

Dr. Kejie Zhao

Li-ion batteries: when mechanics meets chemistry

Abstract:

High-energy density Li-ion batteries are ubiquitous in portable electronics, and are being implemented to power electric vehicles. A Li-ion battery is a system that dynamically couples electrochemistry and mechanics. During charge and discharge of a Li-ion battery, the amount of Li in the electrodes varies substantially, causing the host electrodes to deform. The deformation induces a field of stress, which may lead to fracture or morphological change. Lithiation reactions in batteries lead to rich phenomena of mechanics in the electrodes, such as large deformation, plasticity, fracture, and fatigue. Likewise, mechanics influences the chemistry of lithiation in a significant manner. Stress affects reactions at the interface between the electrode and electrolyte, diffusion of Li in the electrode particles, and phase transformations of the electrode materials. In this talk, I will highlight the intimate relation between mechanics and electrochemistry in Li-ion batteries. Theories of diffusion-induced stresses, coupled Li diffusion and large elastic-plastic deformation, concurrent chemical reactions and flow, and fracture of electrodes will be illustrated. First-principles simulations and experimental measurements that emphasize the mechanisms of reactions and deformation will also be discussed.

Bio: Kejie Zhao is currently a Postdoctoral Associate in the Department of Nuclear Science and Engineering and Materials Science and Engineering at MIT (<http://web.mit.edu/kzhao/www/index.html>). He received his Ph.D degree in Engineering Science in 2012 from Harvard University, and obtained his bachelor's and master's degrees from Xi'an Jiaotong University in China in 2005 and 2008 respectively. His research interests include mechanics of energy materials, multiscale modeling of materials science, environment-sensitive fracture, and mechanical behaviors of amorphous materials.

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