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Journal of Electrochemical Energy Conversion and Storage

Guest Editorial

Special Issue on Multiphysics Coupling in Energy Storage

In recent years, a critical need has emerged to accelerate innovation of energy storage devices with the goal of improving device performance (energy and power), safety, and reliability for diverse applications ranging from vehicle electrification to renewable energy integration and grid storage. Lithium-ion batteries, for example, are leading the race for electric drive vehicles, while alternative chemistries like sodium-ion batteries are receiving renewed attention for grid applications. A commonality among these energy storage devices is that they are complex, dynamic systems composed of mixed functional materials. These materials support a multitude of coupled physicochemical processes encompassing electronic, ionic, and diffusive transport in electrode and electrolyte phases, electrochemical and phase-change reactions, and stress generation in multiscale porous electrodes. The performance and lifetime of such electrochemical energy storage devices are therefore dependent on complex reaction and transport processes spanning across multiple length and time scales. Continued improvement of electrochemical energy storage devices for vehicle electrification, renewable energy integration, and grid storage depends on understanding the underlying multiscale, multiphysics processes. Computational models and characterization of mechanical, thermal, and electrochemical processes play an important role in providing insight into coupled multiphysics interactions.

Within this context, a U.S. National Science Foundation and ASME-sponsored symposium on Multiphysics Coupling in Energy Storage was held at the 2015 ASME International Mechanical Engineering Congress and Exposition. The ASME Advanced Energy Systems Division's Technical Committee on Electrochemical Energy Conversion and Storage organized a multisession symposium during which experts were invited from industry, research laboratories, and academia to present the latest energy storage challenges in their field. This symposium addressed several key issues related to multiphysics behavior of the energy storage devices, including: (1) opportunities and challenges in Li-ion chemistry and beyond (such as Li–air and Li–S); (2) coupled electrochemical, thermal, and mechanical physics; (3) modeling and characterization of physical processes across length scales; (4) mesoscale physics of microstructure–transport–chemistry interactions; (5) degradation processes controlling safety and lifetime; and (6) origin and evolution of safety events, such as thermal runaway. Following the theme of this symposium, this special issue of the ASME *Journal of Electrochemical Energy Conversion and Storage* presents a series of works addressing multiphysics behavior in the energy storage devices.

Three papers providing reviews relevant to understanding multiphysics processes in batteries are included. Shah et al. provided a review of multiscale thermal measurements in Li-ion batteries spanning efforts to characterize thermal properties, heat generation, thermal management, and thermal runaway. Multidisciplinary challenges inherent to thermal measurement in the presence of coupled multiphysics transport phenomena are discussed. Nelson et al. provided a brief review of 3D X-ray imaging focusing on applications of X-ray nanotomography and microtomography toward observation of Li-ion batteries and related components. Examples of ex situ, in situ, and in operando X-ray imaging are addressed along with the application of 3D mesoscale data in simulation efforts. Finally, Xu and Zhao reviewed observations on mechanical–electrochemical coupling related to diffusion, interfacial charge transfer reactions, and growth of lithiated phases pertinent to degradation in Li-ion battery electrodes.

The research papers included in this special issue address experimental and computational approaches applied in the pursuit of understanding coupled multiphysics phenomena in batteries. Several of these papers address phenomena occurring within electrode microstructures. Stein et al. presented a study on the electrochemical performance effects of high energy ball milling on $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ cathodes. The effects of milling time and speed on cathode rate capability and the underlying physical properties governing performance are supported with computational studies. Mesoscale simulation of electrochemical, mechanical, and thermal phenomena within composite electrodes is addressed by Roberts et al. A computational approach for mesoscale simulation is presented with supporting example investigations. Mistry et al. also presented a mesoscale model describing the interaction between electronic and ionic conduction paths within porous composite electrode structures. This work underscores the need for composite electrode preparation strategies supported by accurate microstructural characterization and complimentary modeling approaches. Jithin et al. applied the lattice Boltzmann method toward the study of Li–O_2 batteries at the pore-scale based on idealized microstructures simulated based on macroscopic properties of the porous electrodes. The influence of mass transfer on Li–O_2 battery performance degradation is highlighted. Ramos-Sanchez et al. addressed the mechanisms of solid-electrolyte interphase (SEI) layer formation in Li-ion batteries using quantum mechanical and kinetic Monte Carlo methods. They highlighted the initial stages of SEI growth and pertinent side reaction for organic solvents based on a hierarchical modeling approach.

While a majority of the papers herein focus on electrode materials at the mesoscale and below, additional components and scales are addressed. In particular, Love discussed temperature-dependent lithium dendrite morphologies and their mechanical interaction with polymer separators. The local mechanical properties of the separator are also addressed as key factor in separator–dendrite mechanical interactions. At the cell and battery module level, Lopez et al. also evaluated thermal management strategies using a computational model that couples fluid dynamics and conjugate heat transfer with lithium-ion battery thermal and electrochemical response. The combination of active and passive thermal management methods is assessed from a standpoint of module configuration and phase-change material properties.

Organizing this special edition has been a challenging but rewarding process. This would not have been possible

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