Image-Based Digital Twin for Assessing the Coupled Electro-Chemo-Mechanical Behavior of Li-ion Batteries

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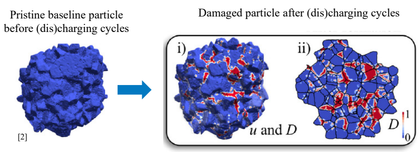
Introduction

What behavior is being modeled? → Electro-chemo-mechanical cathode cracking

- Electro-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.

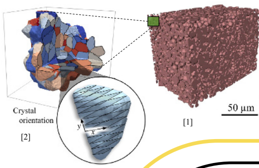


Red areas indicate damaged cathode particle zones; blue areas indicate undamaged zones.

Where in a battery is this damage occurring?

- Electrode materials are made up of many particles, and each particle has a polycrystalline microstructure.
- This work investigates a single particle in the cathode, which is commonly made of a Nickel Manganese Cobalt (NMC) material.

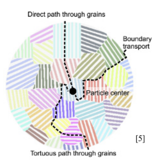
Within a single cathode particle, there are many grains.



NMC cathode materials are made up of a collection of particles and voids.

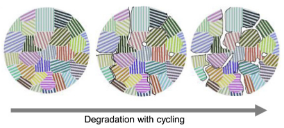
What causes electro-chemo-mechanical cracking?

- A combination of phenomena:



1. *Cathode Composition:*

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



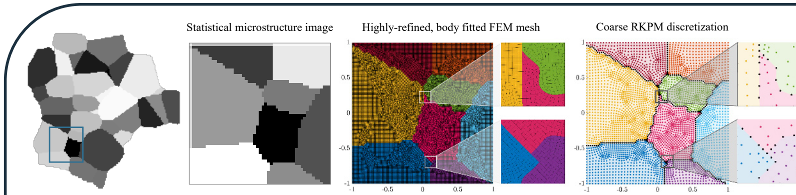
2. *Charge Cycling:*

- 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?

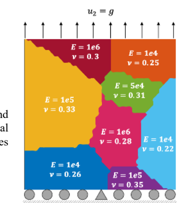
- Electro-chemo-mechanical cracking leads to reduced battery life.
- When these cracks form, they inhibit the movement of lithium, making it difficult to charge Li-ion batteries.

Graphs/ Diagrams



Discretizations

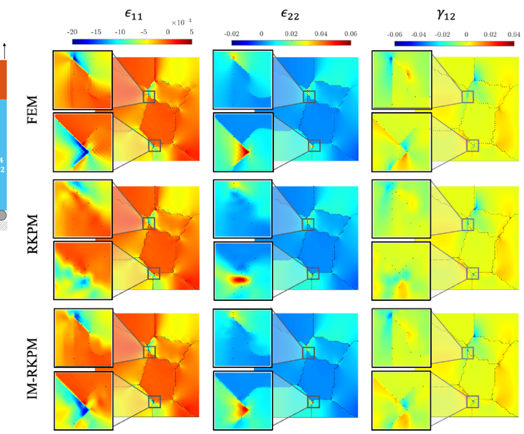
- Image-based geometry
- FEM discretization has 62,852 elements and 63,354 nodes.
- RKPM discretization has 4,195 nodes.



Loading conditions and heterogeneous material properties

Model Verification

Numerical tensile test of image-based domain.



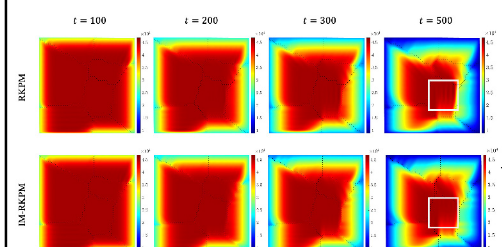
Zoomed-in views around some interesting triple junctions are displayed to better compare the methods' performance.

Observations

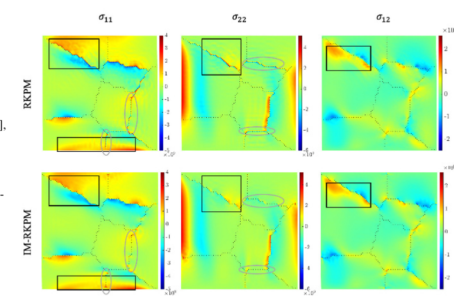
- All methods show good agreement with the FEM reference solution.
- IM-RKPM captures sharp strain discontinuities while maintaining coarse discretization.

Research Highlights

- Model construction transitions directly from pixels to node locations, and transient electro-chemo-mechanical coupling simulates (dis)charging effects.
- Anisotropic material properties capture nonuniform expansion/contraction, which leads to stress and damage largely along grain boundaries.



The concentration is plotted throughout time, visualizing nonuniform diffusion and oscillation reduction (boxed) when using IM-RKPM over RKPM.

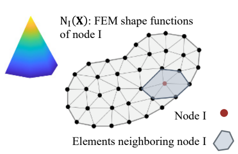


Final stress profiles are compared at $t = 500\ [s]$, showing oscillation reduction (boxed) and nonphysical stress discontinuities relieved (circled) when using IM-RKPM over RKPM.

Methods

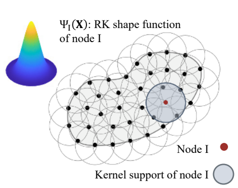
Finite Element Method (FEM)

- A meshed method that spatially discretizes a domain into elements with an explicit mesh.
- Widely used in industry
- The solution accuracy can drastically depend on mesh quality, making meshing tedious at times.
- Used for model verification in this work



Reproducing Kernel Particle Method (RKPM) [3,4]

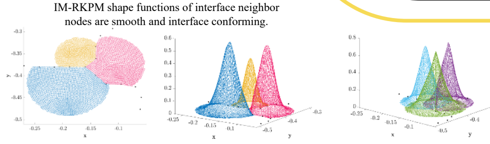
- A meshfree method that spatially discretizes a domain without explicit mesh connectivity, unlike FEM.
- No problems with mesh entanglement/distortion
- Commonly used for large-deformation problems and fracture mechanics, like other meshfree methods.
- RKPM can yield an extremely smooth function, making it challenging to represent material discontinuities without Gibbs oscillations.



Interface Modified RKPM (IM-RKPM) [10]

- Minor modification of the standard RKPM
- A distance-based kernel scaling terminates neighboring kernels along material interfaces.
- Naturally introduces different types of discontinuities into the true field or derivative field to avoid Gibbs oscillations.

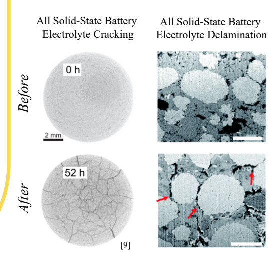
IM-RKPM shape functions of interface neighbor nodes are smooth and interface conforming.



IM-RKPM shape functions of interface nodes incorporate weak discontinuities into the approximation.

Discussion/Conclusion

- IM-RKPM captures strain discontinuities, even with 15x less nodes than FEM.
- Incorporation of IM-RKPM's distance-based kernel scaling drastically reduces Gibbs oscillations and nonphysical stress discontinuities.
- High stress zones largely follow the grain boundaries and exhibit strong discontinuities between grains, as expected.



Future Work

- Visualize crack opening/closing in coupled simulations
  - Capture time-dependent crack growth and battery degradation over lifetime use
- Extend meshfree model to capture arbitrary and more realistic particle geometries
- Apply method to all solid-state battery materials cracking and delamination models (example images at left).

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