

Simulation of Degradation Processes in Lithium-Ion Batteries Using Python Modelling

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Abstract – Solid Electrolyte Interphase (SEI) growth and lithium plating are two degradation mechanisms that limit the lifespan of lithium-ion batteries, which are widely used in grid-scale energy storage, electric vehicles, and portable gadgets. A pseudo-two-dimensional (P2D) electrochemical-thermal model based on Python is presented in this study to predict battery degradation processes under different operating situations. The model depicts how capacity fading and an increase in internal resistance are affected by temperature, C-rate, and depth of discharge. The simulation results provide insights into battery aging and optimization.

Keywords: battery degradation, temperature, lithium plating, Solid Electrolyte Interphase (SEI), depth of discharge (DOD), C-rate

I. INTRODUCTION

Electric vehicles, portable devices, and grid-scale energy storage are all made possible by lithium-ion (Li-ion) batteries. Li-ion cells suffer from increasing internal impedance as a result of chemical aging and progressive capacity fading, which is widely referred to as State of Health (SoH), despite their high energy density and cycle stability. The development of the Solid Electrolyte Interphase (SEI) layer on the anode surface is one of the main aging processes [1].

Lithium plating is a crucial degrading mechanism in addition to SEI development, particularly in unfavourable circumstances like low temperatures or high charging rates.



Fig. 1. Lithium plating on a battery electrode; the right electrode shows signs of heavy deposition [2]

When lithium deposits onto a battery electrode, it stops additional ion transport, a process known as lithium plating. Extreme lithium plating is visible on the electrode on the right, in Figure 1.

While high temperatures speed up chemical processes and SEI formation, low temperatures decrease lithium-ion mobility, raising the danger of plating. Internal resistance is

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further increased by calendar aging and extended high states of charge (SOC). Particle breakage, increased resistance, and dendritic development can all be brought on by mechanical stress. Irreversible capacity loss is further accelerated by lithium plating at low temperatures or high C-rates.

Due to electrolyte reduction processes that produce lithium carbonate (Li_2CO_3) and other inorganic species, SEI development consumes active lithium and raises internal resistance.

Local overpotentials and lithium-ion concentration, which are impacted by charging voltage and current rate, determine the rate of SEI growth. SEI develops during lithium intercalation as well as at the electrode surface.

We use a P2D model that connects SEI development to electrode behavior in order to investigate and measure these degradation processes.

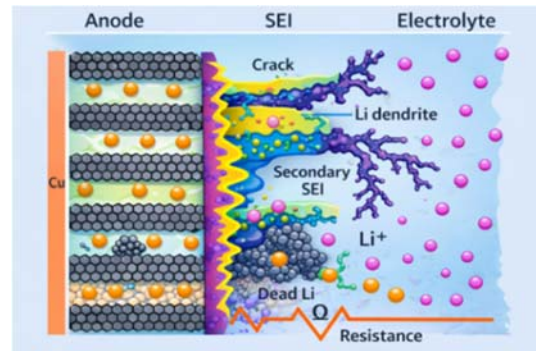


Fig. 2. Anode degradation process brought on by lithium plating

The Figure 2. illustrates the flow of lithium ions (Li^+) from the cathode to the graphite anode via the electrolyte. Li_2 cannot completely intercalate into the graphite at low temperatures or high C-rates, it deposits as metallic lithium on the anode surface. This creates fractures the SEI layer, raises internal resistance, lowers capacity, and may result in safety problems like short circuits [1].

II. LITHIUM PLATING

When metallic lithium deposits on the graphite anode during charging, especially at low temperatures, high C-rates, or high states of charge, this is known as lithium plating. This event shortens the battery's life, fades its capacity.

Although most mitigation solutions are still restricted to experimental research, they concentrate on sophisticated electrode materials, optimal cell design, and customized

charging protocols. For lithium-ion batteries to operate safely and effectively, particularly in fast-charging applications, it is essential to comprehend, identify, and manage lithium plating [3].

