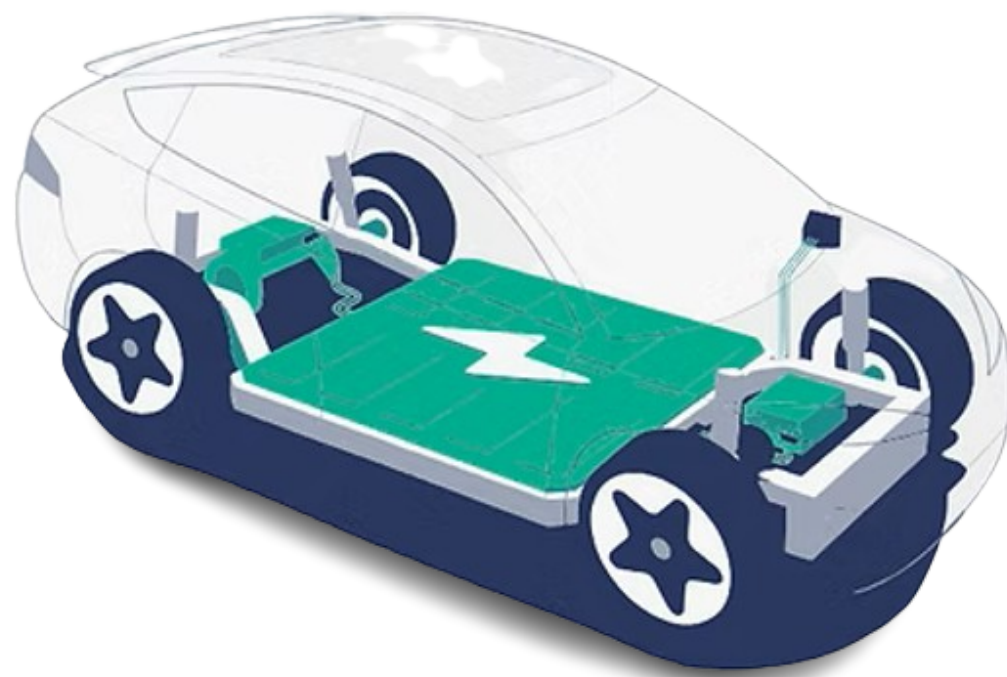


Data-driven prediction of battery cycle life before capacity degradation

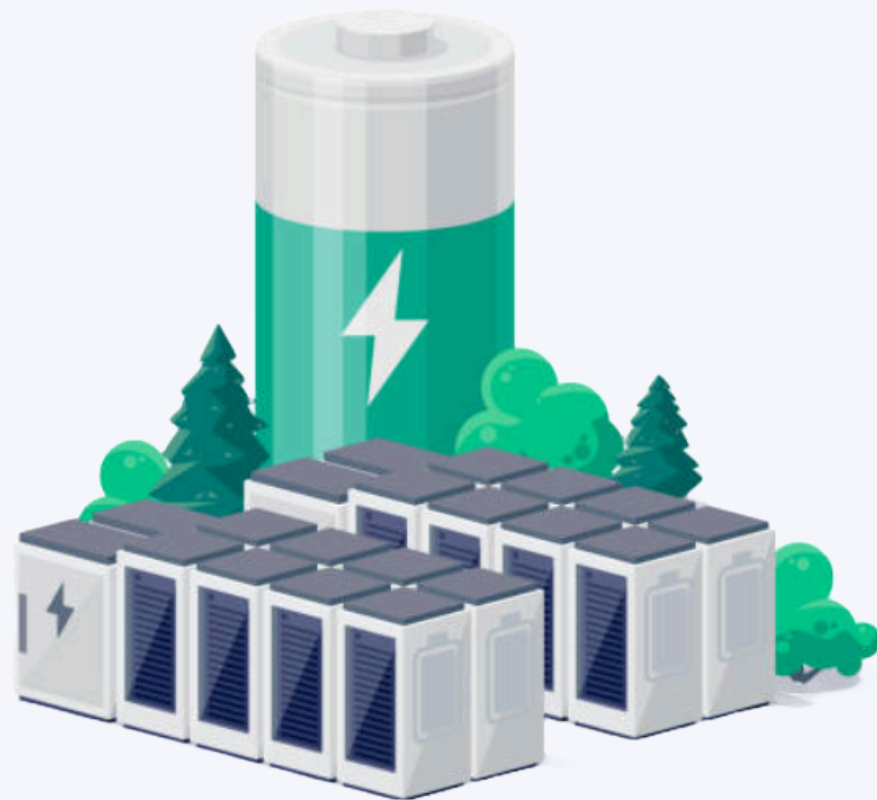


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SIGNIFICANCE

- Battery degradation takes hundreds of cycles to appear, making traditional testing slow and expensive.
- Battery life is hard to predict early, as even similar cells often behave very differently.
- Machine learning enables early prediction by detecting hidden degradation patterns from initial cycles.
- Early prediction unlocks faster cell development, quality grading, and better life expectancy estimates for manufacturers and end users



