A Fatigue Analysis for Lithium-ion Batteries
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Introduction and Background

Energy Storage Need
- Batteries provide the vital storage link between energy generation and consumption around the world.
- Energy demand is increasing, thus new generation facilities are being built and require large scale batteries to store energy for future transmission or backup power.
- Oil prices and CO₂ emissions are also increasing, driving the need for transportation alternatives (EV and PHEV).

Simulation Method and Results for LiFePO₄

Simulation Set-Up for 2-Phase interface

Fracture and Fatigue Analysis
- Choose LiFePO₄ due to long cycle life (~2000 cycles), wide op. temps. (-20 to 60°C) and superior thermal stability (safe, incombustible cells).
- Varying sized particles with varied initial crack sizes (nm scale) are analyzed via fracture mechanics.
- Plane Stress, plate-like particles are used with loading according to misfit strains (observed during lithium insertion, FePO₄ → LiFePO₄).
- Mode dependent stresses, Strain Energy Release Rates (G), and Stress Intensity Factors (K) are calculated using ANSYS software.

Objective
- As it is known batteries experience capacity loss (power loss) over time as the electrode materials degrade, this research investigates the effects of cycling induced stresses and fatigue on LiFePO₄ cathode (positive electrode) particles to elucidate an understanding for crack propagation and fracture.

Conclusion
- Crack propagation and fracture is highly dependent on mode (I or II), misfit %, and particle size.
- Smaller particles show reduced G (crack driving force). Max is always near L/d=0.5.
- Fatigue cycle life estimate of 1800 cycles is fairly consistent with manuf. reported value (2000).
- Understanding what happens at the nm-scale provides insight into what bulk-scale modifications could be made to improve the performance and life of batteries.

Bibliography
A Synergistic Approach to Visualize and Understand Tissue-Cell Mechanical Interactions

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Introduction and Background

Current Knowledge: Heart valves constantly experience different stress states during cardiac cycles.

Current Limitations: How tissue-level mechanical forces can translate into altered cellular stress states is unknown, which hinders a better understanding of the relationships between the mechanical stimuli, cellular mechanotransduction, cell migration, matrix synthesis, and tissue remodeling.

Methods and Results

Microstructural Evolutions via Finite Element Simulations
- Histology were prepared with H&E stains. Photomicrographs were obtained via an optical microscope.
- Circumferential aligned collagen fibers were notable in pulmonary valve leaflets.
- The non-linear anisotropic, and heterogeneous nature of heart valve extracellular matrix is incorporated into our FEA.

Stress Distributions in Heart Valve Tissues
- The corresponding mechanical stress distributions under biaxial stretching around cells are computationally calculated via FEA.
- The feature of inhomogeneous microstructure is apparently illustrated, and most local peak stresses are located around nuclei.
- Higher mechanical stimulation occurs around the boundary, rather than in the belly area of the heart valve; therefore, cellular activities could be stronger around the boundary.

Discussions and Conclusion
- Cellular mechanotransduction might be directional-dependent due to higher stresses are observed in the circumferential direction via our finite element analyses.
- Current study provides new models for better understanding tissue-cell interactions in heart valves.
- Stress distribution is highly emphasized as a result of biomechanics related to collagen secretion, tissue structure integrity and remodeling influenced by mechanical forces.
- Virtual experiments of heart valve tissues provide translational models to clarify the force transmission roles of heterogeneously distributed collagen fibers and the force receiving roles of randomly distributed cells in the matrix.
Phase boundary is experimentally observed aligned with bc plane. Phase boundary moves along the a-direction, while lithium diffusion is along the b-direction. An interfacial zone with a finite thickness exists between FePO₄ and LiFePO₄ phase. Strain energy affected phase transformation path (Simulation approach: Anisotropic thermal expansion).

The Needs for Lithium-ion Batteries:
- e.g. Energy storage units for electronic products and transportation (EVs/PHEVs).

Motivations:
- Capacity loss during high charging/discharging rate.
- Experimentally observed particle fracture.
- A need for anisotropic diffusion model for LiFePO₄.

Characteristics of Lithium-Iron-Phosphate (LiFePO₄):
- One dimensional lithium diffusion (along b-axis).
- Two phase system, Li-rich phase (LiFePO₄) and Li-poor phase (FePO₄).
- Anisotropic volume change.

Methods and Results

Phase Boundary Movement
- Phase boundary is experimentally observed aligned with bc plane.
- Phase boundary moves along the a-direction, while lithium diffusion is along the b-direction.
- An interfacial zone with a finite thickness exists between FePO₄ and LiFePO₄ phase.
- Strain energy affected phase transformation path (Simulation approach: Anisotropic thermal expansion)

Anisotropic Diffusion Model
- Accumulated strain energy indicates that the phase boundary movement along the a-axis is favored.
- Based on the simulation and available experimental data, we assume the diffusion mainly happens in the interfacial zone.
- A single particle could be considered as a combination of many diffusion channels.
- The lithium-ion concentration profile in each channel within the interfacial zone could be calculated by 1D Fick’s law.

Discussions and Conclusion
- Mechanical stress evolution is related to the lithium diffusion and phase transformation path in the particle.
- The interfacial zone is formed due to the strain energy and lithium diffusion mainly happens in this area.
- During discharging, the diffusion channels are fully filled progressively while the interfacial zone sweeps through the particle along the a-direction.
- This anisotropic diffusion model helps explain the diffusion process in a single LiFePO₄ particle and contributes to a better prediction of the stress development.
Biomechanical Properties of Skin
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Introduction and Background

Current Knowledge:
Collagen fibers arrangements within skin tissue determine its strength and its anisotropic behavior.

