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Modeling and simulation of the non-equilibrium process for a continuous solid-solution system in lithium-ion batteries

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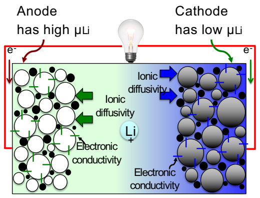
Introduction and Background

Introduction:

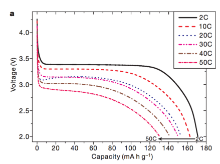
- Lithium-ion batteries are critical to modern and emerging technologies such as electric vehicles, high-power tools.
- It stores and release energy by Li-ion's diffusion between anode and cathode.

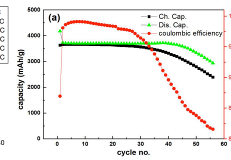


Current Problems of Li-ion battery

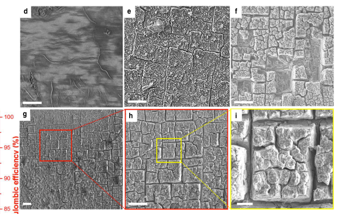
(a) Poor power performance under high C-rate[1]

(b) Irreversible capacity loss after cycling and limited life time under high C-rate[2]



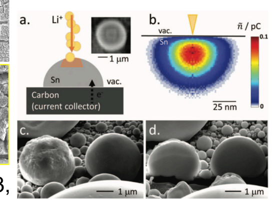


(c) Electrodes' cracks and failure[3]



Si anode SEM images after (d) 3, (e) 8, (f) 50 and (g–i) 30 cycles. Scale bar, 20μm (d–h), 3 μm (i).

(d) Li-ion diffusion were affected by mechanical deformation[4]



Li-ion diffusion under FIB doping

Objective:

- Describe and predict electrical potential, capacity, stress and strain under high C-rate (dis)charging.
- Predict Li-ion battery performance under various C-rates.
- Develop approaches to improve Li-ion battery's cyclic life at high C-rate

Methods and Current Results

Model Architecture based on Continuum Mechanics and Non-Equilibrium Thermodynamics

Constitutive models

$$\dot{\Omega} = \dot{\Omega}\left(\lambda, G, \rho, \mathbf{g}, \dot{\mathbf{e}}^{(e)}, \boldsymbol{\sigma}, \dot{\mathbf{e}}, \kappa, x_{(k)}, \boldsymbol{\varepsilon}^{(e)}\right)$$

$$\mu_{(12)} = \mu_{(12)}\left(x_{(k)}, \boldsymbol{\varepsilon}^{(e)}, \rho\right)$$

$$ds = \sum_l -\bar{\gamma}^{(l)ij} d\bar{\varepsilon}^{(l)}_{(2)ij} + c_{Vx}\frac{dT}{T} + \left(\frac{\partial s}{\partial x_{(\alpha)}}\right)_{\varepsilon_{(2)},T} dx_{(\alpha)}$$

Momentum equation

$$\rho\frac{d\mathbf{v}}{dt} = \nabla\cdot\mathbf{p} + \sum_k^K \rho_{(k)}\mathbf{F}_{(k)}$$

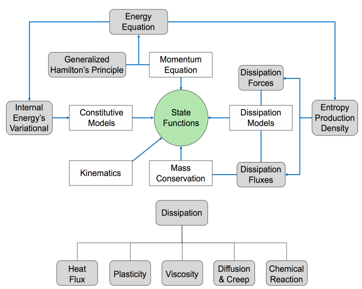
Dissipation models

$$\lambda^{(P)\pm} = C^{(p)\pm}\exp\left(-\frac{E_A^{(p)\pm}}{RT}\right)$$

$$\tau^{(e)} = \tau^{(e)}\left(\dot{e}^{(e)}, \lambda^{(P)\pm}\right)$$

$$J_{(k)} = -\frac{L^{(kq)}}{T}\cdot\nabla T - \sum_k \frac{L^{(kk')}}{T}\cdot\nabla(\psi_{(K')} - \psi_{(n)}) - \frac{L^{(ke)}}{T}\cdot\nabla\phi$$

$$r_+^{(j)} = C_+^{(j)\prime}\exp\left(\alpha^{(j)}\beta\sum_k \mu_{(k)M}\delta^{(kj)}\right)$$



