Lithium-Metal Battery Degradation Dataset from Continuous Cycling Experiments

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ARTICLE INFORMATION

Article title

Lithium-Metal Battery Degradation Dataset from Continuous Cycling Experiments

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Keywords

Lithium-metal battery data set, degradation, capacity loss

Abstract

Lithium-metal batteries are promising next-generation batteries but but their limited lifetime and safety concerns remain key challenges for real-world deployment. The dataset presented in this paper contains current and voltage data, from which the capacity is calculated from 23 different lithium-metal battery cells, encompassing four different design configurations and nominal capacities. The cells were manufactured at Sakuu Corp., and the data were collected in its R&D laboratory. The cells underwent continuous cycling with a constant-current (CC) discharge and a constant-current constant-voltage (CC-CV) charge at different C-rates and voltage cutoffs at room temperature. Each cell experiences capacity loss from repeated cycling due to degradation mechanisms that lead to the formation of dead or inactive lithium, electrolyte depletion and increase in impedance during cycling. The voltage, current, and capacity data for each cycle are presented in the dataset. This dataset can be used for developing models and strategies to predict cell lifespan, accelerating design to improve performance and durability.

SPECIFICATIONS TABLE

Subject	Engineering & Materials science
Specific subject area	Lithium-metal battery aging
Type of data	Table(.mat format)
Data collection	Sakuu Corp. collected the data by applying a constant-current constant-voltage (CC-CV) charging input profile, a CC discharging profile, and recording the output voltage. The charging C-rates and voltage cutoffs used vary for different cells, and

	the cells were all discharged at 1C. The cycle-by-cycle capacity was calculated from the discharge and charge current data, along with the respective equivalent full cycle (EFC) is included in the dataset.
Data source location	Institution: Sakuu Corp. City, State: San Jose, California Country: United States of America
Data accessibility	Repository name: Lithium-Metal Battery Degradation Dataset from Continuous Cycling Experiments Data identification number: DOI 10.17605/OSF.IO/5DQWG Direct URL to data: https://osf.io/5dqwg/?view_only=608e4c22acdd483591d1d55b74a81401
Related research article	Uppaluri, M., Xu, L., Ma, W., Aliahmad, N., Saatchi, A., Littau, K., Onori, S. ,"Clustering and Predicting Early Capacity Fade Trajectories in Lithium-Metal Batteries using Data-Driven Approaches" *manuscript under preparatation* (2025).

VALUE OF THE DATA

- The dataset consists of current, voltage and calculated charge/discharge capacities data from 23 cells of four different design configurations of lithium-metal cells that were developed at the lab-scale. The cells comprise a lithium-metal anode and a nickel-manganese-cobalt cathode (NMC 811). They are grouped based on the differences in the cell design specifications, such as number of layers in the cell, electrolyte design or electrode thickness, and are cycled under varying charge C-rates, and discharged at 1C, with different voltage cutoffs.
- These cells were continuously cycled at room temperature with a constant current (CC) discharge and constant current constant voltage (CC-CV) charge protocol. The number of cycles that the cells underwent ranges from 250-650 cycles. The charge and discharge C-rates and the cutoff voltages are listed in Table 1.
- The discharge and charge capacity with respect to equivalent-full-cycles (EFC) are calculated from the current and voltage data and reported in the dataset, as an indication of the state-of-health (SOH) of the cells.
- The value of this dataset lies in its ability to help researchers develop models and derive insights for estimating cell SOH and forecasting the performance of emerging battery technologies. These insights can guide design decisions to extend battery lifespan.
- To the best of the authors' knowledge, this dataset is the first to offer battery-aging data from lithium-metal battery cells with diverse performance profiles.

