Purdue School of Materials Engineering Presents

Peter G. Winchell Distinguished Lecture Series

Seminar

Date: Fri., Sept. 7, 2012

Time: 3:30 – Seminar

Place: ARMS 1010

4:45 – Refreshments

Armstrong Atrium

PURDUE MATERIALS ENGINEERING

Infinite Possibilities

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Chemical Engineering & Mathematics

Phase Separation Dynamics in Li-ion Batteries

ABSTRACT

High-rate Li-ion batteries increasingly involve electrode materials, such as iron phosphate and graphite, which undergo phase separation into Li-rich and Li-poor phases upon intercalation of lithium. New dynamical phenomena arise because phase separation occurs in nanoparticles, limited by surface reactions and far from equilibrium. A general phase-field theory of ion intercalation kinetics is developed, which unifies the Cahn-Hilliard equation with Butler-Volmer and Marcus kinetics for intercalation reactions. For individual nanoparticles, the theory predicts surface-nucleated intercalation waves at low current, which relax to striped morphologies determined by elastic coherency strain. Above a critical current, typical of battery operation, phase separation is suppressed. At moderate currents, unstable "quasi-solid solutions" lack the time to fully phase separate. In porous electrodes, the theory predicts macroscopic reaction fronts and mosaic instabilities at low current, giving way to smooth, diffusive intercalation at high current. These results help to explain the revolutionary performance of $LiFePO_4$ as a cathode material in nanoparticle form. The general theory can also be applied to water sorption in concrete and other adsorption phenomena with hysteresis.

SHORT BIO

Martin Z. Bazant is broadly interested in materials physics and applied mathematics, motivated by problems in chemical engineering. His PhD in condensed matter physics (Harvard, 1997) produced a popular interatomic potential for molecular dynamics simulations of silicon ("EDIP"). He joined the MIT Department of Mathematics in 1998 and did seminal work on diffuse charge dynamics and "induced-charge electro-osmosis" (including the most cited paper in the *Journal of Fluid Mechanics* since 2004). He joined the Department of Chemical Engineering in 2008 and founded an experimental laboratory focusing on novel electrochemical systems for water desalination and energy conversion. His group combines theory with experiment and draws students from chemical engineering, mechanical engineering, mathematics, physics, and materials science. His honors include the Paris Sciences and Joliot Chairs from ESPCI, Brilliant Ten (2007) from *Popular Science Magazine*, and a Career Award from the Department of Energy.