Data: State-of-health estimation of lithium-ion batteries subjected to different ageing conditions via electrochemical impedance spectroscopy and machine learning

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Cell Specification:

Table 1: Specifications of the cell as provided by the supplier

Manufacturer	LiFun Technologies
Cell stack type	stacked
Format	pouch
Chemistry (Anode)	artificial graphite
Chemistry (Cathode)	NMC622
Nominal capacity	1 Ah
Voltage range	3–4.2 V
Max. continuous charge/discharge current	1.5C/5C
Electrolyte composition	1 M solution of $LiPF_6$ in EC/EMC 3:7 and 2 wt.% VC

Test description

The dataset contains electrochemical impedance spectroscopy (EIS), cycling data, and reference performance test (RPT) measurements acquired from 1 Ah NMC622|artificial graphite pouch cells at different stages of ageing. Potentiostatic EIS measurements were performed using a Zahner Zennium with a 10 mV perturbation signal in multisine mode, with the cells placed in a Binder climate chamber maintained at 25 °C. After each cycling interval, the cells were allowed to rest for at least 12 h before the EIS measurements to minimize transient effects associated with the preceding charge–discharge operation and to ensure consistent measurement conditions. All impedance measurements were performed at 50 % SoC, determined from the remaining measured cell capacity. The measured impedance spectra initially covered a frequency range from 10 mHz to 20 kHz and comprised 67 frequency points. During subsequent measurements, the frequency range was extended to 50 kHz, resulting in 74 frequency points. The cells were aged under 14 different cycling conditions, defined by variations in charging current rate, discharge current rate, temperature, and rest time after charging and discharging. Three replicate cells were assigned to each ageing condition, resulting in a total of 42 cells in the test matrix. One cell under condition TM13 failed prematurely during cycling; therefore, 41 of the 42 cells completed the planned cycling protocol. The ageing experiments began with an initial RPT, followed by 50 charge–discharge cycles. During the first 150 cycles, intermediate EIS measurements were performed after every 50 cycles. Thereafter, the EIS measurement interval was increased to 100 cycles. After cell formation, the pouch cells were mechanically constrained between steel pressure plates with the screws tightened to a torque of 0.6 Nm. The mechanical constraint was

maintained throughout the ageing experiments and was not adjusted during EIS measurements. The RPTs included a C/20 capacity measurement performed at 25 °C using a Neware CT-4008T-5V6A.

Table 2: Cycling test matrix

Test ID	Temperature [°C]	C-rate	D-rate	Rest time [h]
TM1	25	0.5	0.5	2
TM2	45	0.5	1.5	2
TM3	45	0.5	0.5	0
TM4	45	1.5	1.5	2
TM5	25	0.5	0.5	0
TM6	25	1.5	1.5	0
TM7	25	1.5	0.5	2
TM8	25	0.5	1.5	2
TM9	45	1.5	1.5	0
TM10	45	0.5	0.5	2
TM11	25	0.5	1.5	0
TM12	45	0.5	1.5	0
TM13	45	1.5	0.5	2
TM14	45	1.5	0.5	0

EIS data description:

The raw EIS data are provided within the .zip archive “EIS_measurement_data.zip”. The EIS data are compiled in the folder “EIS_Measurement_data”, which contains 14 subfolders, each corresponding to one of the test conditions listed in Table 2, as well as a “capacity_data.xlsx” file containing the measured C/20 charge and discharge capacities of the cells in two separate sheets. The test-condition folders are named according to their respective test IDs (TM1–TM14). Each test-condition folder contains three separate subfolders for the replicate cells cycled under that condition. For example, the TM1 subfolder contains three other folders, “TM1_1”, “TM1_2”, and “TM1_3”, corresponding to the three replicate cells tested under condition TM1. Within each cell folder, the EIS measurements are provided as *.txt* files and are ordered chronologically according to the measurement sequence. The sequence begins with the initial EIS measurement performed after cell formation and continues through the subsequent measurements during ageing, up to the final measurement after 2150 cycles. The file names indicate the measurement sequence and the corresponding cell. For example, “00_tm-daf-1-1.txt” represents the initial EIS measurement of the first replicate cell tested under TM1, while “23_tm-daf-1-1.txt” represents the final EIS measurement of the same cell after 2150 cycles. The cell naming convention used for the EIS files is retained in the “capacity_data.xlsx” file located in the folder “EIS_measurement_data”. Each EIS measurement file begins with a metadata header, followed by the measurement data organized into columns: measurement number, frequency, real impedance, imaginary impedance, significance, and time.

PS: The raw cycling and RPT data for all test conditions are available upon request. Please contact me if you are interested in this data.

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