The simulation results in Figure 3. show how voltage, temperature, and time all play interdependent roles in the beginning of lithium plating during charging. The anode potential falling below 0 V over a specific capacity range indicates when lithium deposition takes place, while the temperature rise illustrates how the charging rate and thermal conditions interact. These findings support the "Bermuda triangle" theory by confirming that lithium plating is not caused by a single parameter but rather results from a combination of operating conditions. For safer, longer-lasting batteries, intelligent charging techniques that regulate both voltage and temperature are crucial.

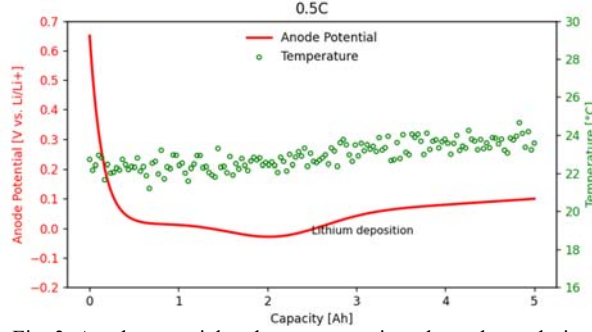


Fig. 3. Anode potential and temperature interdependence during charging at 0.5C, signifying the beginning of lithium plating

III. ELECTROCHEMICAL-THERMAL P2D MODEL

The P2D (DFN) model describes how lithium ions and electrolyte concentrations, electrode potentials, and temperature evolve within a battery cell, offering mechanistic insight into its behaviour, performance, and aging.

The interfacial electrochemical reaction between the solid active material and the electrolyte is described using Butler–Volmer kinetics, which links local lithium concentrations, electrochemical potentials, and temperature to the reaction current density:

$$j = i_0 \left[\exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(-\frac{\alpha_c F \eta}{RT}\right) \right], \quad (1)$$

where i_0 is the exchange current density, α_a and α_c are the anodic and cathodic charge transfer coefficients, and η denotes the interfacial overpotential defined as:

$$\eta = \Phi_s - \Phi_e - U(C_{s,\text{surf}}). \quad (2)$$

Here Φ_s and Φ_e represent the solid and electrolyte-phase potentials, respectively, and U is the open-circuit potential as a function of the surface lithium concentration in the solid particle [7].

Equivalent-circuit models (ECMs) and other low-order empirical models are commonly used in conventional

battery state estimates and control in modern Battery Management Systems (BMSs). ECMs are computationally efficient, but they cannot forecast internal electrochemical states like SEI growth or lithium inventory loss (LLI), and their parameters have no direct physical meaning, which limits their validity to the specific operating conditions in which they were calibrated. On the other hand, lithium-ion transport, reaction kinetics, and temperature effects across the electrodes and electrolyte are mechanistically described by physics-based models, especially the pseudo-two-dimensional (P2D) electrochemical model created by Newman and associates. Despite its higher computational requirements, the P2D model is a great option for advanced control, monitoring, and degradation studies because it can be expanded to account for aging phenomena, such as SEI layer formation and LLI, and accurately captures battery dynamics over a wide range of operating conditions [8].

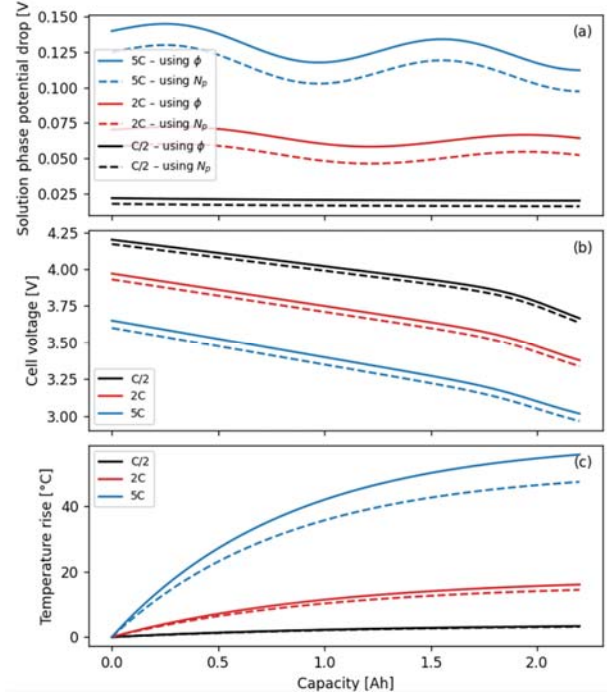


Fig. 4. The electrolyte potential loss, terminal voltage, and cell temperature of a Li-ion battery during discharge at various C-rates

