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Accurate Prediction of Li-Ion Cell Behavior during External Shorting Event using AutoLion™

Introduction

The external short of a Li-ion battery in field application can readily lead to dangerous or even catastrophic failure. A typical BMS may monitor cell current, voltage, and surface temperature as a metric for safety, and as such accurate prediction of these variables by AutoLion™ is of great value to the designer. In this case study, we validate the current, voltage, and local temperature prediction of AutoLion-3D™ by comparing the simulated results with data for an 18650 NMC/graphite cell, proving the ability of AutoLion™ to accurately predict the response of an externally shorted Li-ion cell. Experimental data for internal temperature of the 18650 cell was acquired by use of a novel reaction temperature sensor (RTS) probe. In the process of performing validation, we also highlight that the cell's surface temperature fails as an indicator of the cell safety condition, as an approximately 45ºC difference between cell center and surface temperatures was observed at peak conditions.

Software Used

- AutoLion-3D™

Setup

- A 1.6Ah NMC/graphite 18650 cell was designed in AutoLion-3D™ to represent the corresponding experimental cell.
- The cell was externally shorted for 16s using the AutoLion-3D™ shorting model. A constant 12 mΩ shorting resistance was applied across the battery terminals.
- No shutdown separator, ceramic coated safety layer, PTC, or any other safety devices were employed in the cell design.
- There was natural convection cooling from the exterior surface of the cell. In the simulation a convection heat transfer coefficient of h = 20W/m^2/K was used; ambient/initial temperature was 25°C.
- Initial state of charge (SOC) of the cell (before short) was 1.
- Temperature data for validation was acquired from experiment by use of a novel reaction temperature sensor (RTS) for cell-internal temperature and surface-mounted thermocouple for surface temperature. Current data was acquired by use of a low-resistance shunt resistor. Details can be found in references [1-3].

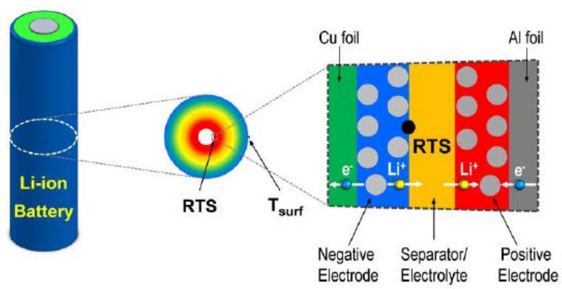

Figure 1. Diagram of 18650 cell embedded with reaction temperature sensor (RTS), along with surface-mounted temperature probe [3].

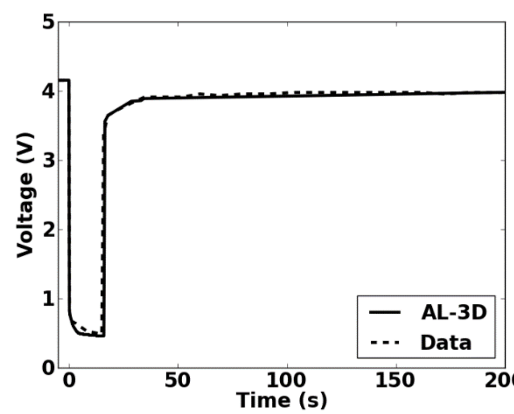

Figure 2. Simulated and experimental cell voltage during external short.

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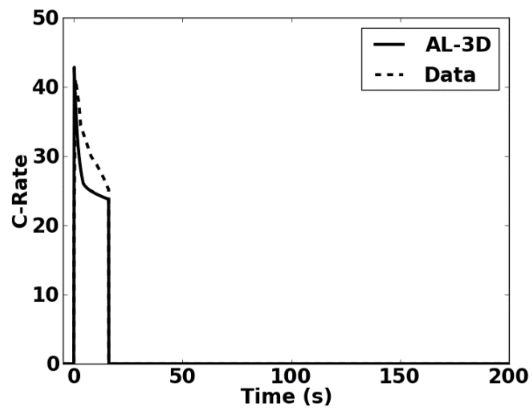

Figure 3. Simulated and experimental cell current (C-rate) during external short.

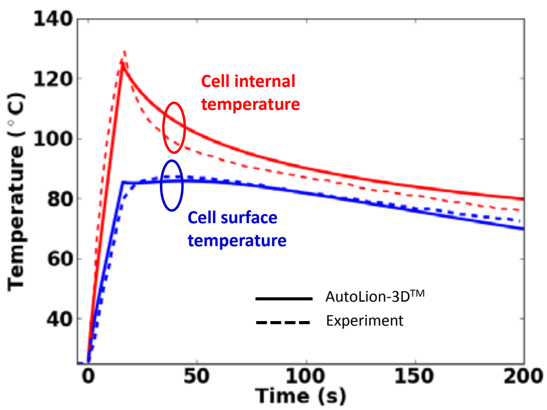

Figure 4. Simulated and experimental temperature during external short. Red curves represent cell-internal temperature at center of cell, blue curves represent surface temperature; dashed lines represent data and solid lines are simulation.

Summary, Analysis, and Conclusions

- Figures 2-4 above highlight an overall good agreement for simulated and experimental voltage, current, and local temperature over the entire shorting process. A maximum error of approximately 2% was observed for voltage, 10% for current, and ~4% error for local temperatures at the peak time (~16s).
- Figure 4 highlights that the cell-center temperature reaches 130ºC while the cell surface temperature reaches only ~ 85ºC at the 16s mark, a staggering difference of 45ºC. Given that thermal runaway will ensue when cell temperature reaches ~ 150-200ºC at any point in the cell, ***clearly a BMS that uses surface temperature measurement as a direct indicator of safety will fail to accurately capture the danger level of the cell***, potentially leading to catastrophic failure.
- The validation shown here proves that ***AutoLion™ can reliably be used to assess the safety of Li-ion batteries in the design phase, before a cell is built***. An AutoLion™ user can readily modify the cell design (internal structure for power vs. energy cell, active material types, form factor of the battery, etc.), and very quickly determine its quantitative effect on battery safety. Much greater iteration in the design phase is achievable through use of AutoLion™.

References

[1] Zhang, G.S., Cao, L., Ge, S., Wang, C.Y., Shaffer, C.E. and Rahn, C.D., "In-Situ Measurement of Li-Ion Battery Internal Temperature," 224th ECS Meeting, Abstract# 538, San Francisco, CA, USA, October 27-November 1, 2013

[2] Zhang, G., Cao, L., Ge, S., Wang, C.Y., Shaffer, C.E. and Rahn, C.D. (2014). "In Situ Measurement of Radial Temperature Distributions in Cylindrical Li-Ion Cells," *Journal of the Electrochemical Society*,161, A1499-A1507

[3] G. Zhang, L. Cao, S. Ge, C. Y. Wang, C.E. Shaffer, and C.D. Rahn, "In Situ Measurement of Temperature Distribution in Cylindrical Li-Ion Cells," 226th ECS Meeting, Cancun, Mexico, October 9, 2014