

Temperature and composition dependence of structural phase transitions in $\text{Ca}(\text{Ti}_x\text{Zr}_{1-x})\text{OGeO}_4$

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ABSTRACT

The solid solubility of CaTiOGeO_4 with CaZrOGeO_4 and the structural phase transitions occurring in this solid solution as a function of temperature and composition were examined using in situ high temperature X-ray powder diffraction. Structural phase transitions were identified based on the determination of spontaneous strain. The transition $P2_1/a$ - $A2/a$, which is typical for titanite and CaTiOGeO_4 , was observed in samples with Zr concentrations up to 10%. The addition of Zr destabilizes the ordered $P2_1/a$ phase and T_c decreases accordingly. The aristotype structure of titanite in space group symmetry $A2/a$ was observed for intermediate compounds. Compounds with high Zr contents exhibit a triclinically distorted titanite structure. Their structure was modeled in space group $A\bar{1}$. The triclinic structure appears at Zr contents of about 70% with T_c close to ambient temperature. Further increase of the Zr content stabilizes the triclinic structure and leads to an increase of T_c up to $T_c = 488$ K in CaZrOGeO_4 .