Modeling C-rate Dependent Diffusion-Induced-Stresses in Lithium-Ion-Battery Materials

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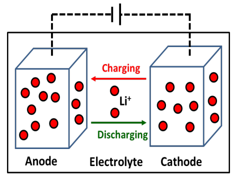
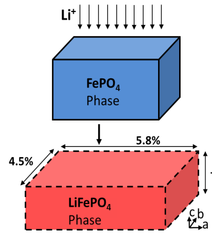
Background and Objectives

- **The needs for high C-rate lithium-ion batteries.**
- **Lithium insertion during charging/discharging → Diffusion-Induced-Stress.**

Li-ion batteries for electric vehicles

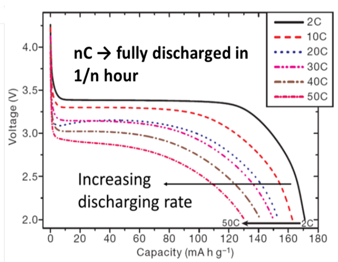


How Li-ion battery works

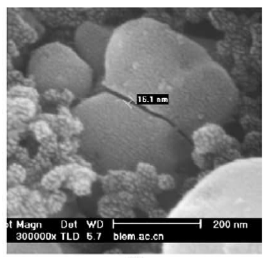


Volume change during Li-insertion

- **Capacity loss is observed at high C-rates.**
- **Particle fractures and crack growth are observed after cycling.**



B. Kang et al., 2009

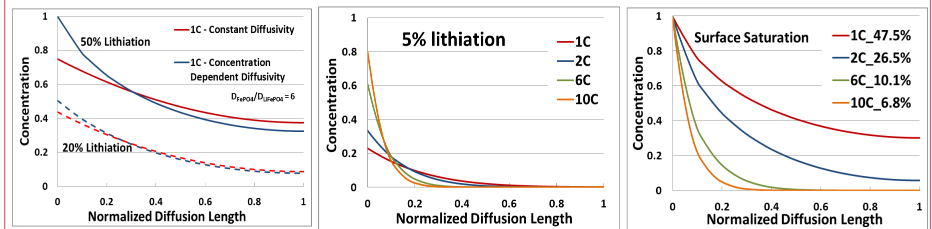


Wang et al., 2005

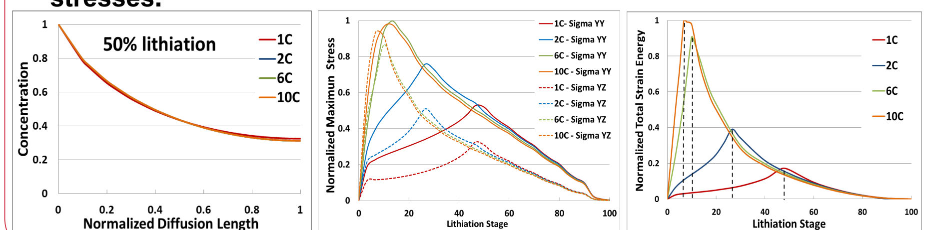
Objective:
Investigate how C-rate might affect diffusion-induced- stresses inside materials?

Results

- **Concentration dependent diffusivity cannot be neglected.**
- **Higher C-rate → Higher concentration gradient.**
- **Surface concentration saturation occurs faster at higher C-rates.**



- **Concentration profiles become the same after 50% lithiation stage.**
- **Higher C-rate → Higher concentration gradient → Higher strain energy.**
- **Higher C-rate → Higher concentration gradient → Higher internal stresses.**

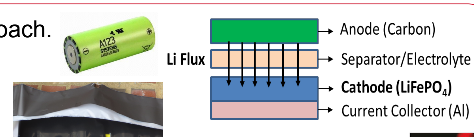


Method

- Apply the thermal stress analysis approach.

Heat Flux $q = -k\dfrac{\partial T}{\partial y}$

Mass Flux $J = -D\dfrac{\partial \phi}{\partial y}$



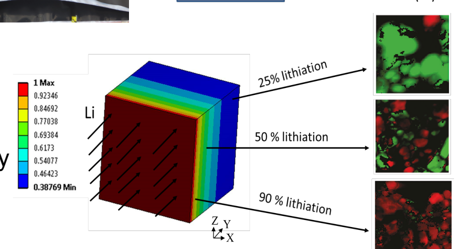
Four cases are studied: 1C, 2C, 6C, 10C

- Finite element model by ANSYS.
- Concentration dependent material property

$$[C(x)] = x[C]^{LiFePO_4} + (1-x)[C]^{FePO_4}$$

- Concentration dependent diffusivity

$$[D(x)] = x[D]^{LiFePO_4} + (1-x)[D]^{FePO_4}$$



10 μm cube

G. Brunetti et al., 2011

Conclusions

- **The concentration dependent diffusivity need to be incorporated in the simulation model since it will affect concentration profiles.**
- **Higher C-rates (more Li-ions pumped into the material in less time) will result in higher concentration gradients inside materials, leading to higher strain energies and internal stresses. Thus the tendency for the particle fracture is higher at high C-rates.**
- **The results of the current study suggest that lowering the concentration gradient could help reduce internal stresses inside battery materials and therefore reduces the capacity loss of the lithium-ion battery.**