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An Integrated Experiments and Modeling of Lithium-ion Battery

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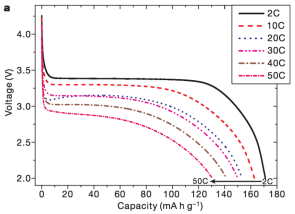
Introduction and Background

Introduction:

- Lithium-ion batteries are critical to modern and emerging technologies ranging from electric vehicles, high-power tools and wearable electronics to prosthetic limbs and exoskeletons for the physically disabled.

Objective:

- Describe and predict electrical potential and capacity characteristic under high C rate (dis)charging.
- Predict li-ion battery's lifetime under different C rate
- Supply approach to improve Li-ion battery's cycle time and high C-rate performance.



Kang & Ceder, *Nature* 458, 190-193 (03/12/2009)

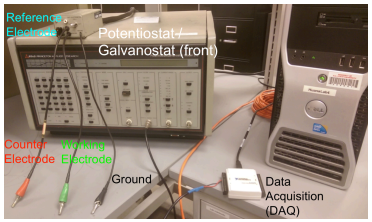
Research steps and plan:

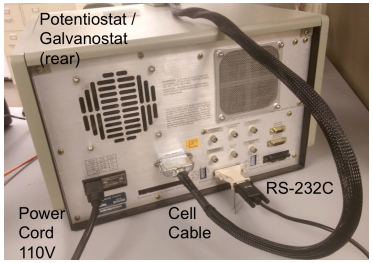
- Design an experimental measure system
- Data collection of open circuit potential (OCP) vs. state of (dis)charging
- Measure voltage responses under different C-rates
- Develop a macroscopic thermodynamic model to describe OCP
- Develop a macroscopic thermodynamic model to describe voltage response with varied C-rates
- Develop micro- and meso-scale models based on quantum & statistical mechanics

Methods and Current Results

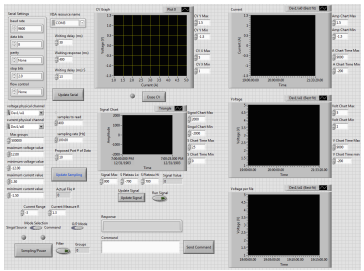
Equipment:

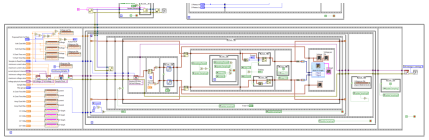
EG&G Princeton Applied Research 273 potentiostat / galvanostat

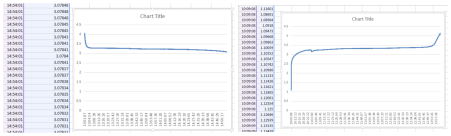


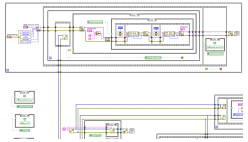


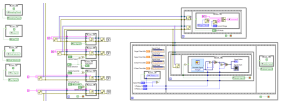
LabVIEW Program and Theoretical Modeling



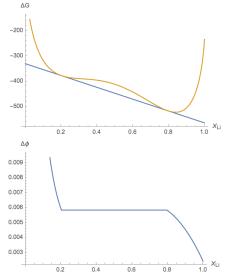








- Anode $Li \rightleftarrows Li^+ + e^-$
- Cathode $Li^+ + FePO_4 + e^- \rightleftarrows LiFePO_4$
- 1st Law $dU = \delta Q + \delta W + \sum_i \mu_i dn_i$
- Usable energy $FE = \Delta G = \Delta H + \Delta(TS)$
- Nernst equation $E = E^0 - \frac{kT}{ne} \ln \frac{[Red]}{[Ox]}$



Model is according to Esther Bohn et al., *Journal of The Electrochemical Society* (2013)

Detailed Experimental Setup

1. Connect potentiostat/galvanostat to a commercial Li-ion battery
2. Establish communications between the potentiostat/galvanostat and the computer via the RS 232C cable and a data acquisition device DAQ 6009
3. Script a LabVIEW program to control and receive feedbacks from the potentiostat/galvanostat.
4. Script a LabVIEW program to record experimental data, and the results will be used to verify the developed theoretical model

Macroscopic OCP Modeling

1. Based on continuum mechanics, strain energy will be incorporated into the energy conservation equation.
2. Identify energy resulted from solid electrodes during (dis)charging, and transform the energy to electrical energy. Derive equations for electric potential vs.state of charge.
3. Compare simulation results with experimental data to calibrate the model.

Conclusion

- The completed research will provide a solid interface and mathematical structure to better describe lithium ion batteries
- Proper usage of Potentiostat/Galvanostat requires much more research and detailed knowledge of lithium ion batteries
- Macroscopic model replied on comprehension of continuum mechanics and thermodynamics, and OCP model should be based on equilibrium and reversibility.
- Due the the influence high C-rate, the system is not reversible, however. Kinetics should be included.
- Quantum and statistical models will be developed and they could accurately describe battery (dis)charging procedure.

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