

cMorph: Scientific Software for the Large Chemomechanical Deformation and Microstructure Evolution of Battery Materials

Software simulates metallic anode microstructures under mechanical load to predict dendrite formation, enabling the design of customized battery architectures for dendrite suppression.

Among the flourish of research conducted on alternative sources of energy, battery systems have a great potential for growth. Lithium-ion batteries seem to be the most promising of these systems. Unfortunately, there is still a lot to learn about the efficiency and electrochemistry related to these batteries. For example, dendrite formation on the metallic lithium anode due to deformation from an external mechanical load significantly reduces the battery's longevity; however, this dendrite formation is difficult to predict and account for during battery construction.

Researchers at Purdue University have developed software that simulates the deformation and evolution of heterogeneous microstructures with electroplating and/or electrodisolution. This model consists of three subcomponents that use electrochemical fields, predict deformation, and exchange data. Simulation of the evolution of metallic anodes can be utilized to predict the dendrite formation of battery cycling. This allows for the possibility of designing battery architectures for customized dendrite suppression, nucleation, and growth.

Advantages:

- Simulates deformation and evolution
- Electroplating
- Electrodisolution

Potential Applications:

Technology ID

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Category

Energy & Power Systems/Energy Storage
Robotics & Automation/Simulation, Digital Twins, & Industrial Automation
Materials Science & Nanotechnology/Advanced Functional Materials

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-Dendrite formation

-Systems with external mechanical load

TRL: 5

Intellectual Property:

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Keywords: lithium-ion batteries, dendrite formation, battery simulation software, metallic lithium anode, electrochemistry, electroplating, electrodisolution, microstructure evolution, battery longevity, dendrite suppression