BACKGROUND

Lithium-metal batteries are considered promising candidates for next-generation energy storage due their high theoretical capacity and energy density.[1,2] These batteries face challenges related to lifespan and safety due to the non-homogeneous structures or dendrites that form due to lithium plating on the negative electrode during charge, the growth of the solid electrolyte interphase (SEI) layer, and the accumulation of inactive lithium, which results in irreversible lithium loss and increased cell resistance.[2,3,4] The data set presented in this paper provides valuable insights into the capacity fade behavior of lithium-metal batteries and can serve as a foundation for developing strategies to improve battery design and extend lifespan. The dataset includes 23 cells undergoing cycling for varying durations, with cycle counts ranging from 250 to 650 cycles. It contains current and voltage time series data, and the calculated discharge and charge capacity data, which can be used to train, calibrate and validate models for SOH estimation and remaining useful life (RUL)/end-of-life (EOL) predictions. [5,6,7]

DATA DESCRIPTION

The dataset consists of current and voltage time series data from 23 lithium-metal cells, the data set also include the calculated capacity ion charge and discharge with lithium metal anodes and NMC-811 cathodes, that were repeatedly cycled at room temperature. This dataset was collected at Sakuu Corp., a lithium-metal battery manufacturing company based in San Jose, CA (https://www.sakuu.com/). The 23 cells in the dataset are classified into four different groups, based on the cell design specifications (such as number of layers in the cell, electrolyte design or electrode thickness) and the operating conditions at which they have been cycled. Each group of cells underwent continuous cycling consisting of the following sequence:

- Constant Current and Constant Voltage (CC-CV) charging at varying C-rates and cutoff voltages.
- Constant Voltage (CV) charging to a specified cutoff voltage.
- Rest period of 600 seconds after each charging event.
- CC discharging at 1C.
- Rest period of 600 seconds after each discharging event.

Table 1 summarizes nominal capacities for each of groups, number of cells in each group, the charge/discharge C-rates, CC charge and discharge cutoff voltages, current cutoff C-rates for CV charging. The cells were cycled from a range of approximately 250 to 650 cycles.

Table 1. Summary of the nominal capacities, the lower and upper cutoff voltages during constant current charge, and the current cutoff during CV charging.

Group	Nominal Capacity, Q_0 (mAh)	Number of cells	Charge Current (C-rate)	Discharge Current (C-rate)	Low Voltage Cutoff (V)	High Voltage Cutoff (V)	Current Cutoff (C-Rate)
1	3.8	6	3 cells@ C/5, 3 cells@ C/2	1C	3	4.3	0.05
2	1000	5	C/5	1C	2.8	4.3	0.02
3	1000	7	4 cells @C/5, 3 cells@ C/3	1C	2.8	4.2	0.02
4	327	5	C/5	1C	3	4.3	0.05

The dataset consists of measured charge and discharge current and voltage profiles for each of the cells. Both charge and discharge capacities were calculated and included in the dataset. The discharge capacity was determined using the following equation:

$$Q_{dis}^{(i)} = \frac{1}{3600}\int_{t_0}^{t_f(i)} |I_{batt}(\tau)|d\tau \quad (1)$$

where t_0 and $t_f(i)$ are the initial and final time for the discharge, determined by the time just after the end of the rest period, and the time at which the cell reaches the low voltage cutoff (shown in Table 1) respectively, during a given cycle i. In this dataset, charge current is positive, while discharge current is negative, expressed in units of milli Ampere (mA). The current integral is divided by 3600 to provide the capacities in milli Ampere-hour (mAh).

Similarly, the charge capacity is given as:

$$Q_{chg}^{(i)} = \frac{1}{3600}\int_{t_0}^{t_f(i)} I_{batt}(\tau)d\tau \quad (2)$$

where t_0 and $t_f(i)$ are the initial and final time for the CC-CV charge, determined by the time after the rest period, and the time at which the cell reaches the current cutoff after CV charge (shown in Table 1) respectively.

