Energy Storage Technologies

Coupled Kinetic, Thermal, and Mechanical Modeling of Focused Ion Beam Micromachined Electrodes

Background

Development and design of electric vehicles (EVs), hybrid, plug-in hybrid, and all electric, is one of the primary research directions for reduction of vehicle emissions and reduction of U.S. dependence on foreign oil. Lithium- (Li-) ion-based electrochemical energy storage technology is the primary candidate for the electrification of vehicle drivetrains. Ongoing collaborative research between companies and research institutions provides evidence of the high potential for use of Li-ion batteries in EVs. However, despite the attractive features of Li-ion battery systems and a wide range of applications in smaller scale devices such as consumer electronics, the service life of Li-ion battery systems is still limited due to degradation of electrode materials with repeated charging and discharging cycles.

Technology

It is commonly accepted that Li-ion battery life is limited due to continuous capacity loss. During battery operation, Li ions are shuttled between cathode and anode when the battery is being charged and discharged. One of the degradation mechanisms is related to the development of internal stresses in electrode particles due to repeated Li insertion and removal. The stresses ultimately result in cracks in and fracture of particles. To explore the mechanical side of battery degradation mechanisms, Oak Ridge National Laboratory has partnered with the University of Michigan on a project using the equipment and intellectual capabilities of both institutions, as well as those of the Shared Research Equipment Collaborative Research Center of the U.S. Department of Energy Office of Science, Basic Energy Science Program. The project targets the fundamental understanding, description through mathematical modeling, and controlled experimental validation of internal stress generation in and morphology change of electrode particles in Li-ion batteries.

Status

Experiments are being performed on model systems represented by microscopic specimens of electrode material. The modeling work is being done on preselected geometries of specimens to

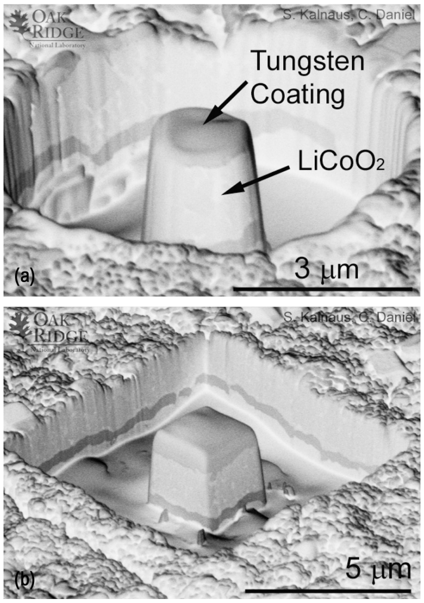

Figure 1: FIB machined specimens with: (a) circle and (b) square as a base shape.

Benefits

- *Fundamental understanding of electrode failure mechanisms.*
- *Model development for accurate life prediction.*
- *Guidance for future development of novel electrode materials and structures with longer life and higher performance.*

validate the constitutive approach. Different cathode materials are being investigated, including $LiCoO_2$, $LiMn_2O_4$, and $Li_4Ti_5O_{12}$. At the preliminary stage, sample electrode specimens were micromachined from the layer of $LiCoO_2$ deposited by physical vapor deposition on the gold current collector. Fabrication of samples was performed using a Hitachi NB5000 dual beam focused ion beam– (FIB–) scanning electron microscope (SEM). Two of the samples are shown in the SEM pictures in Figure 1.

Preliminary computational results were obtained based on a cylindrical homogenous $LiMn_2O_4$ particle. Intercalation-induced stresses during a discharge process (current density i = 2 A/m^2) were simulated using a stress-diffusion coupling model. Three cases were considered to quantify the stress level (Figure 2): (a) a single particle, (b) two agglomerated particles, and (c) two particles combined by a polyvinylidene fluoride (PVdF) binder.

Figure 2 shows the von Mises stress distribution at the end of the discharge process, where the Li concentration reaches the stoichiometric maximum. In a single particle [case (a)], the stress is larger along the upper edge, where the gradient of lattice spacing is more severe. In case (b), there is a stress concentration at the connection between two particles. However in case (c), there is no stress gradient around that connection due to the presence of Li-free binder, and the stress level and distribution are similar to the case of a single particle.

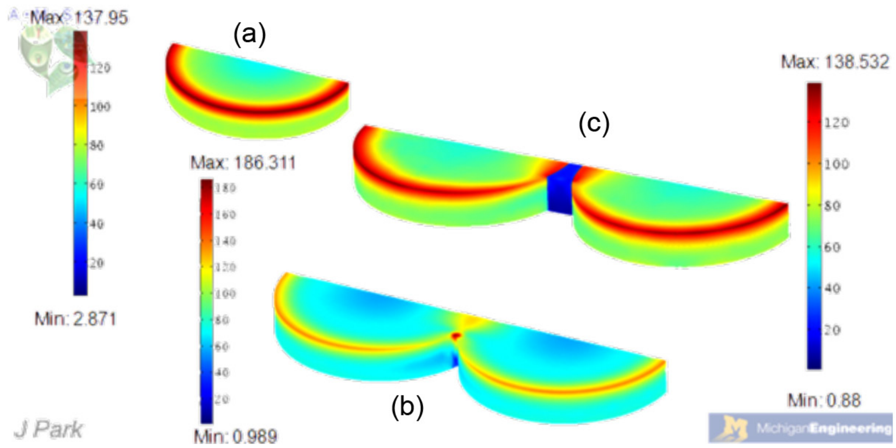

Figure 2: Von Mises stress distribution (in megapascals) in cathode particles at the end of discharge: (a) = the single particle case, (b) = two agglomerated particles, and (c) = two particles combined by a PVdF binder.

Contacts

Claus Daniel
Oak Ridge National Laboratory
(865) 241-9521
danielc@ornl.gov

David Howell
Team Leader
Hybrid Electric Systems Subprogram
U.S. Department of Energy
(202) 586-3148
david.howell@ee.doe.gov

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