How battery Degrades (Literature review)

Lithium-ion batteries degrade over time and usage due to a variety of intertwined physical and chemical processes. Major degradation mechanisms include:

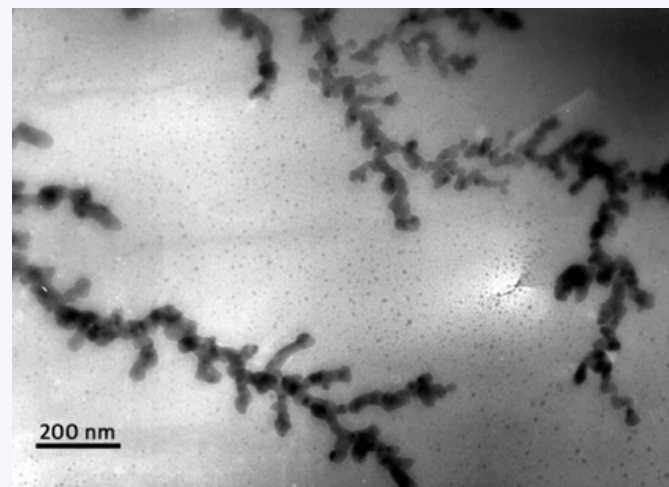
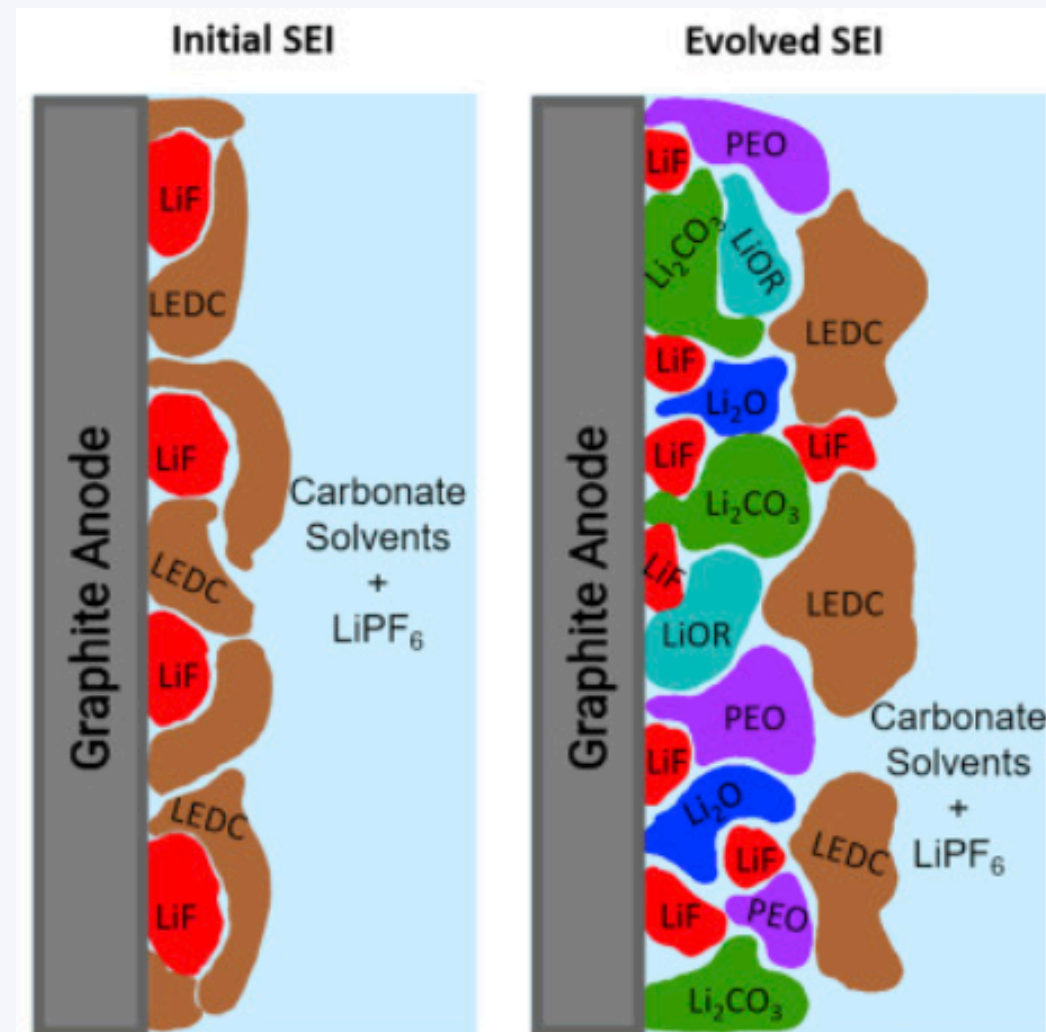
- Solid Electrolyte Interphase (SEI) growth
- Lithium plating
- Positive electrode (cathode) structural changes and decomposition
- Particle fracture (both electrodes)

Degradation mechanisms lead to:

- Capacity Fade → Battery stores less energy with time, so devices run shorter. Caused by loss of active lithium and electrode degradation.
- Power Fade → Battery struggles to deliver power quickly. Due to increased internal resistance and electrode damage.
- Safety Risks → Aging raises chances of swelling, overheating, or fire. Triggered by lithium plating, gas formation, or internal shorts.

