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A Generalized method of modeling evolution process for a continuous solid-solution system in lithium-ion batteries

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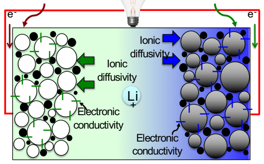
Introduction and Background

Introduction:

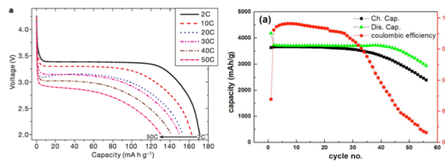
- Lithium-ion batteries are critical to modern and emerging technologies such as electric vehicles, high-power tools.
- It stores and release energy by Li-ion's diffusion between anode and cathode.



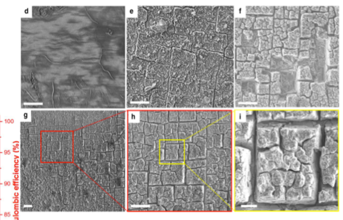
Current Problems of Li-ion battery

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

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

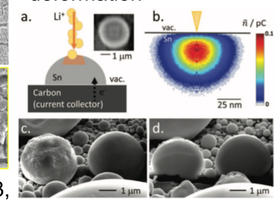


(c) Electrodes' cracks and failure[3]



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]



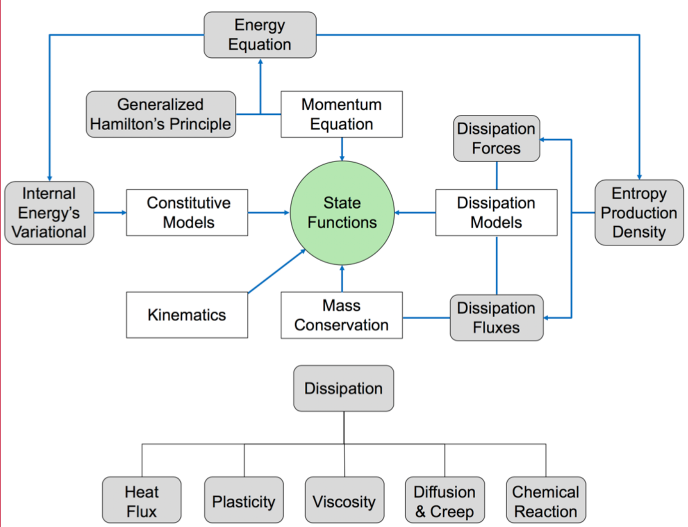
Li-ion diffusion under FIB doping

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

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

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

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

Momentum equation

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

Kinematics

$$e_{(2)ij}=\frac{\partial\varepsilon_{(2)ij}}{\partial t}=\frac{1}{2}\frac{\partial g_{(2)ij}}{\partial t}$$

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

Dissipation models

$$f=\left(\tau^{(p)ij}-\frac{1}{3}\tau^{(p)k}{}_{k}g^{ij}_{(2)}\right)\left(\tau^{(p)}_{ij}-\frac{1}{3}\tau^{(p)k}{}_{k}g_{(2)ij}\right)-\frac{8}{3}\Upsilon^2$$

$$\dot{\boldsymbol{\tau}}^{(e)}=\boldsymbol{\eta}\dot{\boldsymbol{e}}$$

$$\boldsymbol{J}_{(k)}=-\frac{\boldsymbol{L}^{(kq)}}{T}\cdot\underline{\nabla}T-\sum_{k}\frac{\boldsymbol{L}^{(kk')}}{T}\cdot\underline{\nabla}(\psi_{(k')}-\psi_{(n)})-\frac{\boldsymbol{L}^{(ke)}}{T}\cdot\underline{\nabla}\phi$$

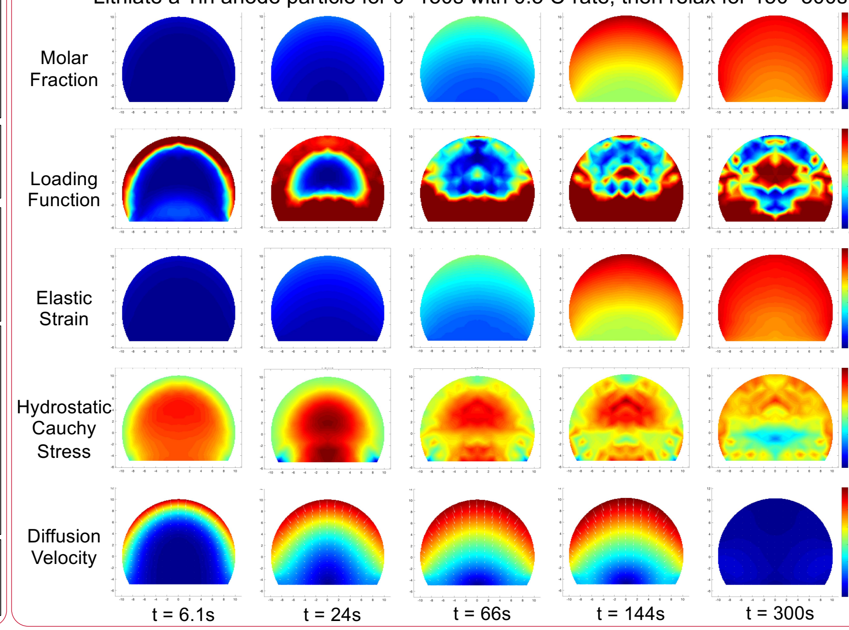
$$r^{(j)}_{+}=C^{(j)\prime}_{+}\exp\left(\alpha^{(j)}\beta\sum_{k}\mu_{(k)M}\delta^{(kj)}\right)$$

Mass conservation

$$\rho\frac{dx_{(k)}}{dt}+\nabla_i J^{i}_{(k)}=\sum_{j}\xi^{(j)}_{(k)}J^{(j)}$$

Numerical Simulation

Lithiate a Tin anode particle for 0~150s with 0.5 C-rate, then relax for 150~300s



Future Work

- Understanding the loss of power density and capacity involving interdisciplinary theories and models.
- 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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