Topology Optimization of Lithium-Ion Battery Electrode Micro-structure Morphology for Reduction of Damage Accumulation and Longevity of Battery Life

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Introduction

With the ubiquitous use of Lithium-Ion batteries (LIBs) in such areas as mobile devices comes the increased demand for further commercial applications. These batteries are greatly desired for use in efficient energy storage systems for clean and renewable power sources and the electrical transportation industry. LIBs are not yet technological mature to met various commercial demands. Due to operational standard of modern LIBs, the following challenges for example,: (1) lower than desired effective traveling distance due to limited LIB capacity, (2) unsuitable LIB lifespan and (3) relatively high maintenance and battery replacement costs collectively make electrical vehicles impractical for large-scale consumer production. A major contributor to this bottle-neck in development is battery degradation mechanisms, specifically multiphysics fracture of electrode active materials for intent and purposes.

The concept of induced multiphysics damage is very important in the modeling of LIBs but is not fully understood. Importance of understanding damage evolution stems from the notion that damage is attributed to causing irreversible capacity loss and limited LIB longevity. Therefore, understanding this phenomenon allows for methods of increasing effective capacity, battery life and reducing damage formation. This presentation will therefore address the development of an advanced multiphysics, brittle material, continuum damage scheme, and understanding the effects of micro-structure morphology on damage generation in LIB Silicon anodes.

Use of COMSOL Multiphysics

To model the coupled electrochemical and solid mechanical physics of the LIB, the mechano-diffusion governing equations are implemented through *Equation-Based Modeling*. The *General Form PDEs* are coupled through the mechanical fields (stress $\boldsymbol{\sigma}$, strain $\boldsymbol{\epsilon}$, displacement $\bar{u}$) and the diffusion field (concentration c).

$$Solid\ Mechanics : \nabla \cdot \boldsymbol{\sigma}(\bar{u}, \boldsymbol{\epsilon}, c, \mathbf{D}) = 0$$

$$Diffusion : \dot{c} = \nabla \cdot \boldsymbol{J}(\bar{c}, \boldsymbol{\sigma}, \boldsymbol{D}).$$

To appropriately model the damage accumulation $\boldsymbol{D}$ of the system, the evolution law is implemented through *Domain ODEs and DAEs*, specifically *Distributed ODEs* to capture the maximum damage quantity $\boldsymbol{D}_{max}$ over a desired time interval:

$$\dot{\boldsymbol{D}}_{max} = \dot{\boldsymbol{D}}(\boldsymbol{\sigma}, c) * H(\dot{\boldsymbol{D}}) * H_{\boldsymbol{D}_{max}}(\boldsymbol{D}).$$

Due to the continuity of the finite element implementation within COMSOL, the greater benefits of parallel computing comes from the use of the *Cluster Computing* study node in convergence studies and the use of the *Cluster Sweep* study node in parametric and more advanced shape optimizations (in future works).

Results

An initial finding that supports previous works in the field is that the inclusion of anisotropy yields marginal affects on mechanical and electrochemical responses for a material such as crystalline Silicon.

It is expected however that the inclusion of anisotropy into the continuum damage laws will significantly affect the behavior of damage evolution dependent of the specific crystal orientation. Future-works will illustrate the affects of shape optimization on stress and damage generation for models of 2D and 3D periodic micro-structure morphologies as seen in Figure 1.

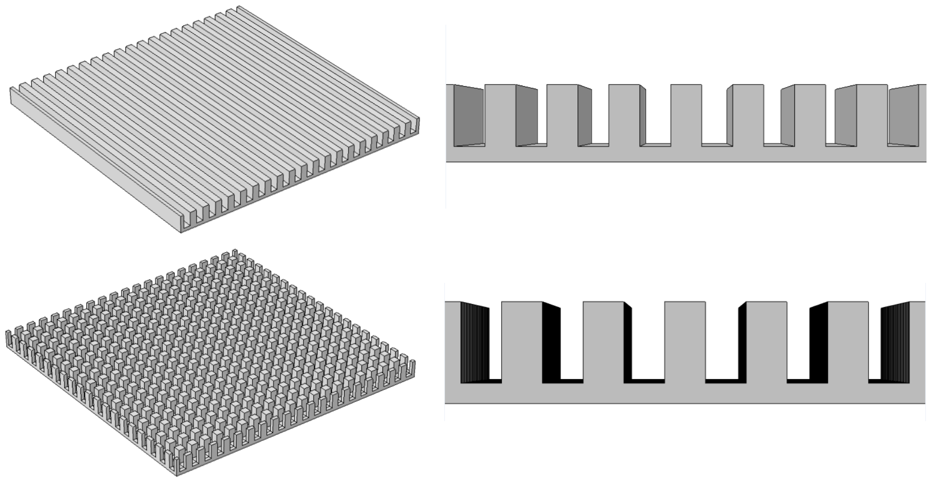

Figure 1: 2D and 3D Pristine Base Micro-structures for Optimization

Conclusion

Thus far, study shows that modeling materials such as cubic crystal silicon does not significantly benefit from inclusion of anisotropy in the mechano-diffusion governing equations. This is due to the marginal anisotropic elastic properties and isotropic diffusion of crystal silicon. The affects of anisotropy are however expected to have great influence on the development of multi-phases of Silicon, anisotropic morphology changes and their influence on damage evolution which will all be addressed in future works. Implementing topology optimization schemes in future works is expected to aide in new design methods to increase resilience of highly stressed electrode surfaces. This will subsequently increase electrode effective capacity and overall LIB performance. Ultimately the assumptions of previous works within the field will be assessed allowing for the modeling of more complex materials and electrode geometries.

References

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