SEI (SOLID ELECTROLYTE INTERPHASE)

- Formed over the negative Electrode.
- During the very first cycle initial SEI layer is formed ~ 10% initial capacity is lost.
- Acts as a solid electrolyte that blocks stops the further reaction of the electrolyte, however the thickness increases.



Dendrites

Reasons for SEI layer increase:

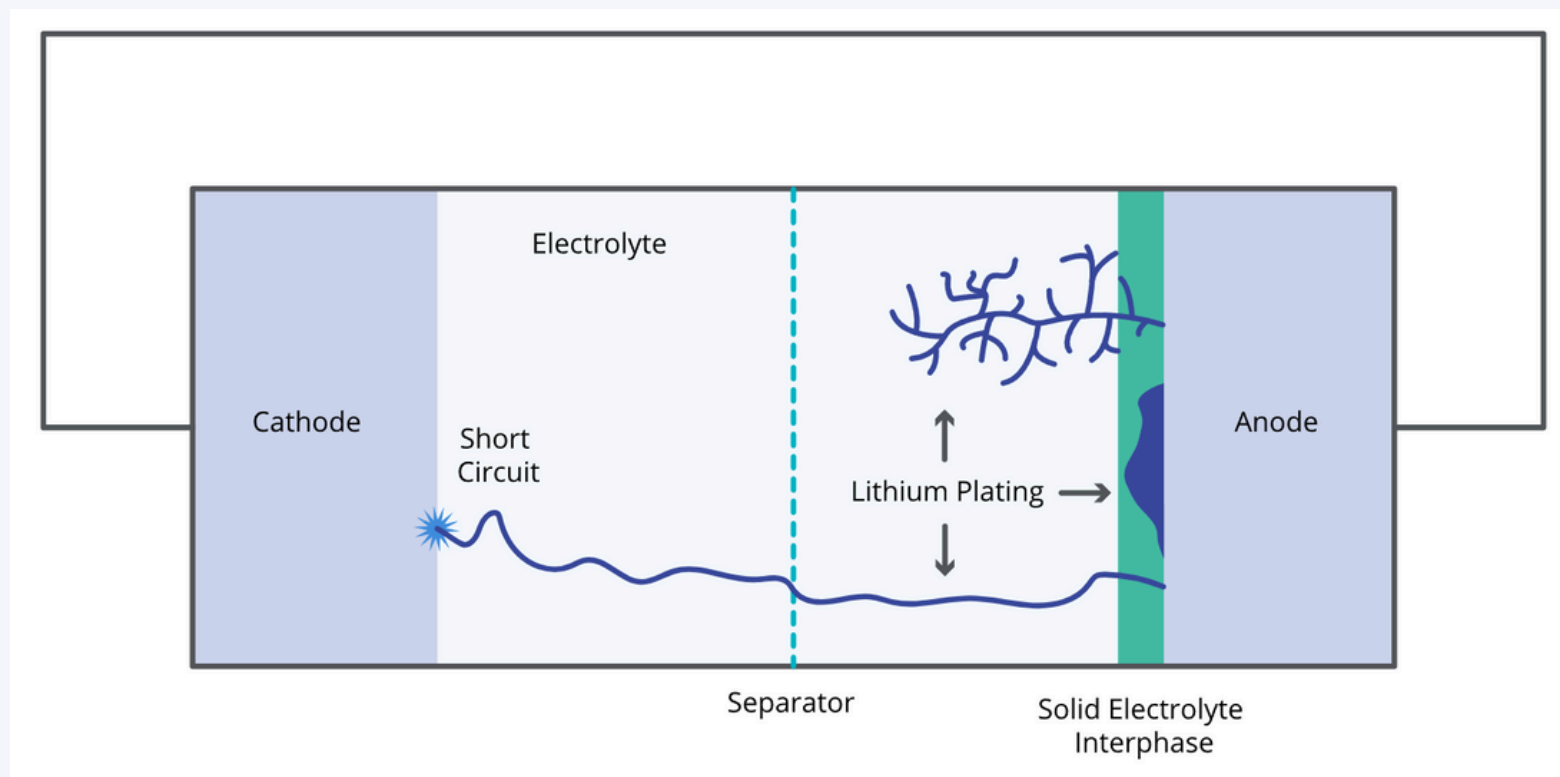
- Solvent diffusion: Electrolyte molecules permeate through pores/defects in existing SEI → react at electrode → form new SEI.
- Electrode cracking: Mechanical stress during cycling exposes fresh graphite surfaces → immediate SEI formation.
- Higher temperature, High currents, High voltage.

