Suppression of Phase Transition Temperature in Aluminum Indium Tungstate and Aluminum Indium Molybdate

C. Lind-Kovacs1, L. Lovings2, D. Dietzel3

The University of Toledo, Department of Chemistry & Biochemistry, 2801 W. Bancroft Street, Toledo, OH, 43606, United States; Xavier University of Louisiana, 1 Drexel Drive, Suite 307, Box 164, New Orleans, LA 70125, United States; Institute for Inorganic Chemistry and Analytical Chemistry, Johannes-Gutenberg University, Duesbergweg 10-14, Mainz, 55099, Germany

Cora.lind@utoledo.edu

Keywords: Phase transition temperature, Scandium tungstate family, Negative thermal expansion

Over the past 25 years, the field of negative thermal expansion (NTE) materials has grown from a scientific curiosity observed in a small number of oxide families to a vibrant field encompassing numerous different compositions, structures and mechanisms. Successful prediction and synthesis of new compositions that may show NTE by substituting atoms in known structure types has significantly expanded the number of materials that display this property. However, control of expansion and phase transition behavior as a function of temperature and pressure remains a challenge in many families of NTE materials. This poster will focus on materials in the scandium tungstate (A2M3O12) family, in which the M-site generally contains Mo or W, while the A-site can be substituted by trivalent cations ranging in size from Al3+ to the smaller lanthanides.[1,2] In this family, NTE is observed in an orthorhombic structure, but many compounds show a reversible phase transition to a structurally related denser monoclinic polymorph with positive expansion upon cooling or when pressure is applied.[3] We recently found that strategic choice of A-site cations can be used to suppress undesired phase transitions to lower temperatures.[4,5]

Aluminum indium tungstates and aluminum indium molybdates were synthesized by nonhydrolytic sol-gel chemistry, and their crystal structures, phase transition and thermal expansion behavior were studied using variable temperature powder diffraction. A significant lowering of the phase transition temperature was observed in both systems for compositions close to the middle of the solid solution series. This suppression is attributed to the large size difference between Al3+ and In3+. Interestingly, samples with much lower phase transition temperatures than those predicted by Vegard’s law also tend to display positive thermal expansion along all cell axes instead of the typically observed negative expansion of orthorhombic A2M3O12 compositions. This may be a result of the strain present in the crystal lattice, which can interfere with the phonon modes that cause NTE in this family.


Funding through U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences (contract No. DE-AC02-06CH11357 to Argonne National Laboratory Advanced Photon Source); National Science Foundation (scholarship No. 1432878 to La’Nese Lovings); Bundesministrium für Bildung und Forschung (scholarship to Dominik Dietzel); BASF (scholarship No. Deutschlandstipendium to Dominik Dietzel); Deutscher Akademischer Austauschdienst (scholarship No. PROMOS to Dominik Dietzel) is acknowledged.