The development of a Li-ion cell under constant-current discharge at C/2, 2C, and 5C is depicted in Figure 4. The solution-phase potential drop ($\Delta\Phi$) between the anode and cathode is shown in panel (a), the terminal voltage is shown in panel (b), and the bulk cell temperature is shown in panel (c). Internal states like local overpotentials and heat generation vary greatly, affecting battery degradation and thermal behaviour, although terminal voltage is comparatively insensitive to the potential model.

The modified MacInnes equation with prefactors $2(1-t_+)$ and $(1-2t_+)$, where t_+ is the cation transference number, is the crucial formula for calculating the diffusion potential's contribution to the overall cell voltage [8].

The Figure 5. illustrates how the discharge rate (C-rate), which is simulated using the P2D model, affects the cell terminal voltage. Higher C-rates cause the voltage to drop more quickly and for greater lithium concentration gradients to form throughout the cell, whereas lower C-rates cause the voltage to drop gradually and evenly. This suggests that quicker discharges produce more noticeable internal gradients, which may have an indirect impact on long-term battery deterioration and SEI expansion [7].

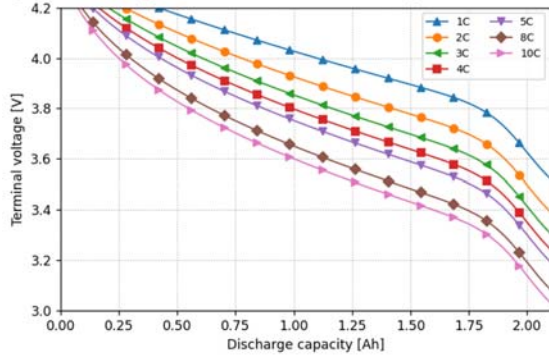


Fig. 5. Cell terminal voltage prediction using a P2D model at various discharge rates

Minimal P2D (DFN) simulation in Python

```
import pybamm
model = pybamm.lithium_ion.DFN()
sim = pybamm.Simulation(model)
sim.solve()
sim.plot()
```

This is the minimum of code needed to use PyBaMM to run a P2D (DFN) battery model in Python. It imports the library, builds the DFN model, does the simulation, and plots the outcomes. For more complex simulations, optional elements like personalized experiments or parameter modifications can be included.

```
experiment = pybamm.Experiment(["Discharge at 1C
until 3.0 V"])
sim = pybamm.Simulation(model,
experiment=experiment)

param = pybamm.ParameterValues("Chen2020")
param.update({"Electrode height [m]": 0.1})
sim = pybamm.Simulation(model, parameter_values=param)
```

First two lines can be added to imitate a particular battery experiment, such as charging or discharging. The next three lines allow you to modify default battery parameters, such as electrode dimensions or material properties, to run a more customized simulation.

IV. TEMPERATURE AND OPERATING CONDITIONS' EFFECTS

Lithium-ion battery deterioration and the beginning of lithium plating are significantly influenced by temperature

and operating conditions. Lithium-ion transport slows down at low temperatures, which increases overpotentials during charging and increases the likelihood of lithium plating, particularly at high charging rates. On the other hand, greater temperatures speed up chemical reactions inside the cell, which increases SEI growth, electrolyte breakdown, and mechanical stresses. These factors all lead to higher cell impedance and reduced capacity.

Next important factor is the charging rate (C-rate). Larger C-rates raise the possibility of lithium plating, whereas deeper DOD and prolonged high states of charge increase electrochemical stress and hurry aging.

Effective thermal management and optimized operating strategies (moderate temperatures, controlled C-rates, and SOC/DOD limits) are therefore crucial for maintaining battery performance and extending life.

Calendar aging is the term used to describe capacity deterioration and a rise in internal resistance that happen over time even in the absence of active cycling of a lithium-ion battery. State of charge (SOC) and storage temperature have a substantial impact on calendar aging, with greater SOC levels and temperatures greatly increasing degradation.

