

# Nonequilibrium thermodynamics of rate-capacity lost phenomena for Li-ion battery

Hongjiang Chen and Hsiao-Ying Shadow Huang

Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC

## Introduction and Background

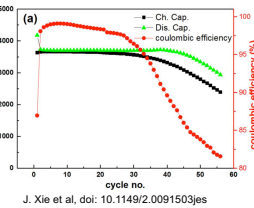
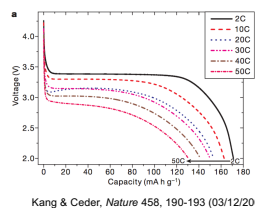
### Introduction:

- 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.

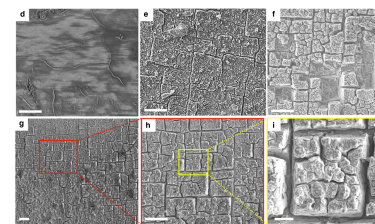


### Current Problems of Li-ion battery

- Poor power performance under high C-rate
- Irreversible capacity loss after cycling and limited life time under high C-rate



### Electrodes' cracks and failure



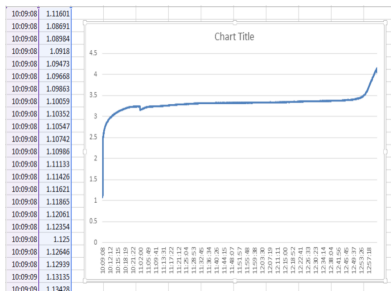
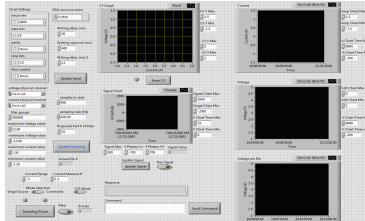
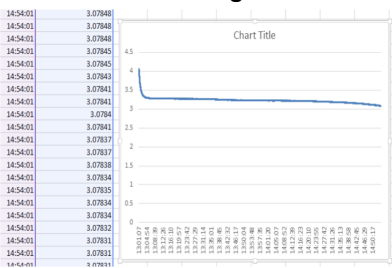
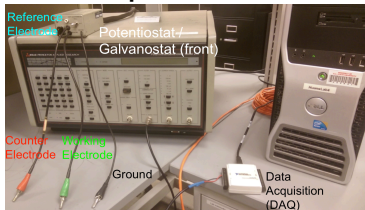
Si anode SEM images after (d)3, (e) 8, (f) 50 and (g-i) 30 cycles. Scale bar, 20 $\mu$ m (d-h), 3  $\mu$ m (i). [F. Shi et al, doi: 10.1038/ncomms11886.]

### Objective:

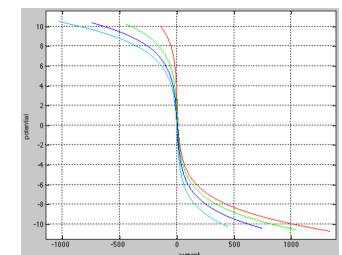
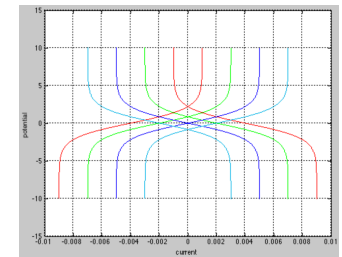
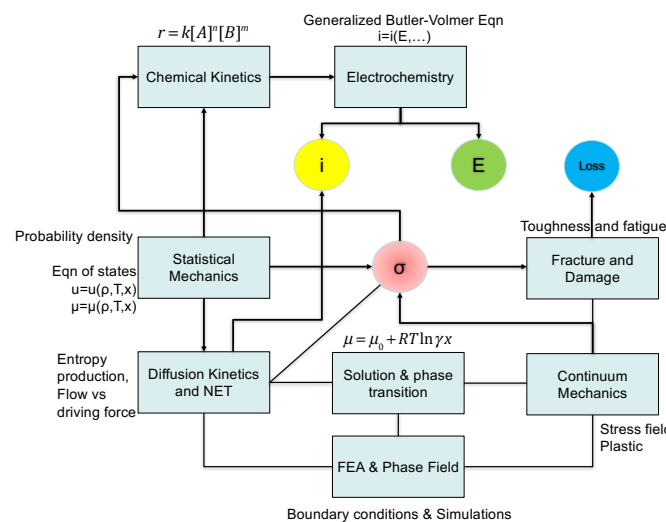
- Describe and predict electrical potential and capacity characteristic under high C-rate (dis)charging.
- Predict Li-ion battery's lifetime under different C-rates.
- Develop approaches to improve Li-ion battery's cycling time and high C-rate performance.

## Methods and Current Results

### Experiment measurement and LabVIEW Program



### Theory Architecture based on Non-Equilibrium Theory



## Conclusion and Future Work

- Understanding the loss of power density and capacity involves interdisciplinary theories and models.
- Develop more comprehensive model with less assumption to achieve accurate prediction.
- Model the equations of states: Chemical potentials and specific internal energy incorporating density, fractions and temperature as independent variables.
- Solve equation groups from the above theory architecture and conduct finite element analyses and phase field simulations.
- Damage and capacity loss modeling.