Mass conservation

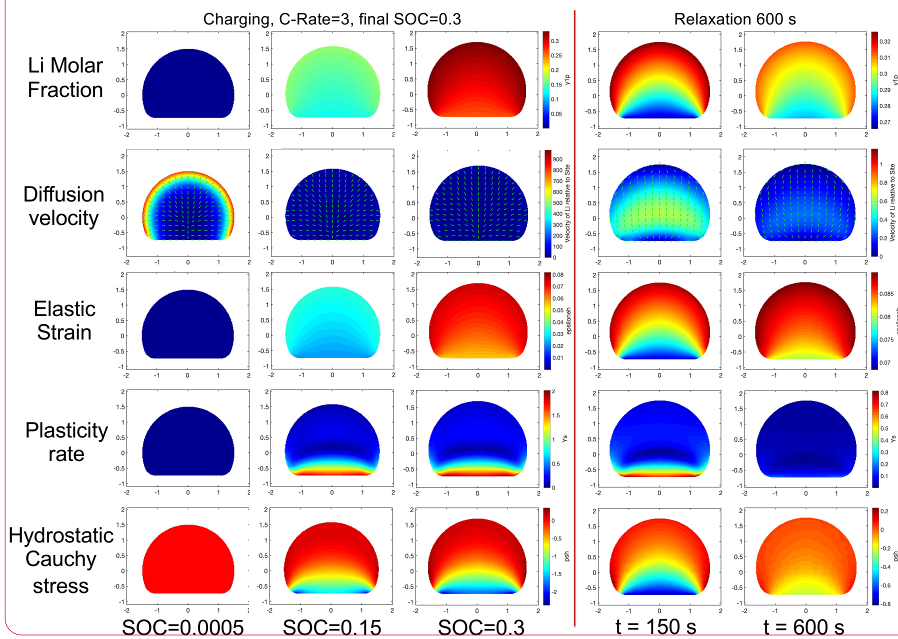
$$\rho\frac{dx_{(k)}}{dt} + \nabla_i J^i_{(k)} = \sum_j \xi^{(j)}_{(k)} J^{(j)} \qquad F\int_V J_M dV = I$$

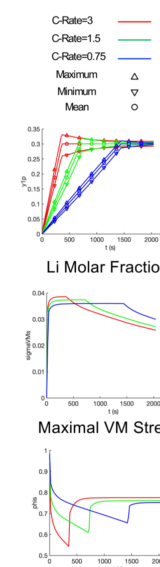
Kinematics

$$\dot{e}_{(2)ij} = \frac{\partial\varepsilon_{(2)ij}}{\partial t} = \frac{1}{2}\frac{\partial g_{(2)ij}}{\partial t}$$

$$\dot{e}_{(2)ij} = \dot{e}^{(e)}_{ij} + \dot{e}^{(p)}_{ij} \qquad \dot{e}_{(2)ij} = \frac{1}{2}\left(\nabla_i v^L_{(2)j} + \nabla_j v^L_{(2)i}\right)$$

Numerical Simulation





Future Work

- Simulate whole (dis)charging process and cycling
- Use the finite different method to obtain stress evolutions with phase transformation during cycling.
- Developing algorithms to simulate continuous plasticity-elasticity interface. Damage and irreversible capacity loss modeling.

[1] Kang & Ceder, Nature 458, 190-193; [2] J. Xie et al, doi: 10.1149/2.0091503jes; [3] Shi et al, doi: 10.1038/ncomms11886; [4] Saya Takeuchi et al., doi:10.1149/2.1161606jes

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