Sandia National Laboratories

Energy, Climate, &
Infrastructure Security

Battery Reliability Science at Sandia

Sandia has unique, powerful methods to directly observe battery materials at the nanometer scale during electrochemical charging and discharging. These techniques, when combined with other Sandia activities, allow researchers to understand mechanisms that limit batteries' performance lifetimes and impact their response to abusive conditions.

Vision

To enhance the nation's security and prosperity through sustainable, transformative approaches to our most challenging energy, climate, and infrastructure problems.

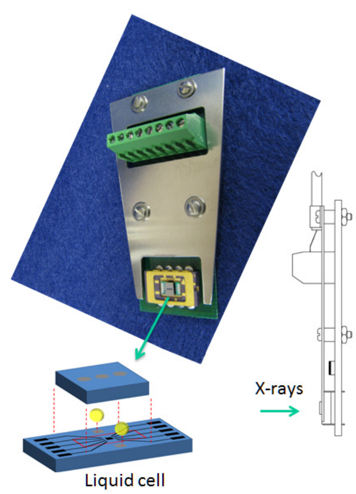
Transitioning from fossil-fueled to electrified vehicles depends on developing batteries that are increasingly economical, reliable, and safe. A vehicle battery is a large investment and carries with it a requirement for a long, reliable life. Substantially improving battery performance requires greatly improving the energy storage community's fundamental understanding of the complex processes active in batteries, particularly those that degrade a battery's service lifetime.

As a lithium-ion battery discharges and then is recharged, lithium ions physically move from the anode to the cathode (called lithiation and delithiation). A myriad of chemical, electrochemical, and microstructural changes result from these two processes. Over the thousands or cycles needed for automotive applications, these processes stress the battery causing it to degrade and eventually fail. By *directly* studying the atomistic lithiation and delithiation processes, Sandia has been able to elucidate structural and chemical changes that battery materials undergo. This work has led to a new understanding of the charging and deformation process not possible with ex situ techniques.

These in situ techniques allow Sandia to isolate single particles of battery materials as well as sections of battery electrodes in order to study changes in particle structure and the creation of defects that cause degradation over the battery's life. This work enables materials or design strategies that reduce or eliminate the defects/degradation—making batteries more reliable and long lasting.

Scanning Transmission X-Ray Microscopy (STXM)

Sandia has developed a new technique that allows scanning transmission x-ray microscopy to be used to study the highly reactive chemistries in batteries. This technique allows the researcher to identify the chemical state (charge state) *in addition to* the spatial distribution of the different chemical species in the battery with tens of nanometers resolution.



The special sample mount for in situ STXM observations/ experiments.

U.S. DEPARTMENT OF ENERGY

Quantitative nanoscale electrochemistry reveals evidence of capacity loss due to SEI thickening using in situ TEM.

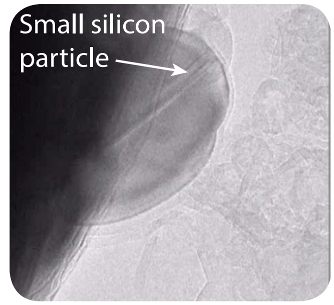
Using Sandia's STXM technique, researchers can discern the chemical and structural information in a full electrochemical cell using real electrolyte and observe the cell as it undergoes charge and discharge cycles. The goal is to quantitatively monitor charging/discharging of a battery's nanoscale electrode materials in the presence of the liquid electrolyte and observe the effects of degradation processes, such as fracture or thickening of the electrolyte decomposition product layer, known as the solid-electrolyte interphase (SEI).

Transmission Electron Microscopy

In December 2010, Sandia was home to breakthrough TEM work that directly observed changes in atomic structure of a SnO_2 nanowire as it underwent lithiation. This experiment demonstrated the power of in situ TEM for directly observing structural changes and the resulting degradation in battery materials during charge-discharge cycling. More recent experiments have shown new mechanisms for lithiation and degradation in anode materials, including the observation of a size-dependent failure mechanism in silicon anode particles.

Developing an understanding of materials' physical changes during charge/discharge can lead to improved electrode architecture, enabling improvements in efficiency, energy density, reliability, safety, and lifetime. Sandia's in situ TEM lithiation experiments are now able to view single nanoscale battery particles and—in a capability unique to Sandia—control and detect charging and discharging currents at the level of femtoAmperes (a quadrillion times less than the charging current in an electric vehicle battery). These studies reveal sources of capacity loss in anode materials, such as SEI layer growth and evolution.

Connections with Other Aspects of Sandia's Battery Research



Sandia is also developing a physics-based numerical simulation capability for tracking thermal history and predicting the onset of thermal runaway in transportation-based, secondary lithium-ion batteries. This simulation capability will enable our researchers to explore and characterize a wide variety of operational conditions and their associated thermal histories—so that potential safety and stability issues of new battery designs can be identified and mitigated before fabrication.

In sum, Sandia presents a unique combination of four strengths: novel in situ diagnostics, state-of-the-art multi-scale mechanistic modeling, custom battery manufacturing and abuse testing, and a strong commitment from management. By combining nanoscale direct observation capabilities with multiscale battery models, Sandia is able to obtain a complete picture of the processes active during battery use that can directly impact new battery material maturation cycle.

This work forms a key component of Sandia's energy storage roadmap and positions Sandia to work with U.S. auto industry, providing future external investment opportunities in a rapidly growing field.

For more information, please contact:

Sean Hearne
Phone: (505) 844-0804
E-mail: sjhearn@sandia.gov
Website: energy.sandia.gov

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2012-6785P