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A Cahn-Hilliard type phase-field model for intercalation in storage particles of lithium-ion batteries

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Abstract
Lithium-ion batteries are a key ingredient in many green technologies such as hybrid and plug-in electric vehicles, and in portable electronic devices such as cellular phones. Battery performance may be compromised by damage in the storage particles in the electrodes. Large stresses develop because of the volume changes associated with the intercalation of lithium, and damage the particles. These stresses result in plasticity, fracture, and delamination between the particles and the surrounding matrix.
In some systems, lithium intercalation has been experimentally observed to proceed through the formation of lithium-rich and lithium-poor phases. The formation and evolution of the phases during intercalation has a significant effect on the stresses generated and consequently on rate of charge. In addition, it has been observed that the particle size affects the phase morphology and may suppress phase separation during intercalation.
A thermodynamically consistent Cahn-Hilliard type phase-field model was developed for species intercalation coupled with large elastic deformations. The theory was implemented in the commercially available finite element program Abaqus/Standard by writing a custom user element.
In this talk, this coupled deformation-intercalation phase-field model will be presented, and its capabilities will be demonstrated through simulations of phase-separation in solids. Specifically, simulations of lithium intercalation in spheroidal particles will be presented and used to study the effects of stress coupling and phase separation on the rate of charge, the morphology of phases, and the levels of stress.

Biography:
Elisha Rejovitzky is a postdoctoral fellow at the Department of Mechanical Engineering at MIT. He completed his undergraduate (BSc) and graduate (PhD) degrees at the Technion – Israel Institute of Technology in the Faculty of Mechanical Engineering. During his PhD he worked on stochastic fatigue modeling and damage accumulation under variable loading. His current research interests focus on coupled intercalation-deformation problems, phase-field modeling, and interaction between multiple storage particles in lithium-ion batteries.

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