SAND2019-5598C

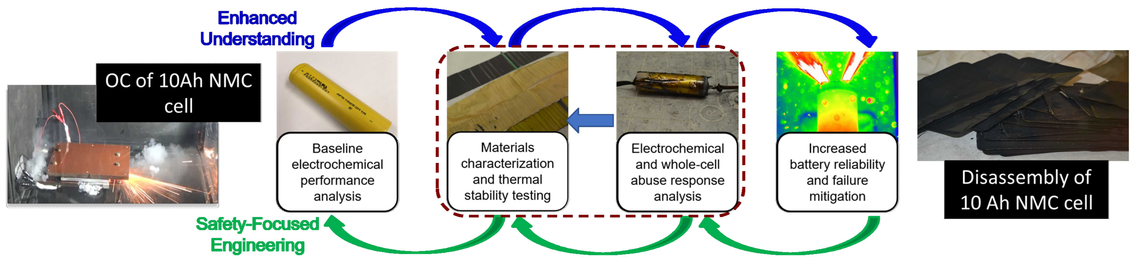
Sandia National Laboratories

Degradation Mechanisms of Overcharged Li-ion Batteries

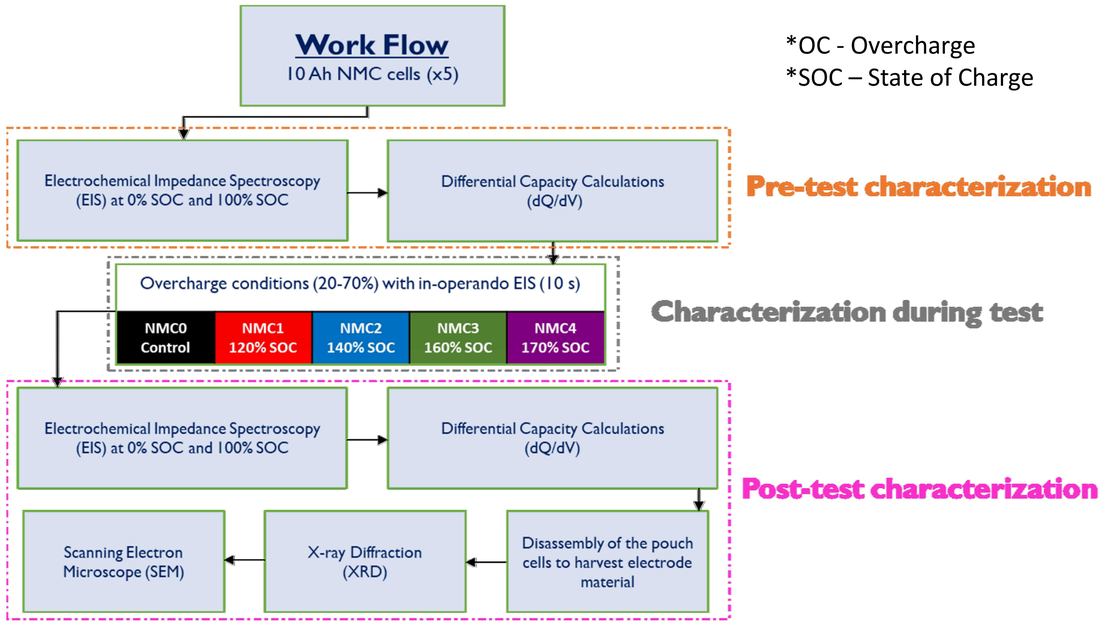
E. Deichmann, L. Torres-Castro, J. Lamb, M. Karulkar, C. Grosso, J. Langendorf, L. Gray and J. Stanley

Introduction

- Stationary energy storage systems (ESS) are increasingly deployed to maintain a robust and resilient grid.
- As system size increases, financial and safety issues become important topics.
- Holistic approach: electrochemistry, materials, and whole-cell abuse will fill knowledge gaps.
- Simple passive monitoring of a cell or battery is often unable to identify the onset of failure until it is too late to intervene.
- The prevention of catastrophic failure requires detection of internal faults well before they have developed to the point of no return.
- Understanding the degradation mechanisms of the battery components during abusive conditions is essential to influence the development of new components designs that are more resilient to abusive conditions.

