

Advanced Materials for Energy Applications

Fundamental understanding, unique characterization facilities, and standardized materials and data form the technological basis for advances in materials for energy-related technologies. We are working to develop the metrology required to relate properties and performance of energy materials to processing/manufacturing routes via understanding the roles of chemistry, phase relations, and microstructure, to establish a sound physical basis for material system design.

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A challenge for the U.S. economy in the new millennium is for both emerging and mature industries to provide environmentally friendly, inexpensive, efficient, compact, and cutting-edge synergistic technologies for energy conversion, distribution, and storage applications. This project aims to facilitate commercialization of energy-related technologies by addressing various near-term and long-term materials issues.

The proliferation of portable telecommunication devices, computer equipment, and hybrid electric vehicles has created a substantial interest in manufacturing rechargeable Li-ion batteries that are less expensive, non-toxic, durable, and small in size and weight. The electronic structure of the electrode materials during the electrochemical cycling is particularly important to the implementation of Li-ion batteries. This year, we studied the electronic structure of the Li-ion deintercalated $\text{Li}_{(1-x)}\text{Co}_{1/3}\text{Ni}_{1/3}\text{Mn}_{1/3}\text{O}_2$ materials with soft X-ray absorption spectroscopy (XAS) at O *K*-edge and metal $L_{\alpha, \beta}$ -edges, in combination with metal *K*-edge XAS spectra in the hard x-ray region to elucidate the charge compensation mechanism. We found that a large portion of the charge compensation during Li-ion deintercalation is achieved in the oxygen site due to the presence of Co.

Characterization of the triple phase boundary in solid oxide fuel cells (SOFC), where the electron- and ion-conducting phases and the gas transport (void) phases meet, is a priority in understanding SOFC performance and durability. By combining studies of the large microstructure scale range, accessible using the NIST-built ultrasmall-angle x-ray scattering (USAXS) facility at the Advanced Photon Source, with anomalous small-angle x-ray scattering (ASAXS) measurements, it has been demonstrated that ASAXS can provide the differential contrast for distinguishing between the ion- and electron-conducting phase morphologies.

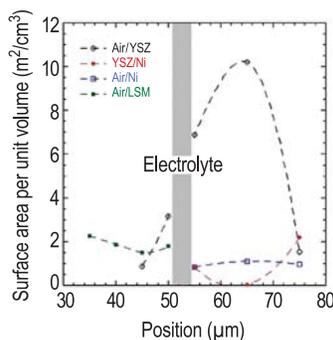


Figure 1: Spatial variation in component phase surface areas.

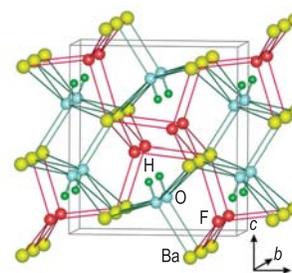


Figure 2: Structure of Ba(OH)F .

Figure 1 shows the spatial variation of the void/solid surface areas involving the ion-conducting yttria-stabilized zirconia (YSZ) and lanthanum strontium manganate (LSM), and Ni that are the electron-conducting phases in the cathode and anode layers.

Phase equilibria data are critical for the coated conductor high T_c materials for cable, generator, fly-wheel, and transformer applications. As an integral part of a DOE R&D program, phase diagrams were developed for the Ba-R-Cu-O (R = Tm and Yb) systems. The “ BaF_2 ” process is a promising method for producing long-length coated conductors. We have investigated the role of low-temperature melt and intermediate superlattice phases in the formation of $\text{Ba}_2\text{YCu}_3\text{O}_{6+x}$ (Y-213). A new Ba(OH)F phase (Figure 2) was discovered that may be related to the low-temperature melting. The interaction of Y-213 with SrTiO_3 substrates was studied in terms of phase equilibria of the Ba-Sr-Y-Cu-Ti-O system.

In collaboration with the University of South Florida, we have characterized the structure and provided x-ray reference patterns for two clathrate phases ($\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ and $\text{Cs}_8\text{Na}_{16}\text{Ge}_{136}$) that are promising candidates for thermoelectric power conversion applications. The structure of $\text{Na}_{1-x}\text{Ge}_3$, which often coexists with $\text{Cs}_8\text{Na}_{16}\text{Ge}_{136}$, was also studied. Defining the industrial needs for thermoelectric metrologies and the uses of combinatorial approaches for materials optimization remain a high priority.

Contributors and Collaborators

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