Current Limitations:
How subjecting skin to stretching changes its biomechanical properties is unknown. Subjecting skin to stretching could reduce the anisotropic properties of skin, creating uniform material properties benefiting many medical applications.

Objectives:
Determining the directional mechanical characteristics of skin tissue is key to understanding how the collagen arrangement affects the mechanical properties of skin tissue.

- To investigate the relationship between collagen fiber orientation and tissue strength via biaxial testing.
- To understand why subjecting skin to stretching has directional mechanical properties. Primarily, the difference in anisotropic properties are determined by comparing non-stretched and stretched samples.

Methods and Results

Directional Mechanical Properties via Biaxial Testing

Equipment:
- Biaxial testing was conducted via a BioTester 5000.
- Porcine epidermis 4 mm square skin samples were tested bi-axially.

Procedure:
- Skin samples were stretched from 0% strain to 35% to 0% over 30 second time period.
- 3 different skin samples were considered:
  - Un-stretched
  - Stretched 1, experienced the most stretch
  - Stretched 2, experienced less stretch
- Stretched samples were subjected to stretching for 24hrs in balloon tissue expander.
- Each sample was tested five times at 0 degrees, 30 degrees and 60 degrees. Only tests 2-5 were considered.

Directional Mechanical Properties in Skin Tissues

- Corresponding stress and material stiffness was calculated for each samples’ rotation.
- Samples’ mechanical properties become most anisotropic and non-linear in Zone 3.
- Comparing material stiffness of the preferred and cross-fiber directions in Zone 3 indicate reduced anisotropic properties.

Discussions and Conclusion

- Reducing anisotropic properties, which eliminates weaknesses, occurs after skin tissue experiences an expansion processes. The expanded skin better serves patients in need of skin graft operations. The current study provides new methods for determining and comparing the directional mechanical properties of skin tissue.
- The collagen fiber distribution in skin tissue becomes more homogeneous by subjecting samples to stretching, indicated by the similar material strengths in the X and Y-directions from the results of biaxial testing; however, preferred collagen alignment directions still exist.
- Longer periods of stretching may have a more significant affect on the reduction in anisotropic properties.
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$_2$O$_4$, LiFePO$_4$[2]).

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

Lithium Ion Diffusion and Dislocation Formation

- Lithium-ion diffuse in the b-direction.
- Lithium diffusion and dislocation formation
- 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 dislocation 1 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 for Multiple Edge and Screw Dislocation

- Lithium ions diffuse in the b-direction.
- Stress variations for arbitrary dislocation directions are investigated.
- Dislocation 2 remains its Burger’s vector as ($b_x=1$, $b_y=0$), while the dislocation 1 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.

Lithium Ion Diffusion and Dislocation Formation

- Kinetics of the dislocation formation due to Li-diffusion
- Mode I/II/III fractures caused by the accumulated dislocations

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

Multiscale Interactions of Mechanics, Microstructures, and Composition of Heart Valve Tissues

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Introduction and Background

- Approximately 250,000 heart valve disease in USA in 2010 [1]. Stenosis and insufficiency are the most common heart valve diseases, which are related to the mechanics of heart valves.
- Objective: Investigated the relationship of mechanical property, collagen fibers microstructure, and collagen concentrations in aortic and pulmonary semilunar valves.
- Function of heart valves:
  1. allow blood to flow through the heart smoothly.
  2. prevent retrograde flow of blood.
- Method of dissection:
  1. Each valve has three leaflets. Cartesian coordinate system was set before dissection.
  2. Leaflet samples were relaxed in HBSS for the physiological condition.

Method and Results

Mechanical Testing
- Biaxial testing was conducted via a BioTester 5000 (CellScale, Waterloo, CAN).
- ~7mm x 7mm sample were cut from leaflets.
- Samples were mounted and tested circumferentially (x-axis) and radially (y-axis).
- Evenly distributed boundary conditions were provided, which eliminates the variability between sample sizes.
- Aortic valves are stiffer in the circumferential direction.
- A greater variance in the directional strength of the aortic valve than in the pulmonary valve was found.

Cellular Analysis
- Tissue-Level:
  - Histology were prepared with Masson or H&E stains. Photomicrographs were obtained via Leica DMLB Microscope.
  - Circumferential aligned collagen fibers were notable in aortic valve leaflets.
- Cellular-Level:
  - Immunohistochemical samples were prepared for a confocal microscope.
  - Direction of actin filaments follows the nuclei long-axis.

Biochemical Analysis
- Collagen extracted from a leaflet sample into solution (0.5M acetic acid: distilled water = 0.029:1 & 50mg Pepsin A), dyed, centrifuged, and dissolved in Alkali reagent.
- A spectrophotometer and standard curve were used to calculate the concentrations.
- Use of distilled water and collagen extraction time may have substantial effects on results.
- Higher collagen concentrations were observed on edge regions than on belly regions of PV leaflets (AV leaflets provided inconsistent location-dependent results).

Discussion

- A relationship exists between the mechanical strength, collagen fiber microstructure, and collagen concentration of a valve leaflet.
- Semilunar valve tissues have nonlinear anisotropy material properties due to the heterogeneous collagen fiber microstructure.
- A higher collagen concentration may be related to greater mechanical strength and may be location dependent.
- The mechanical property of semilunar valve tissues do not depend only on collagen concentration but how collagen fibers are arranged structurally at the microscopy level.