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# Mechanical Stresses at Electrode-Electrolyte Interface in Lithium Batteries

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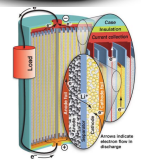
## Introduction and Background

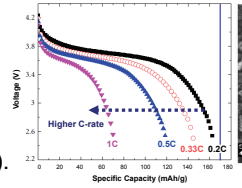
**Promising Power Source; Lithium-ion Batteries :**

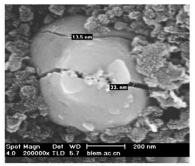
- Low cost, toxicity, high thermal stability, electrochemical performance, and high specific capacity.
- Good potential for electronic devices and transportation (HEV, PHEV, and EV)



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

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



**Motivations:**

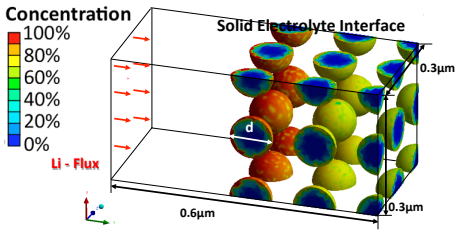
- Significant capacity loss during high charging/discharging current-rate (C-rate).
- Higher stress in the electrode → particle fracture → short circuit.
- A need for computational models considering electrode and electrolyte: ***Fluid-Structure Interactions***.

## Methods and Results

### Phase Transformation during Discharging

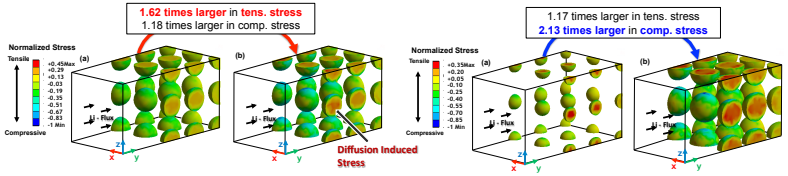
- Diffusion in electrode and electrolyte governed by Fick's second law
- Shrinking-core model for electrode; $Li^+$ transported from surface to center of particles.
- Material property changes coupled with C-rate dependent lithiation stage during discharging.
- Lithiation stage :

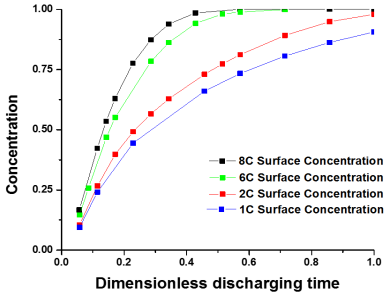
$$\sum_i V_i \left( \frac{\sum_{j=1}^{j=10} \phi_j}{10} \right) \Big/ V_T$$

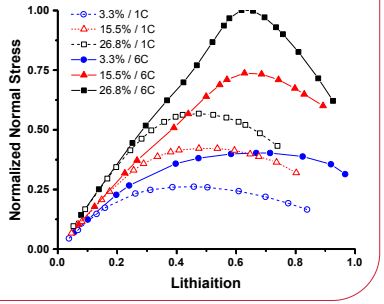



### Effect of C-rate and Volume Fraction on Mechanical Stress at the Electrode-Electrolyte Interface

- Tensile stresses are mainly caused by volume expansion; compressive stress mainly caused by electrolyte fluid pressure
- Tensile stresses are highly affected by C-rate; compressive stress highly affected by volume fraction (i.e., particle size).
- Increase in volume fraction and C-rate increase both compressive and tensile stresses.
- Stress increases initially, followed by a decrease after reaching peak values during lithiation due to concentration gradient (similar trends observed in $LiCoO_2$).
- A need to relief stresses on the electrode-electrolyte interface




## Discussions and Conclusion

- We investigate mechanical stress evolution during lithiation with different particle sizes, C-rates in a half-cell battery system.
- Our simulations demonstrate that both electrode and electrolyte material properties have greater effects when studying mechanical stresses on the electrode-electrolyte interface
- These computational models would aid on mitigating higher stresses in cathode particles to ensure longer battery cycle life.

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