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Thermal expansion and phase transformation behavior in the rare-earth titanate system

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THERMAL EXPANSION AND PHASE TRANSFORMATION BEHAVIOR IN THE RARE-EARTH TITANATE SYSTEM

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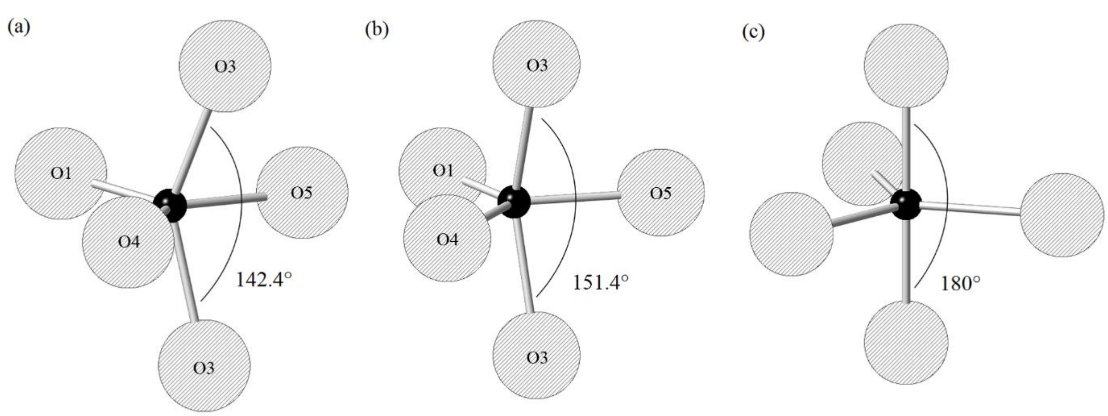
Abstract

The thermal expansion and phase transformation behavior in the rare-earth titanate system has not been well understood. Much of the previous work in this material system was performed *ex situ* and reveals little information about the thermal expansion, mechanisms behind this expansion, and the relationship between the orthorhombic and hexagonal phases with temperature.

In this paper, a unique method using a thermal image furnace and synchrotron radiation was employed to monitor crystallographic changes in this material system *in situ* to determine the thermal expansion tensor and describe the mechanism behind such behavior. In addition, this information was paired with insights into the volume expansion, structural elements, and geometric units between the orthorhombic and hexagonal phases to describe a potential pathway between two crystallographic cells which have no group-subgroup relationship. The novel pairing of information to describe a reconstructive transformation in this manner is unique and may be a new method to describe such transformations where few tools currently exist today.

Additionally, a new experimental technique to study the phase transformation kinetics *in situ*, which can avoid traditional pitfalls of such investigations, was used to examine the kinetic parameters describing the orthorhombic to hexagonal phase transformation. While the technique still needs development, it nonetheless describes the transformation kinetics in a sufficient manner for an initial experiment and understanding.



Thermal expansion of hexagonal phase of $DyTiO_5$. The trigonal bipyramidal structural motif around the Ti^{+4} cation at (a) room temperature, (b) 1310 °C, and (c) for the