Multivariate analysis of Thermal Runaway Behaviour in Aged Lithium-ion Batteries

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Lithium-ion batteries (LIBs) are widely employed across various applications due to their high energy density and long cycle life. However, ensuring their safety is a critical issue because of the potential risk of fires or explosions caused by overheating, overcharging, or internal short circuits. Moreover, throughout their cycle life, batteries are subjected to repeated charging, discharging and thermal stress, all of which impact their state of health (SOH). Thermal runaway (TR) is the most critical safety hazard in lithium-ion batteries, leading to their failure due to uncontrolled exothermic reactions triggered by mechanical, thermal, or electrical abuse. In this study, aged cylindrical cells with an NMC cathode were subjected to thermal abuse tests using the standard Accelerating Rate Calorimeter (ARC).This instrument, which is able to simulate adiabatic conditions, was employed to identify critical thermal instability thresholds following the heat-wait-seek (HWS) protocol, enabling precise monitoring of the batteries' thermal behaviour. To assess the state of health, considering the different aging paths of the cells used in the tests, a specific electrochemical characterization was performed using the galvanostatic intermittent titration technique (GITT)[1].This analysis focused on evaluating the progression of capacity fade and the increase in internal resistance, which are key parameters associated with the cell's state of health (SOH). The main objective of this work is to correlate SOH variables with thermal runaway parameters through the application of Principal Component Analysis (PCA). PCA is a technique that captures the direction of the maximum variance of the given data through converting potentially correlated variables into a set of linearly uncorrelated variables. With its application, key variables that are significantly related to SOH and thermal runaway are summarized and utilized to establish representative features. Such features can be further utilized to analyse cell-to-cell variability in thermal runaway behaviour, with the aim of predicting aging-related changes in thermal performance under abuse conditions.

Keywords: *thermal runaway, ARC, state of health, Principal Component Analysis*

References: *[1] Kirkaldy, Niall, et al. "Lithium-ion battery degradation: measuring rapid loss of active silicon in silicon–graphite composite electrodes." ACS applied energy materials 5.11 (2022)*

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