Impact of SEI on cell performance:

- Initially, the SEI layer is thin and the performance is not affected much.
- In early stages, the SEI prevents the e⁻ from anode surface from mixing with the electrolyte.
- As the cell ages, the SEI layer thickens and starts interfering with the major chemical reactions inside the cell.
- Beyond a certain thickness, the anode's ability to absorb the lithium ions reduce. Thus, the ions instead get deposited on the SEI layer, initiating the growth of the dendrites.

LITHIUM PLATING

- Li deposits on the Negative Electrode (NE) surface instead of entering graphite.
- Occurs when Li^+ ions arrive faster than graphite can absorb.
- Can be thermodynamic (NE fully lithiated, no space left) or kinetic (fast charging, cold T).



Reasons for Lithium Plating:

- Low temperature: slows down Li^+ intercalation.
- High SoC: NE nearly full, no room for more Li^+ .
- High charging current (fast charging): ions arrive faster than insertion rate.
- High voltage: favors plating over intercalation.
- Local defects: separator flaws, electrode cracks, uneven surface → localized plating.

Impact of Lithium Plating on Cell Performance:

- Reversible plating: some Li can be stripped (recovered).
- Irreversible plating: plated Li reacts with electrolyte → forms SEI or gets isolated as dead lithium.
- Capacity fade: Loss of Lithium Inventory (LLI).
- Power fade: Pore clogging increases resistance.
- Safety risk: Metallic Li can form dendrites, puncturing separator → internal short circuit & fire hazard.

PARTICLE FRACTURE

Reasons behind Particle Fracture:

- It occurs due to large volume changes in electrode materials during lithiation/delithiation, creating stress and cracks

What makes it worse:

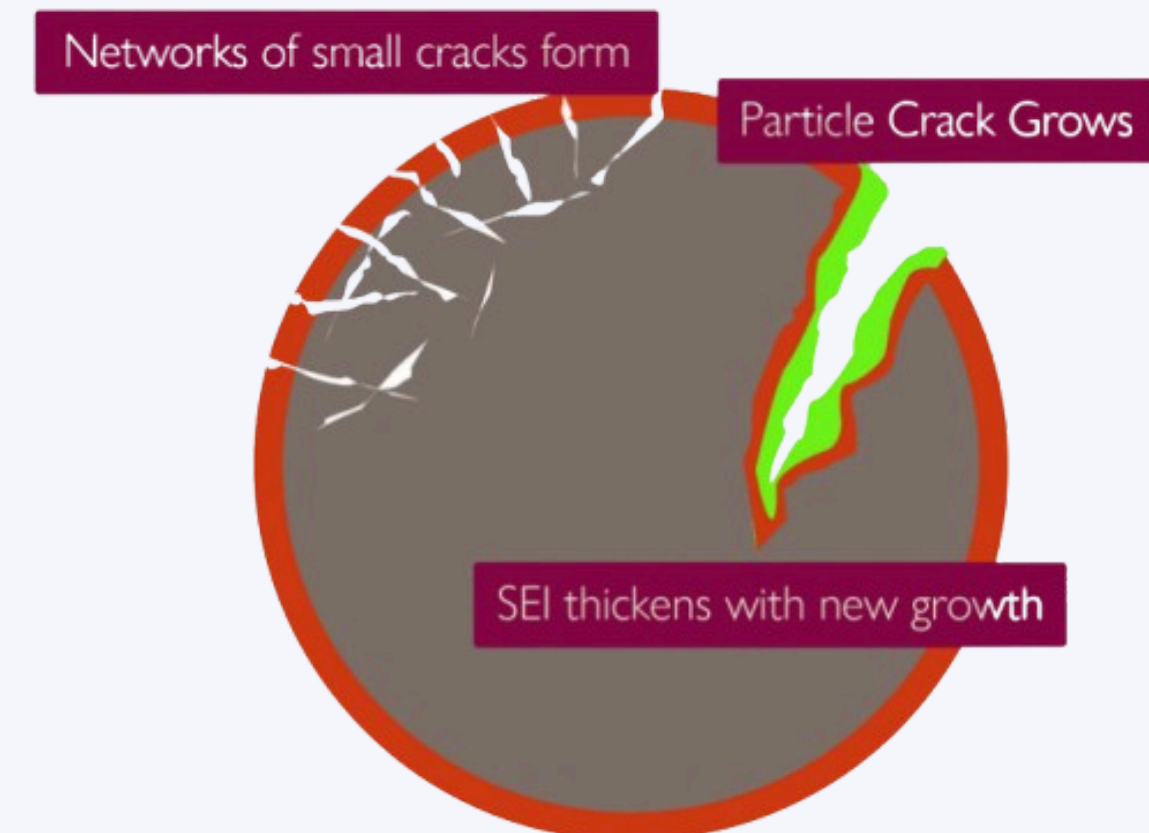
- High/Low temperatures
- very deep charging/discharging
- fast charging
- stresses during making of batteries