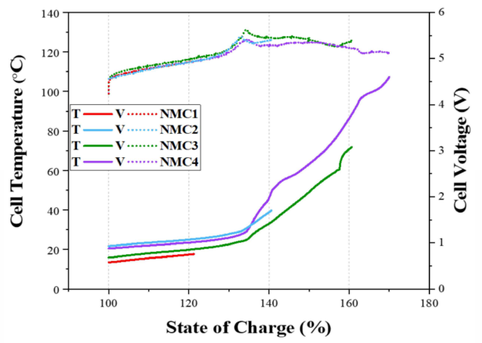


Methodology



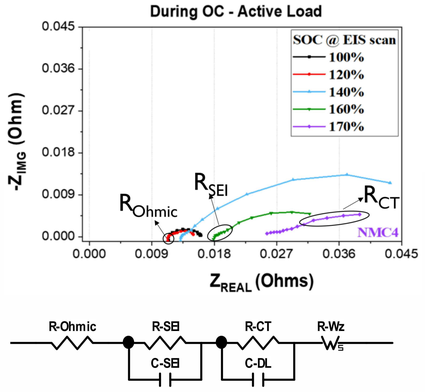
*OC - Overcharge
*SOC – State of Charge

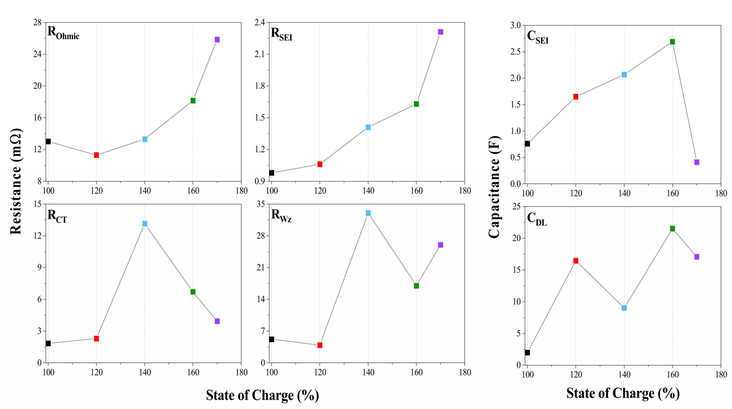
Overcharge Effects on Cell Temperature and Voltage



- Four individual NMC cells were overcharged to 120%, 140%, 160%, and 170% SOC
- The overcharge % was determined based on the nominal capacity of the cell (10Ah)

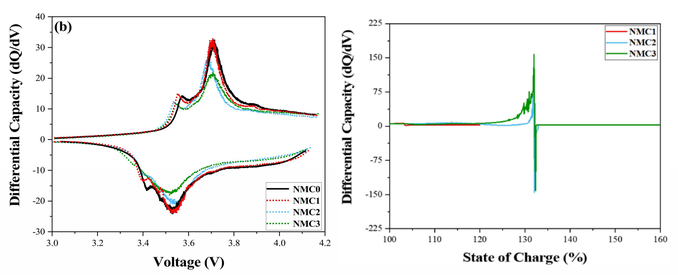
NMC4: 100-170% SOC In-operando EIS





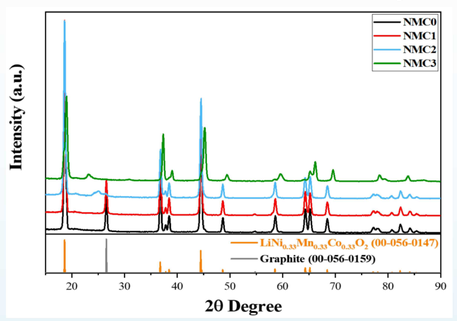
- The R_{SEI} slightly increased after each level of overcharge as well as the C_{SEI}, which could indicate a growth in the SEI layer
- The R_{CT} significantly increased after 140% SOC and subsequently decreased for high SOC's

Differential Capacity

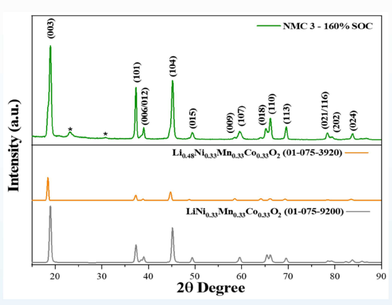


- The dQ/dV for NMC1 (120% SOC) exhibits no change in the redox processes of the cell
- NMC2 and NMC3 presented a decreased dQ/dV, characteristic of loss of active material
- The dQ/dV calculated during the OC procedure identified a redox reaction between 130-135% SOC

X-ray Diffraction: Cathode



- Significant changes observed above 140% SOC (NMC2)
- NMC3 (160% SOC) diffraction peaks shifted to higher degree values, indicating a general shrinkage of the lattice. Lattice parameters ***a*** and ***b (a=b)*** confirmed this conclusion since a decrease from 2.866 Å to 2.817 Å was identified
- Rietveld refinement for NMC3 (160% SOC) presented a combination of phases with 86% lithiated NMC and 14% delithiated NMC, suggesting a decomposition of the cathode and loss of lithium inventory

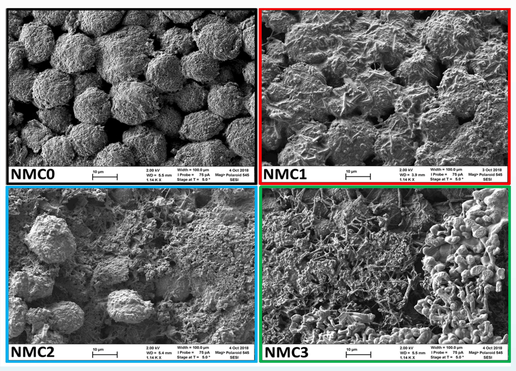


Rietveld Refinement of NMC3 based on lithiated NMC (green pattern) vs. delithiated NMC (orange pattern)

Phase	% (+/- 5%)
Lithiated NMC	86
Delithiated NMC	14

SEM: Anode

Electrodes harvested at 0% SOC (fully lithiated cathode).



Summary

- Several overcharge procedures were applied to 10 Ah NMC single cells
- The electrochemical and structural characterization indicated a clear marker of degradation for the cells at 140% SOC
- The XRD diffractogram for 160% SOC indicated significant decomposition of the cathode and loss of lithium inventory, which could also be attributed to Li plating on the anode

Funded by Dr. Imre Gyuk through the U.S. Department of Energy; Office of Electricity. A special thanks to the following people for thoughtful discussions, advice, and experiment design: C. Orendorff, S. Ferreira, Yuliya Preger, R. Shurtz and J. Hewson.

Sandia National Laboratories