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Electrochemical Nonequilibrium Thermodynamics

Martin Z. Bazant

Departments of Chemical Engineering and Mathematics
Massachusetts Institute of Technology

Visiting Professor, GCEP Chair
Materials Science and Engineering, SUNCAT Center
Stanford University

ABSTRACT: Li-ion batteries often involve electrode materials, such as iron phosphate and graphite, which separate into different stable phases upon intercalation of lithium. In these and other systems, bulk thermodynamic relaxation competes with surface electrochemistry, leading to the fundamental question: *What is the reaction rate during a phase transformation?* A consistent answer is provided by a mathematical theory that unifies and extends the Cahn-Hilliard and Allen-Cahn equations for chemical kinetics and charge transfer*. The reaction rate depends on concentration gradients, space charge, coherency strain, and other thermodynamic non-idealities. The theory predicts some surprising new mesoscale phenomena, such as current-induced suppression of phase separation in nanoparticles and mosaic instability in porous electrodes, which have since been observed experimentally, not only for Li-ion batteries, but also for other chemical systems, such Li-air batteries, catalyst nanoparticles and patchy colloids.

Lecture 1: Chemical Kinetics and Nonequilibrium Thermodynamics

Lecture 2: Applications to Li-ion Batteries

* Recommended reading: M. Z. Bazant, *Accounts of Chemical Research*, 46:1144 (2013).

Biography

Martin Z. Bazant is the E. G. Roos (1944) Professor of Chemical Engineering and Mathematics at the Massachusetts Institute of Technology. After a PhD in Physics at Harvard University (1997), he joined the MIT faculty in Mathematics (1998) and then Chemical Engineering (2008), where he currently serves as Executive Officer. His research combines theory, computation and experiments in diverse fields, with emphasis on electrochemistry and electrokinetics. His contributions have been recognized by the Alexander Kuznetsov Prize in Theoretical Electrochemistry (ISE), Global Climate and Energy Project Chair (Stanford), Paris Sciences Chair (ESPCI), Brilliant Ten (Popular Science), Lighthill Lecture in Applied Mathematics (IMA), Winchell Lecture in Materials Science (Purdue), and Corrsin Lecture in Fluid Dynamics (Johns Hopkins). He serves on the editorial board of *SIAM Journal of Applied Mathematics* and *Scientific Reports* and is the Chief Scientific Advisor for Saint Gobain Ceramics and Plastics, Northboro R&D Center.