What happens after cracking:

- particles lose contact with each other
- newly formed surfaces due to cracking accelerate SEI formation
- Eventually electrode part break off resulting into loss of battery capacity

The Silicon Problem:

- Si which can store much more energy than graphite but it expands almost 4 times when charging
- This again rises the concern about cracking and damage to battery life
- Efforts have made by allowing Si with C to lower this effect but it was still not perfect.



POSITIVE ELECTRODE STRUCTURAL CHANGE AND DECOMPOSITION

- It's a chemistry-dependent degradation, which varies with the chemistry of the positive electrode.

Impact on Battery Degradation:

- Very less active material left results in capacity fade.
- Higher resistances resulting into power fade.
- Gas formation is associated with safety risks.
- Dissolved metals can damage the anode too.

When does this type of decomposition accelerate:

- At high voltage(Higher State of Charge)
- High Temperature
- In the presence of moisture.

What happens inside:

- Its crystal structure changes from a nice layered form to less stable forms(spinel, rock salt, etc.)
- Oxygen atoms can escape, reacting with the electrolyte and forming gases such as CO₂ and CO.
- Some Metals (like Ni,Mn,Co) dissolve into the electrolyte and move to the negative side
- Nickel and Lithium can “swap places” inside the crystal, blocking Li⁺ movement.
- Acid(from moisture in the electrolyte) makes things worse by dissolving more metals.
- A thin film (pSEI) forms on cathode surface, just like SEI on the anode.

CONCLUSIONS FROM ALL THESE MECHANISMS:

- These mechanisms generally do **not work out individually**; they are complexly **coupled**.
- There are many other mechanisms that play a role in degradation; however, all mechanisms can be grouped into **key categories** based on their impact:
 - Loss of active material
 - Loss of Lithium Inventory
 - Stoichiometric drift due to electrode imbalance
 - Increasing the Internal Resistance
- Degradation broadly depends on:
 - Temperature
 - State of Charge (SoC)
 - Load
 - Materials.
- Experiments with models are essential for lifetime prediction.



DATA DESCRIPTION

- In collaboration with **MIT** and **Stanford**, the **Toyota Research Institute (TRI)** released two high-throughput cycling datasets covering **357** commercial LFP/graphite cells (**A123 Systems APRI8650M1A, 1.1 Ah**).
- **Objective:** Study the effect of fast-charging protocols on ageing
- **Charging:**
 - **72 profiles** (single-step) up to ~80% SOC
 - From 80–100%: 1C CC–CV charge at 3.6 V, cutoff = 1/50C–1/20C (~22–55 mA)
- **Discharge:** Standardized 4C constant current (~4.4 A) to 2.0 V
- **Conditions:** 30 °C chamber, data logged from **cycle 2 to EOL** (80% capacity ≈0.88 Ah)
- **Data recorded:** The dataset contains **in-cycle** measurements (voltage, current, temperature, charge/discharge capacity) and **per-cycle summaries** (capacity, internal resistance, charge time)
- **Cycle life range:** 150–2300 cycles, depending on charging protocol.

Battery Information

Parameters	Value
Nominal Voltage	3.3 V
Nominal Capacity	1.1 Ah
Upper cut-off voltage	3.6 V
Lower cut-off voltage	2.0 V
Cell anode	Graphite
Cell cathode	LiFePO4



ORGANIZATION OF DATA IN THE DATASET

- 124 cells data is divided into 3 batches, each batch contains data of some cells.

1×46 struct with 8 fields

Fields	policy	policy_readable	barcode	channel_id	cycle_life	cycles	summary	Vdlin
1	'3_6C-80PER_3_6C'	'3.6C(80%)-3.6C'	"EL150800460514"	"1"	1190	1×1189 struct	1×1 struct	1000×1 double
2	'3_6C-80PER_3_6C'	'3.6C(80%)-3.6C'	"EL150800460486"	"2"	1179	1×1178 struct	1×1 struct	1000×1 double

- Each cycles column contains the data collected within every cycle of a particular battery.

