Challenges and Rewards Using High-Temperature Diffraction

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This talk will provide an overview of research at ORNL using high-temperature x-ray and neutron scattering methods. These studies typically are seeking more than simple search-match phase ID at fixed temperatures, but also phase fractions, lattice parameter changes, often time-resolved, and consequently the experiments are more complex, and the analyses are more demanding. The sample morphology can also have an important impact on the data quality, as simulating “real world” synthesis or operating conditions will often take the operator far from the ideal of finely ground, equiaxed, randomly oriented powders, and this needs to be carefully considered in the design and analysis of the experiment. A careful evaluation of the potential for systematic errors is often valuable in experimental design, and also in interpretation of such data.

An array of commercial and “in-house” sample environments are available for such studies at ORNL, and their suitability and limitations will be discussed. Specific examples that will be highlighted will include studies of phase transformations in vanadium oxide thin films, reaction pathways and kinetics in synthesis of photovoltaic thin films, in-situ studies under reactive atmospheres, and high-pressure studies.