

A high-temperature diffraction study of the solid solution CaTiOSiO_4 - CaTiOGeO_4

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ABSTRACT

The structure of CaTiOGeO_4 (CTGO) has been refined using single crystal X-ray diffraction data. CTGO is isostructural with titanite, CaTiOSiO_4 . The displacive $P2_1/a$ - $A2/a$ phase transition analogous to titanite has been studied by in situ heating X-ray powder diffraction and transmission electron microscopy. The transition is accompanied by the disappearance of superstructure reflections, $k + l = 2n + 1$, which are replaced by diffuse scattering for $T > T_c$. The diffuse scattering is seen as streaks along \mathbf{b}^* in high-temperature TEM SAD. Lattice parameters as a function of temperature and composition were determined by X-ray powder diffraction between room temperature and a maximum of 1123 K. Strain analysis of CTGO indicates a transition temperature of $T_c = 588 \pm 4$ K and the additional occurrence of an isosymmetric anomaly at $T_i = 800 \pm 25$ K. There is complete solid-solution along the join $\text{CaTiO}(\text{Ge}_x\text{Si}_{1-x})\text{O}_4$. The lattice parameters across the solid solution vary continuously and the structural phase transitions were identified based on the determination of spontaneous strain associated with the transitions. The e_{11} and e_{13} components dominate the strain tensor. All compositions across the solid solution exhibit close to tricritical behavior and nearly constant scalar strain.