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A Dislocation Based Stress Development in Lithium-ion Batteries

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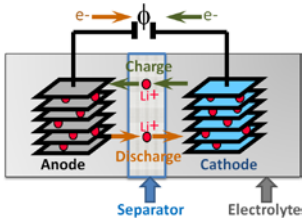
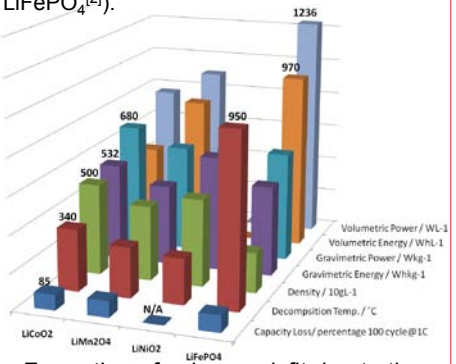
Introduction

The Needs for Li-ion Batteries

- Energy storage is becoming a vital link between energy supply and demand.
- Portable electronic devices require batteries with high volumetric energy density. Electric drive transportations require batteries with high gravimetric energy density.
- Li-ion battery has both high volumetric & gravimetric energy densities[1].



- Battery Components: Electrolyte, Separator, Anode, Cathode ($LiCoO_2$, $LiNiO_2$, $LiMn_2O_4$, $LiFePO_4$[2]).

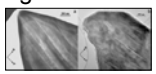


- Formation of volume misfit due to the coherent interface[3]. Dislocations are induced during (dis)charging.

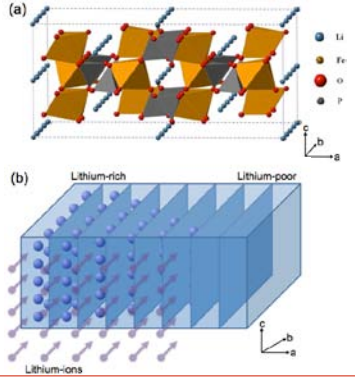
Method & Results

Lithium Ion Diffusion and Dislocation Formation

$LiFePO_4$ as a modeling system.
Cracks along c-axis is observed[4].

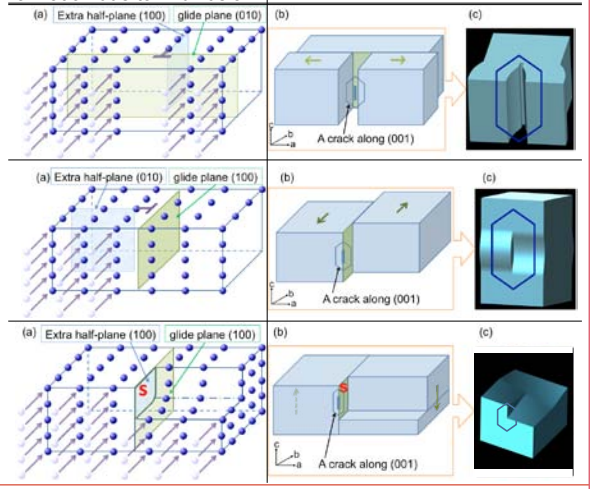


Lithium-ion diffuse in the b-direction.



(I) Kinetics of the dislocation formation due to Li-diffusion

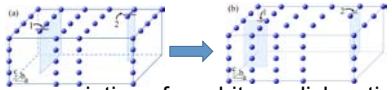
(II) Mode I/II/III fractures caused by the accumulated dislocations



Stress Field for Multiple Edge and Screw Dislocation

Multiple dislocations present in particles

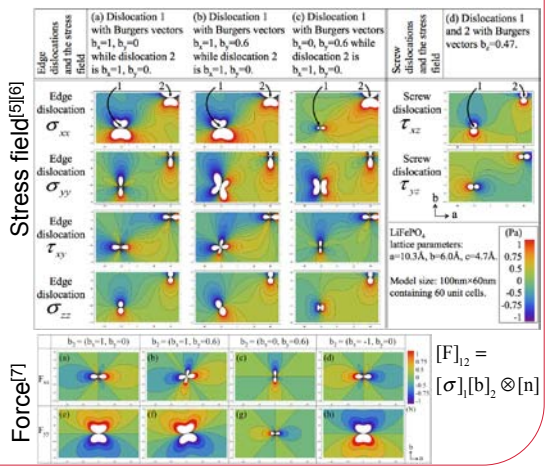
Dislocation 1 rotation



- Stress variations for arbitrary dislocation directions are investigated.
- Dislocation 2 remains its Burger's vector as (b_x=1, b_y=0), while the dislocation1 rotates from 0° to 90°
- Superposition method issued to obtain the stress field of multiple dislocations in anisotropic $LiFePO_4$ material.
- The stress fields manifesting between dislocations are numerically calculated via Mathematica.

Stress field[5][6]

Force[7]



$$[F]_{12} = [\sigma]_1[b]_2 \otimes [n]$$

Conclusion

- We reported three different lithium intercalation-induced dislocation mechanisms explaining experimental observed cracks.
- It is observed that mechanical stresses between two edge dislocations could be minimized when they are orthogonal to each other.
- The force field might be one key factor that push and attract lithium ion in the crystal and results in the capacity fade.
- The results provide links between stress fields and the observed structural failure in lithium-ion batteries.

Bibliography

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