1×1189 struct with 9 fields

Fields	discharge_dQdV	t	Qc	I	V	T	Qd	Qdlin	Tdlin
1	[]	[]	[]	[]	[]	[]	[]	[]	[]
2	1000×1 double	1087×1 double	1087×1 double	1087×1 double	1087×1 double	1087×1 double	1087×1 double	1000×1 double	1000×1 double
3	1000×1 double	1117×1 double	1117×1 double	1117×1 double	1117×1 double	1117×1 double	1117×1 double	1000×1 double	1000×1 double

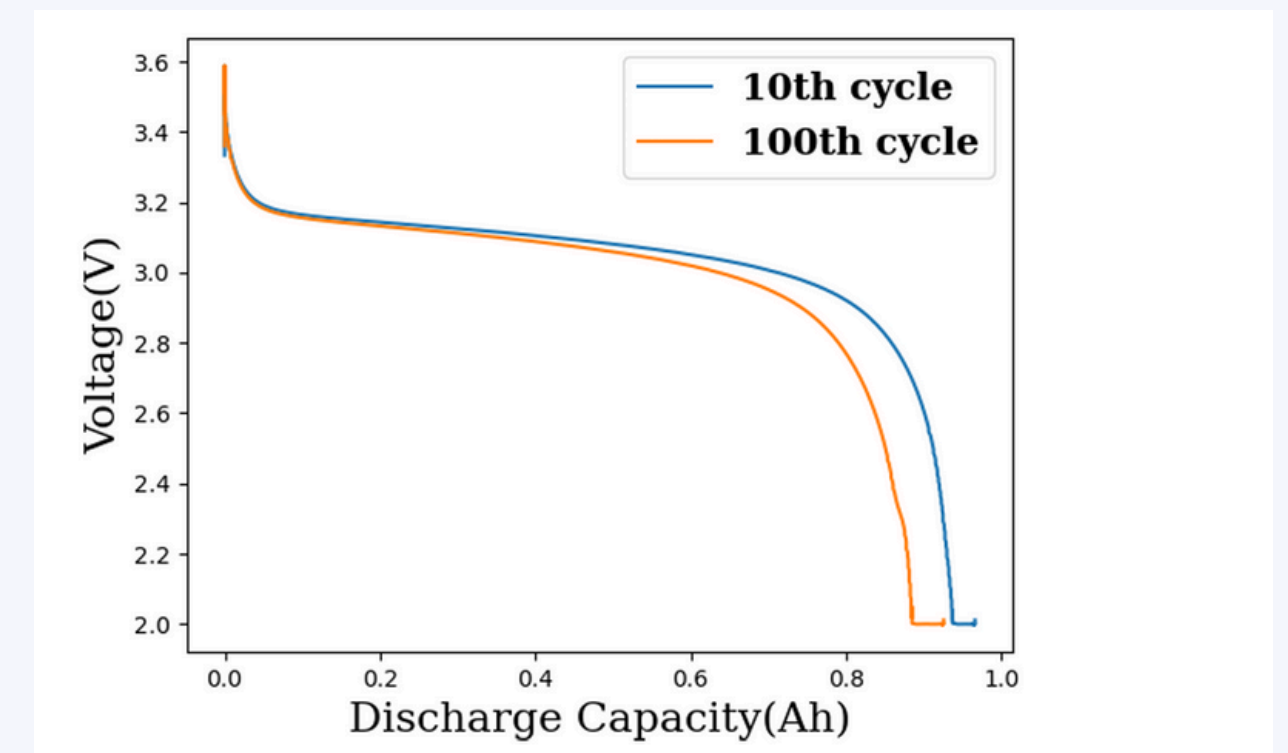
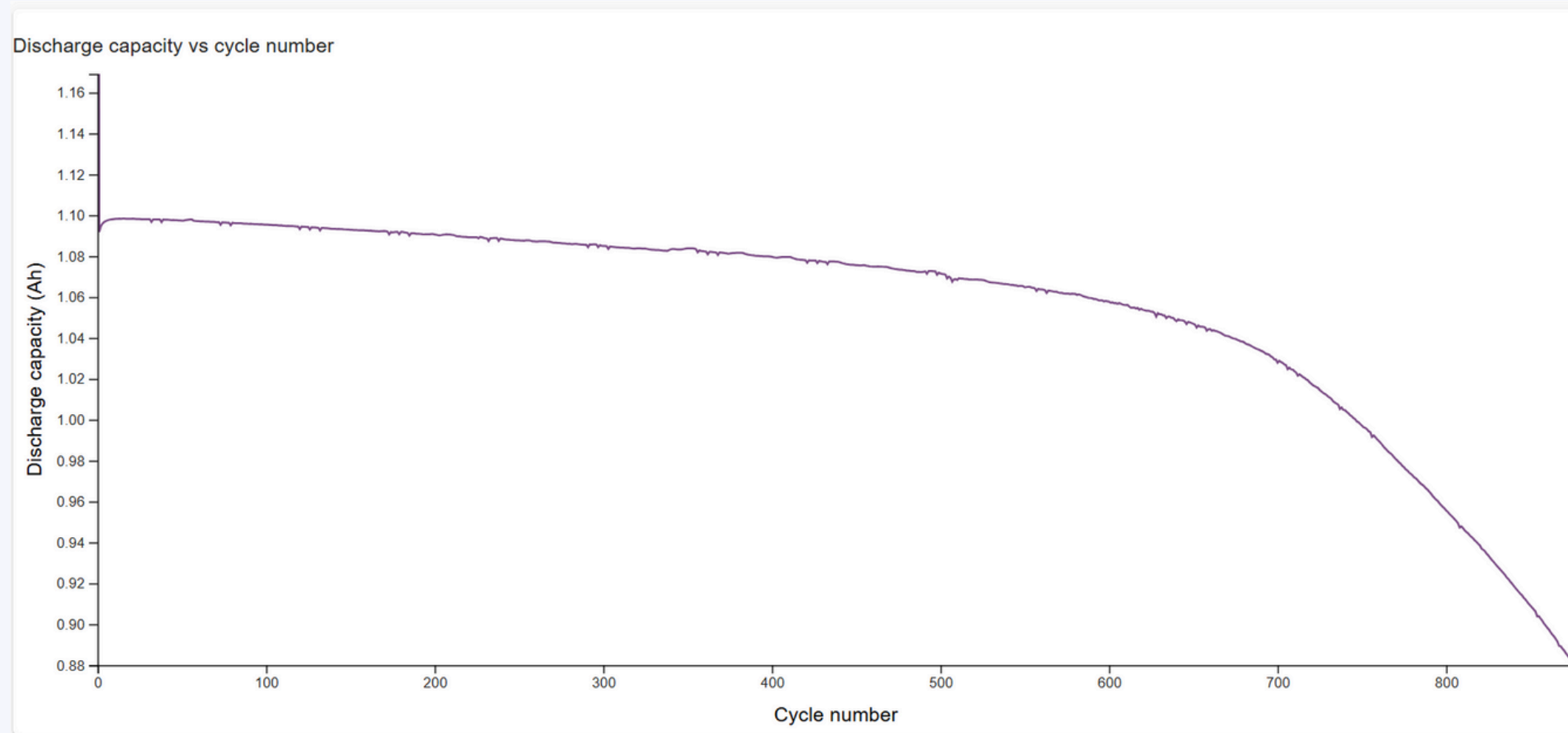
- If we, see the summary column of the data set

