Thermal Expansion and Phase Transformation Mechanism in the Lanthanide Di-titanate System

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Characterization of the thermal expansion in the lanthanide di-titanates is important for their use in high-temperature piezoelectric and dielectric applications. The thermal expansions of most rare-earth di-titanates, $Ln_2O_3 \cdot 2TiO_2$ (Ln = La, Pr, Nd, Sm, Gd, Dy, Er, Yb, Y), in both the monoclinic and cubic room temperature phases, were measured from room temperature to 1600°C. $La_2O_3 \cdot 2TiO_2$ undergoes a monoclinic to orthorhombic displacive transition on heating and the orientation relation between these structures were studied. Crystalline powder samples were synthesized by the solution-based steric entrapment method. High temperature characterization was achieved with a quadrupole lamp furnace. The 3-D thermal expansion coefficients leading to transformation mechanisms were obtained from in-situ synchrotron (APS 33-BM-C) as well as neutron (SNS BL-11A) diffraction. Accurate temperature was determined using Pt as an internal temperature standard. Upon determination of the lattice parameters, the thermal expansion tensor was calculated and visualized using the program CTEAS.