Meshfree Methods for Modeling Chemo-Mechanical Cathode Cracking in Li-ion Batteries

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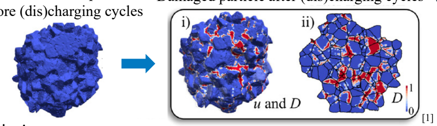
Introduction



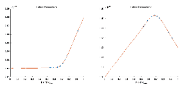
Red areas indicate damaged cathode particle zones; blue areas indicate undamaged zones

What is chemo-mechanical cathode cracking?

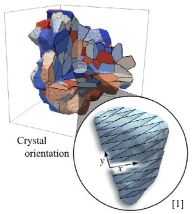
- Chemo-mechanical cracking is a result of uneven swelling and contraction of adjacent cathode grains, which leads to stress concentrations and crack propagation, largely along grain boundaries.

What causes chemo-mechanical cracking?

- A combination of phenomena:



Nonlinear, [Li]-dependent material properties used to determine principal and secondary expansion/contraction coefficients



Cathode Composition:

- Randomly oriented grains
- Strongly anisotropic and nonlinear [Li]-dependent grain material properties can cause grains to expand into and contract away from each other.

Charge Cycling:

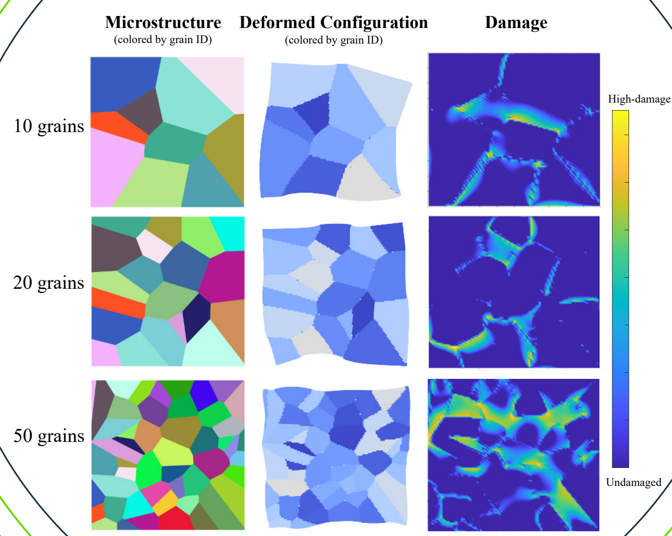
- Lithium moving between electrodes during the (dis)charging process causes expansion and contraction of grains.

What are the implications for damage of Li-ion batteries?

- Chemo-mechanical cracking leads to reduced battery life.
- When these cracks form, they inhibit the movement of lithium, making it difficult to charge Li-ion batteries.

Research Highlights

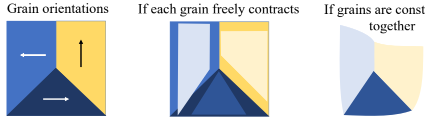
Cathode microstructures are approximated as Voronoi cells, as shown below.



The number of grains within a single cathode particle can vary, so the simulation was run with multiple levels of grain refinement.

Graphs/Diagrams

Test Case 1: Estimated Displacement Field $\Delta[Li] < 0$

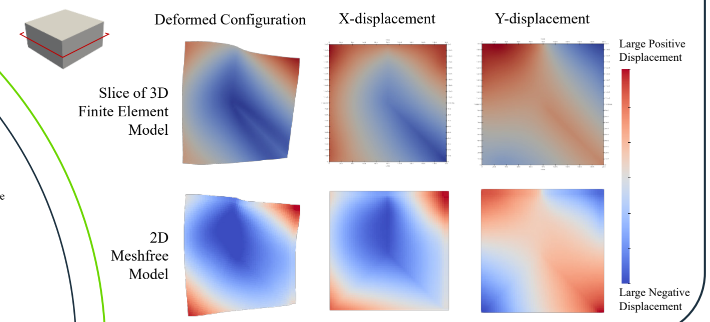


Arrows indicate each grain's principal direction, which expands/contracts ~10x more than the secondary direction.

Test Cases

1. To verify the anisotropic grain orientations, simpler grain structures were used to estimate the deformed configuration.
2. To validate the 2D meshfree model, the displacement fields were compared with a slice from the 3D finite element model.

Test Case 2: Validation With 3D Finite Element Model $\Delta[Li] < 0$



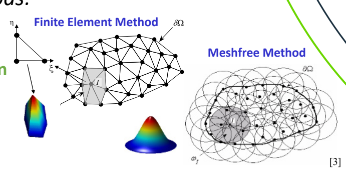
Materials and Methods

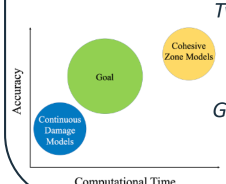
What is a meshfree method?

- A numerical method used to spatially discretize a domain without explicit connectivity from a mesh, like in the finite element method
- The Reproducing Kernel Particle Method is used in this work.

Some advantages of meshfree methods:

- No problems with mesh entanglement/distortion/quality
- Commonly used for large-deformation problems and fracture mechanics
- Straightforward adaptive refinement implementation.





Two main chemo-mechanical models:

- Cohesive Zone Models can accurately capture sharp discontinuities across a crack but are extremely computationally expensive and intractable for 3D problems.
- Continuous Damage Models are easily computed but not well-suited to capture discontinuities.

Goal:

- Use meshfree methods to enhance the continuous damage model's ability to capture discontinuities across a crack and achieve a model that has enhanced accuracy with reduced discretization complexity for chemo-mechanical modeling of cathode grains.

Discussion/Conclusion

- Anisotropic grain material properties and grain rotations can capture nonuniform expansion/contraction, which leads to stress and damage.
- Because the finite element model used for comparison in test case 2 is 3D, the comparison with the 2D meshfree model may not be the most direct benchmark.
- Further efforts in model correlation are being investigated for test case 2.

Future Work

- Capture time-dependent crack growth and battery degradation over lifetime use
- Extend meshfree model to capture arbitrary and more realistic particle geometries
- Couple chemical and mechanical models such that crack formation inhibits localized lithium movement within a cathode particle.

References

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