1×1 struct with 8 fields

Field	Value	Size	Class
cycle	1189×1 double	1189×1	double
QDischarge	1189×1 double	1189×1	double
QCharge	1189×1 double	1189×1	double
IR	1189×1 double	1189×1	double
Tmax	1189×1 double	1189×1	double
Tavg	1189×1 double	1189×1	double
Tmin	1189×1 double	1189×1	double
chargetime	1189×1 double	1189×1	double

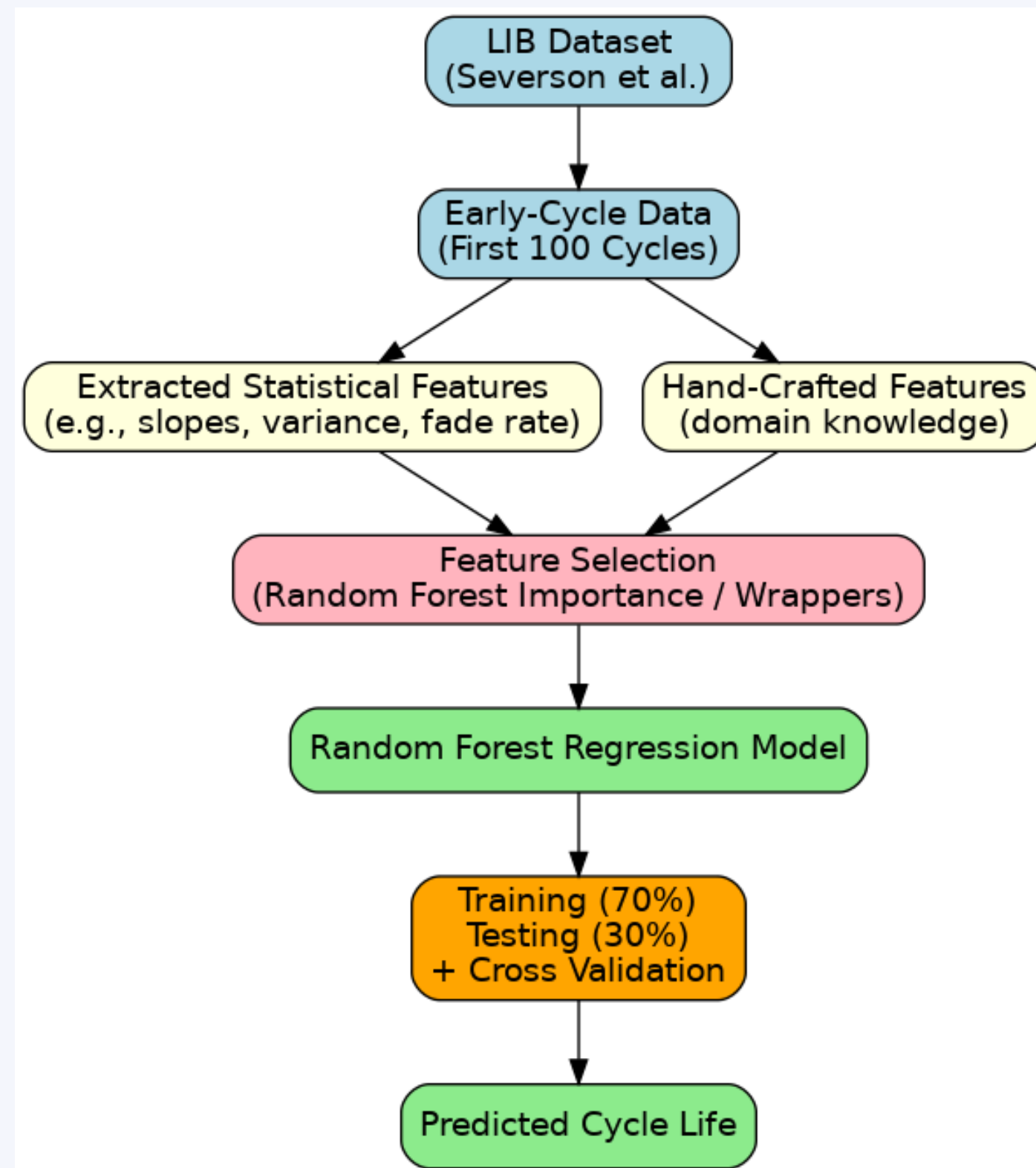
WHAT THE MODEL IS GOING TO PREDICT FROM THE DATA?

