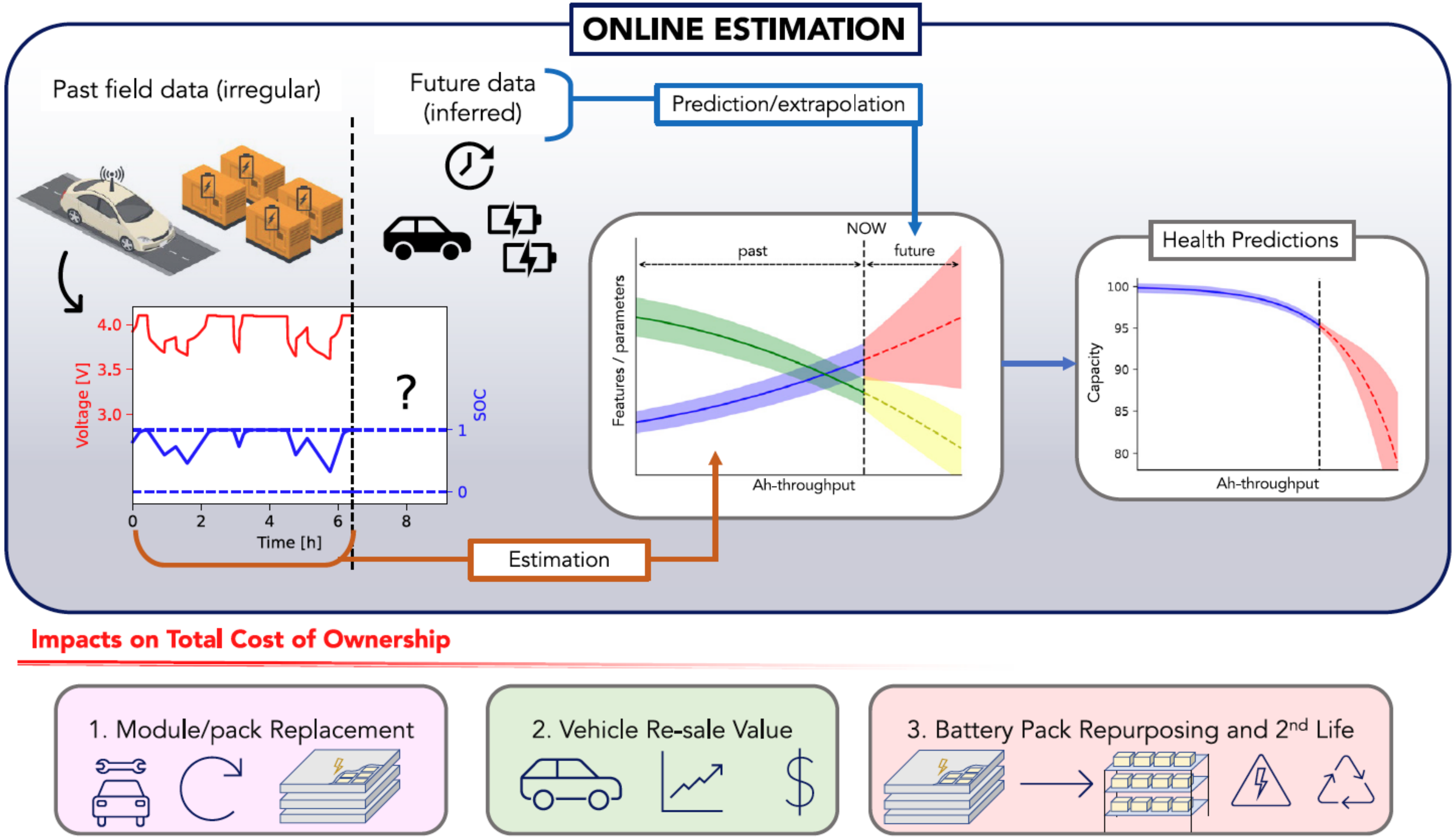
Seeing the Physics Explained Wrinkles and Learning from Field Data



Diagnostics (key features)
Estimation of internal states
Learn pattern
Predict
...

Act:
Manage Assets
Adjust Use & Maintenance
Redesign-Improve

Thank you!

V. Sulzer, et al, "The challenge and opportunity of battery lifetime prediction from field data, Joule Oct 2021