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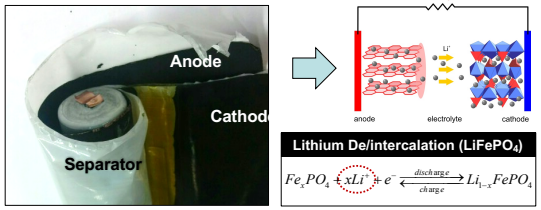
Investigations of Mechanical Stresses in FIB/SEM Reconstructed Battery Materials

Sangwook Kim and Hsiao-Ying Shadow Huang
Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC

Introduction and Background

Promising Power Source: Lithium-ion Batteries

ref. J. Molenda (2011)

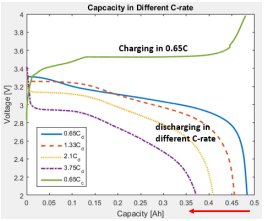


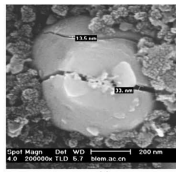
Lithium-Iron-Phosphate ($LiFePO_4$) as a Cathode Material:

- High volumetric energy (970 WhL^{-1}), low exothermic peak temperature (289°C), and low heat flow (-6 Wg^{-1}).
- One dimensional lithium diffusion (along y-direction)
- Li-poor phase ($FePO_4$) → Li-rich phase ($LiFePO_4$); volume expansion.

Motivations:

- Significant capacity loss during high charging/discharging current-rate (C-rate).
- Higher stress in the electrode → particle fracture → short circuit.
- A need for computational models considering reconstructed geometry



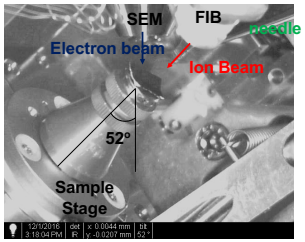


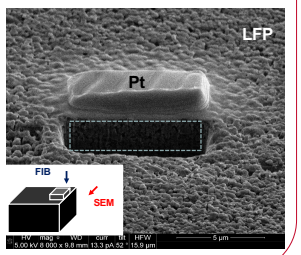
ref. Wang et al. (2005)

Methods

Reconstructed Geometry via FIB/SEM

- **FIB/SEM (NCSU AIF)** was used for sequential FIB (Focused Ion Beam) milling in conjunction with high resolution SEM images.
- Protective layer (Pt) is deposited to ensure **less curtaining effects.**
- After getting sequential images, **image was processed** by ImageJ.
- **3D reconstructed geometry** from 2D images can be imported in both COMSOL and ANSYS

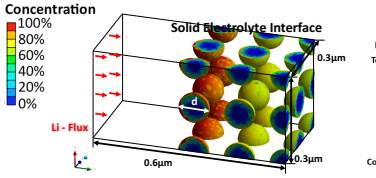


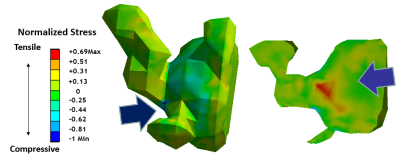


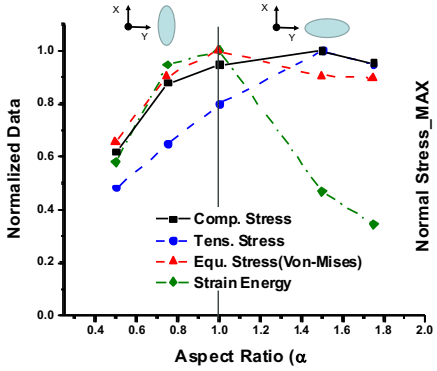
Results

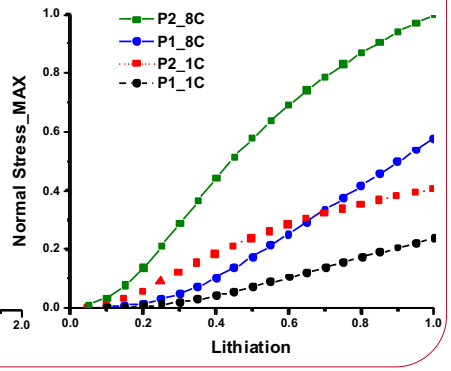
Effect of Geometry Configuration on Mechanical Stress in $LiFePO_4$ Particles

- Material property changes are coupled with **C-rate dependent lithiation stage** during discharging.
- **Tensile stresses** (diffusion induced stress) are highly affected by C-rate; **compressive stresses** (electrolyte) are highly affected by particle geometry.
- Effect of **aspect ratio** is not symmetry in our model due to anisotropic analysis.
- Length along **y-direction** is preferred to be smaller than that along x or z direction.
- Complicated **surface configurations** increase compressive stress rather than tensile stress.









Discussions and Conclusion

- We investigate mechanical stress evolutions during lithiation(discharging) with different C-rates and particle geometry in a half-cell battery system.
- Our simulations demonstrate that both electrode and electrolyte material properties have greater effects when studying mechanical stresses.
- These computational models would aid on mitigating higher stresses in cathode particles to ensure longer battery cycle life.
- Thermal effects will be investigated with reconstructed geometry in the future work.

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