

Elucidating the Structure of Negative Thermal Expansion Materials Using Powder Diffraction

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Negative thermal expansion (NTE) materials have attracted significant attention over the past two decades since this behavior was shown to arise from certain structural features in several families of metal oxides [1]. While much progress has been made in elucidating the structural basis of the NTE phenomenon, phase transitions as a function of composition, temperature and pressure are much less understood. This talk will focus on materials in the scandium tungstate ($A_2M_3O_{12}$) family that deviate from behavior expected based on simple models like the rule of mixtures [2, 3]. 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, or by mixtures of di- and tetravalent cations. In this family, NTE is observed in an orthorhombic structure, but many compositions show a reversible phase transition to a structurally related denser monoclinic polymorph with positive expansion upon cooling. This structure is also commonly observed at very low pressures (<0.6 GPa) upon compression. However, some compositions show a strong suppression of this undesirable transition to much lower temperatures or much higher pressures than expected. The *in situ* characterization of the variable temperature and pressure behavior of these materials relies heavily on powder diffraction studies combined with Rietveld analysis.

[1] J.S.O. Evans *et al.*, Physica B **241** (1997) 311.

[2] A. M. Gindhart *et al.*, Journal of Materials Research **23** (2008) 210.

[3] R. Truitt *et al.*, Materials **8** (2015) 700.