- For each cell, we have the discharge capacity and cycle number data. So, we are going to give only the data of the **first 100 cycles** to the model.
- The model will be provided with the first 100 cycles of discharge capacity data, along with **extracted features**, enabling it to learn patterns and predict the cell's cycle life in alignment with experimental observations.



WORKING FLOW OF THE MODEL

- Below added schematic , is just an overview of how a model works on data.



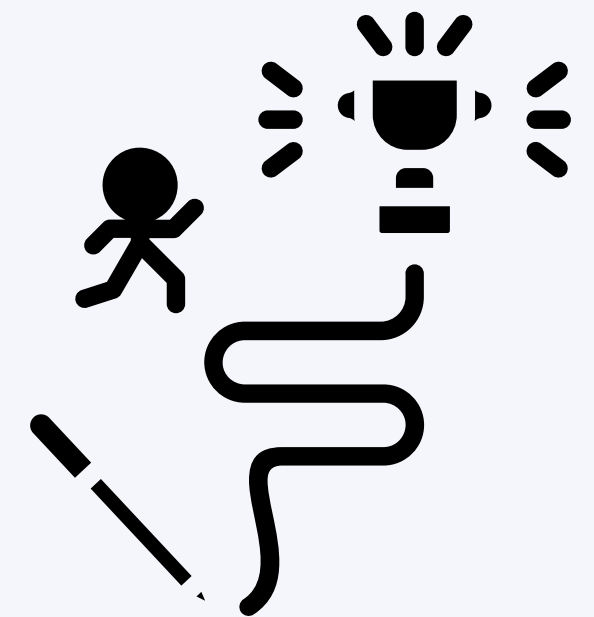
FUTURE WORK

- Extraction of **key features** from the data based on insights from reviewed literature.
- **Model selection** (Elastic Net Regression and Random Forest Regression) for prediction and further development.
- Refinement of the chosen model followed by **validation of results**.



CHALLENGES

- Since the approach is data-driven, extracting **meaningful features** is crucial; otherwise, the model predictions will deviate significantly from experimental results.
- **Choosing the right model** is challenging, as simple models may fail to capture complex degradation pathways, while complex models risk **overfitting** and poor generalization to unseen battery data.



REFERENCES



- Severson, Kristen A., Peter M. Attia, Norman Jin, Nicholas Perkins, Benben Jiang, Zi Yang, Michael H. Chen et al. "Data-driven prediction of battery cycle life before capacity degradation." *Nature Energy* 4, no. 5 (2019): 383–391.
- Edge, Jacqueline S., Simon O’Kane, Ryan Prosser, Niall D. Kirkaldy, Anisha N. Patel, Alastair Hales, Abir Ghosh et al. "Lithium ion battery degradation: what you need to know." *Physical Chemistry Chemical Physics* 23, no. 14 (2021): 8200–8221.
- Celik, Belen, Roland Sandt, Lara Caroline Pereira dos Santos, and Robert Spatschek. "Prediction of battery cycle life using early-cycle data, machine learning, and data management." *Batteries* 8, no. 12 (2022): 266.

THANK YOU