The current, voltage and capacity data for each group is stored in a subfolder within that group. Figure 1 shows the structure of the data within each group. Each cell contains two .mat files: G'x'_Cell'y'_data.mat, that contains the voltage and current data for a given cell y in group x, and G'x'_Cell'y'_capacity_degradation.mat that contains the calculated charge and discharge capacity data of the cell. For instance, for cell 1 in group 1, the "G1_Cell1_data.mat" file contains the time, voltage and current data for each cycle while the "G1_Cell1_capacity_degradation.mat" files contain the charge and discharge capacities along the EFC.

Within the "G'x'_Cell'y'_data.mat" file, there exists structures (Struct) for each cycle, that contain the voltage, current and capacity data during charge, and the voltage, current and capacity data during discharge, as well as the voltage and current data for each full cycle (charge and discharge), rest period included.

The separate discharge and charge capacities for each of the cells were calculated and stored in a separate .mat file. The EFCs were evaluated for each cell and stored in the "G'x'_Cell'y'_capacity_degradation.mat" files. The EFC is defined as

$$EFC(i) = \frac{Ah - Throughput(i)}{2 * Q_0} \quad 3$$

where the Ah-Throughput is the cumulative charge collected at a given full cycle i given by

$$Ah - Throughput(i) = \frac{1}{3600}\int_{t_0}^{t_f^{(i)}} |I_{batt}(\tau)|d\tau \quad 4$$

where t_0 is the initial time of the cycle (start of charge), and $t_f(i)$ represents the final time (end of discharge) of the cycle i.

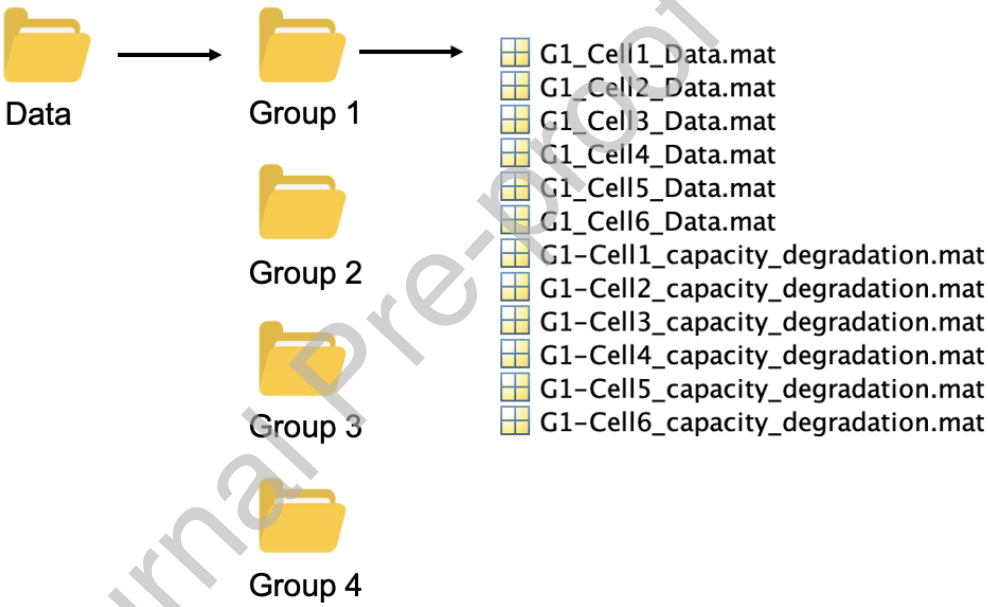

Figure 1. Structure of the overall dataset.

