Investigations of Mechanical Stresses in FIB/SEM Reconstructed Battery Materials

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Introduction and Background

Lithium-Iron-Phosphate (LiFePO₄) 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 (FePO₄) → Li-rich phase (LiFePO₄); 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

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 LiFePO₄ 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.