Showcase of Undergraduate Research and Creative Endeavors (SOURCE)

Apr 24th, 12:00 AM

**Thermodynamics-Based Discovery of New K-La-Zr-O Compounds via Hydrothermal Synthetic Methods**

Thomas Sullivan  
*Winthrop University*

Follow this and additional works at: https://digitalcommons.winthrop.edu/source


This Poster Presentation is brought to you for free and open access by the Conferences and Events at Digital Commons @ Winthrop University. It has been accepted for inclusion in Showcase of Undergraduate Research and Creative Endeavors (SOURCE) by an authorized administrator of Digital Commons @ Winthrop University. For more information, please contact digitalcommons@winthrop.edu.
Research on Thermodynamic-based Discovery of New K-La-Zr-O Compounds

T. Sullivan and M.C. Gelabert

Department of Chemistry, Physics and Geology, Winthrop University, Rock Hill, South Carolina 29733

contacts: sullivant1@mailbox.winthrop.edu, gelabertm@winthrop.edu

Abstract

This project employs aqueous modeling and solid-state synthetic methods for novel compound discovery under mild hydrothermal conditions (≈200°C, 16 atm) – one specific goal for advanced materials development outlined by SC Vision 2025 and NSF’s Big Ideas. Innovative luminescent materials, especially visible-light-emitting scintillators, are desired for improving properties of opto-electronics and other optical material technologies. Guided by aqueous speciation calculations run with OLI Studio, exploratory hydrothermal syntheses are performed in attempt to yield new compounds of the K-La-Zr-O quaternary system, as inspired by several compounds of Na-Y-Si-O and La-Zr-O system, with water-soluble metal salts, chelating agent, water, and base as reactants for synthesis of a new rare-earth optical scintillators, are desired for improving properties of opto-electronics.

Innovative luminescent materials, especially visible-light-emitting scintillators, are desired for improving properties of opto-electronics.

An example of a x-ray powder diffraction is shown. This shows the diffraction pattern for a sample.

Future Work

- Continue SEM/EDS analyses of samples (5A-B,3C)
- Continuation of studies of this and related systems with different compositions of starting materials
- Inclusion of high-temperature solid state investigation of phase diagram(s)

References


Acknowledgments

MADE in SC; SC EPSCoR, NSF #1655740
SURE Program, Winthrop University Department of Chemistry, Physics and Geology
Dr. Marta Gelabert
Dr. Julian Smith

Hydrothermal Synthetic Methods and Materials

Aqueous mixtures of ZrOCl₂, LaCl₃, EDTA, and KOH were prepared with target amounts corresponding to several locations outside the ZrO₂ stability region. Samples (1E remake, ZrA-1, ZrA-3, 4A-8, and 5A-8) were sealed in Teflon-lined autoclaves and maintained at 200 °C for 5 days, then quenched in cold water. Products were centrifuged and washed in distilled water (x2) and then ethanol (x2) to prepare for analysis via optical microscopy (Leica DM 2500M). X-ray powder diffraction (XRD, Rigaku Miniflex 600), and scanning electron microscopy (SEM) with energy-dispersive X-ray (EDS) analysis (JEOL 1610 InTouchScope).

Chemical/yield diagrams are shown for Zr-La system (left) and lanthanum system (right); these diagrams illustrate log molalities of La vs. log molalities of KOH; 99% yield regions for zirconia (ZrO₂) (left) and lanthanum hydroxide [La(OH)₃] (right) are highlighted in green.

Yield Diagrams

Chemical/yield diagrams are shown for Zr-La system. Zirconium subsystem (left), lanthanum subsystem (right). These diagrams illustrate log molalities of La and Zr vs. log molalities of KOH. 99% yield regions for zirconia (ZrO₂) (left) and lanthanum hydroxide (La(OH)₃) (right) are highlighted in green.

Future Work

- Continue SEM/EDS analyses of samples (5A-B,3C)
- Continuation of studies of this and related systems with different compositions of starting materials
- Inclusion of high-temperature solid state investigation of phase diagram(s)

Using optical microscopy, we observe the microstructure of the samples.