V. SOLID ELECTROLYTE INTERPHASE (SEI) GROWTH MECHANISM

The electrolyte and electrode materials determine solid electrolyte Interphase (SEI) composition. In order to stop more electrolyte breakdown, a stable SEI must be thin, ionically conductive, electrically insulating, and able to adapt to variations in anode volume.

Thinner organic-rich SEI layers occur on basal planes of graphite anodes, whereas thicker inorganic-rich layers form on edge planes. When the SEI thickens excessively or stops providing protection, battery performance deteriorates. [5]

```
experiment = pybamm.Experiment([
    "Charge at 0.5C until 4.2 V",
    "Rest for 1 hour",
    "Discharge at 0.5C until 3.0 V"])
param = pybamm.ParameterValues("Chen2020") # ili
drugi set parametara
param.update({
    "Electrode height [m]": 0.1,
    "SEI film resistance [Ohm.m2]": 0.1})
```

This code snippet shows how to define a battery experiment with charge, rest, and discharge steps, and how to adjust key battery parameters such as electrode height and SEI film resistance for a pseudo-two-dimensional (P2D) model simulation in Python using PyBaMM.

The decrease in ionic mobility within the electrolyte brought on by parasitic side reactions and electrolyte breakdown is known as electrolyte conductivity loss. Resistive by-products are produced as a result of these events, which gradually obstruct lithium-ion transport and raise internal cell impedance. The simulated results validate

the exponential sensitivity of conductivity loss to both temperature and SOC, as illustrated in Fig. 6.

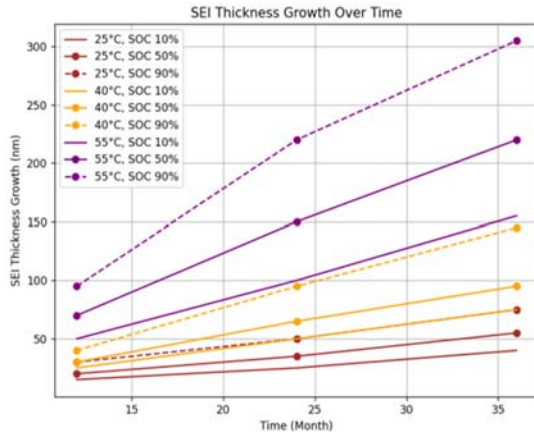


Fig. 6. SEI thickness increase over time at various temperatures and states of charge (SOC)

The graphic in Fig. 7. illustrates how SEI growth and electrolyte degradation are significantly accelerated by high temperature and high state of charge (SOC), which immediately result in higher internal resistance and a decline in battery performance [7].

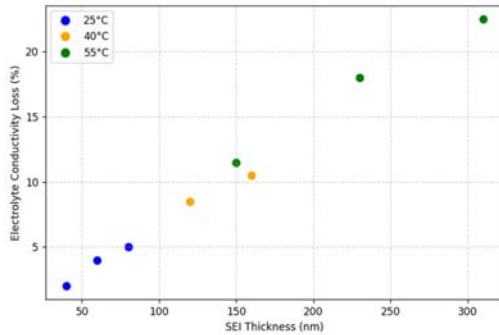


Fig. 7. SEI thickness increase and electrolyte conductivity decrease during 36 months

TABLE II

An overview of the main trends in Li-ion battery degradation

Operating condition	Dominant degradation mechanism	Impact on battery performance
High SOC and temperature	SEI growth	Increased internal resistance and lithium inventory loss
Low temperature and high C-rate	Lithium plating	Capacity loss, formation of dead lithium and safety risk
DOD	SEI thickening and mechanical stress	Accelerated aging and reduced cycle life
Prolonged high SOC storage	SEI and CEI formation	Calendar aging and capacity fade
Moderate temperature and C-rate	Minimal degradation	Improved battery lifetime and stability

VI. CONCLUSION

Table II shows the main degradation mechanisms and their effects on battery performance. Low temperatures and fast charging promote lithium plating, causing capacity loss and safety risks. High SOC and rising temperatures accelerate SEI growth, increasing resistance and reducing lithium. Deep DOD and long high-SOC storage worsen mechanical stress and aging. Moderate conditions improve battery life by slowing degradation.

VII. LITERATURE

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