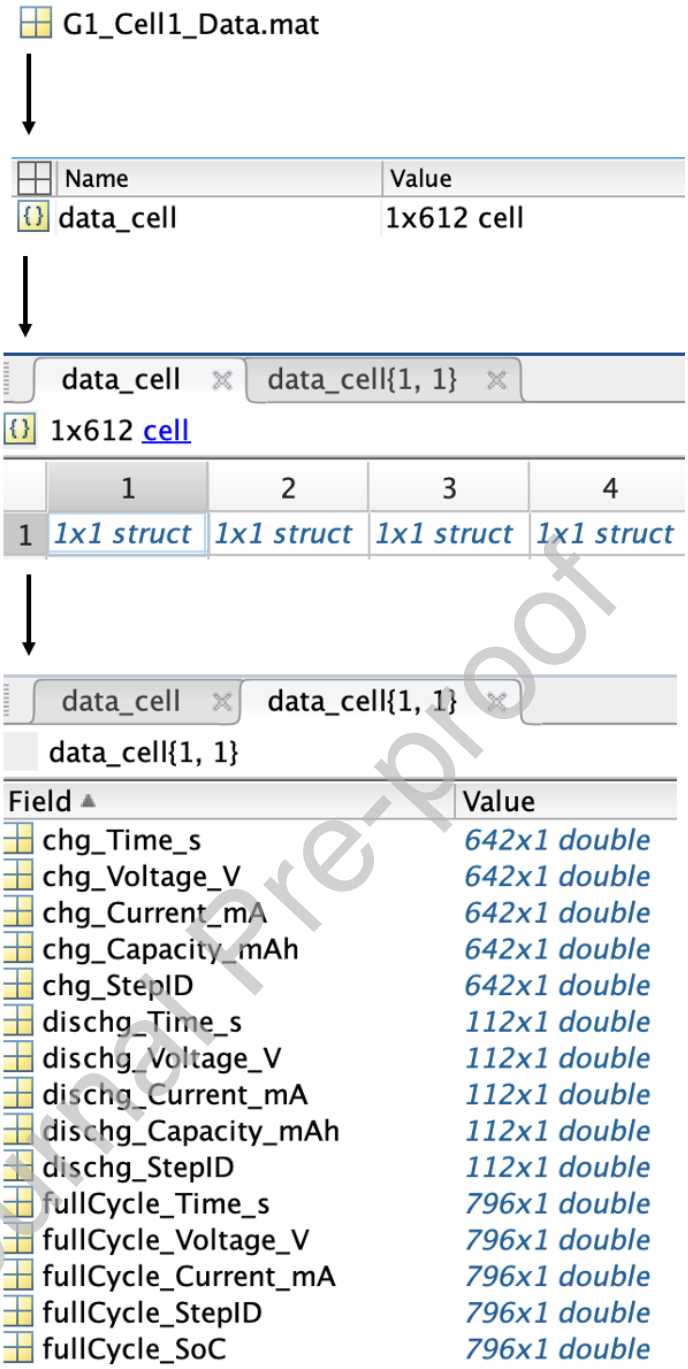

Figure 2. Structure of the “Struct” , containing the current, voltage and capacity data for the charge, discharge process, as well as the current and voltage data for a full cycle.

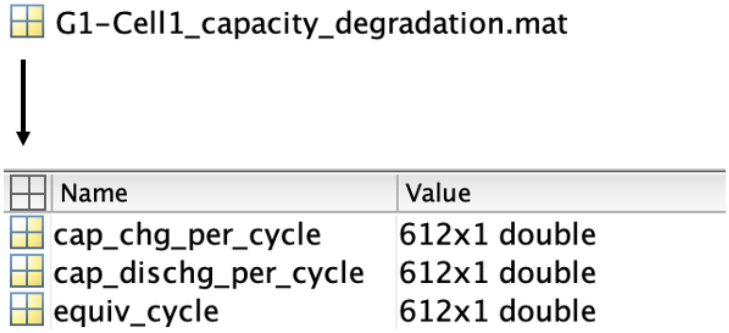

Figure 3. Structure of the charge and discharge capacity data for a given cell, along with the corresponding equivalent full cycle.

EXPERIMENTAL DESIGN, MATERIALS AND METHODS

Each group of cells were cycled using Neware battery testing cyclers at room temperature with a CC discharge and CC-CV charging profile. Each group was cycled with a different CC and CC-CV current (as reported in Table 1). The profiles are shown in Figure 5.

