

Tuning Expansion and Phase Transition Behavior in the Scandium Tungstate Family

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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 talk will focus on materials in the scandium tungstate ($A_2M_3O_{12}$) 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 Al^{3+} to the smaller lanthanides. Compositions in which the A and/or M-site are substituted by aliovalent cations have also been reported, which may adopt cation ordered structures. 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. We recently found that strategic choice of A-site cations can be used to suppress undesired phase transitions to lower temperatures and higher pressures.

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