Massachusetts Institute of Technology
Department of Mechanical Engineering

MMEC SEMINAR SERIES

Mechanics: Modelling, Experimentation, Computation

Tuesdays @ 4:00pm – Room 3-370 **October 28, 2014**

A Cahn-Hilliard-type theory for species diffusion coupled with large elastic-plastic deformations.

Application to Li-ion electrode materials

Lallit Anand, *MIT Dept. of Mechanical Engineering*

I will present a unified framework of balance laws and thermodynamically- consistent constitutive equations which couple Cahn-Hilliard-type species diffusion with large elastic-plastic deformations of a body, and account for the swelling and phase segregation caused by the diffusing species.

A technologically-important area of application of the theory is in the chemo-mechanical analysis of the evolution of large stresses which develop because of the volume changes associated with the diffusion of lithium ions in the active electrode particles of lithium-ion batteries during charge-discharge cycles.

We have numerically implemented our theory in a finite-element program. Using this numerical simulation capability, we have studied

- The problem of spinodal decomposition in the absence of any mechanical deformation.
- The combined effects of diffusion and stress on the lithiation of a representative particle of a phase-separating cathode material.
- The combined effects of diffusion and stress on the lithiation of a representative amorphous silicon anode particle which does not phase- separate, but deforms plastically.

The results from these simulation studies will be presented.

Seminar Host: Pedro Reis (preis@mit.edu)

Please join us for ***refreshments beforehand, outside Room 3-370***

For more information, visit our website at ***http://web.mit.edu/mmec/***
Series Organizers: Ken Kamrin (kkamrin@mit.edu); Pedro Reis (preis@mit.edu); Kostya Turitsyn (turitsyn@mit.edu)

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