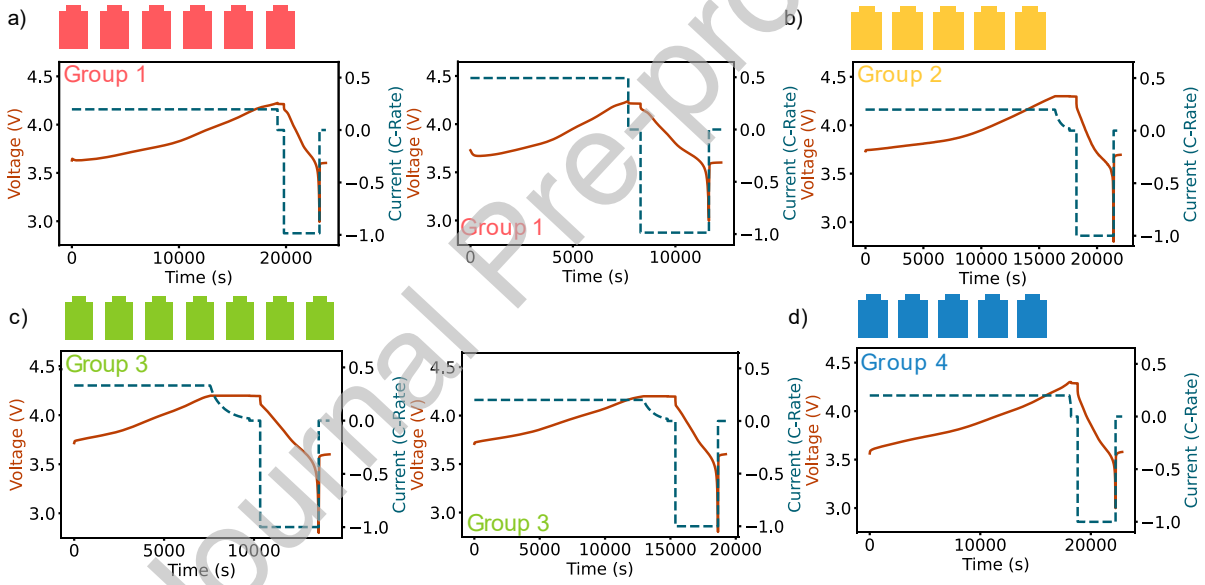

Figure 4. Cycling protocol performed on each of the cell groups.

LIMITATIONS

This dataset consists of only 23 cells, which may which may limit its suitability for comprehensive analysis or certain data-driven predictive models. Nonetheless, the degradation curves exhibit meaningful variations that can provide valuable insights for analysis and modelling.

ETHICS STATEMENT

Hereby, we Maitri Uppaluri, Wenting Ma, Le Xu, Alireza, Nojan Aliahmad, Alireza Saatchi, Karl Littau and Simona Onori assure that for the manuscript “Lithium-Metal Battery Degradation Dataset from Continuous Cycling Experiments” the following is fulfilled:

1.This material is the authors’ own original work, which has not been previously published elsewhere.

2.The paper is not currently being considered for publication elsewhere.

3.The paper reflects the authors' own research and analysis in a truthful and complete manner.

4.The results are appropriately placed in the context of prior and existing research.

5.All sources used are properly disclosed. Literally copying of text must be indicated as such by using quotation marks and giving proper reference.

6.All authors have been personally and actively involved in substantial work leading to the paper and will take public responsibility for its content.

CRediT AUTHOR STATEMENT

Maitri Uppaluri: Analysis, Writing – Original Draft, **Wenting Ma, Le Xu:** Data cleaning, Analysis, **Nojan Aliahmad, Alireza Saatchi, Karl Littau:** Data Collection, **Simona Onori:** Writing – Review & Editing, Supervision, Funding acquisition.

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DECLARATION OF COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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