In situ powder diffraction study of titanite (CaTiOSiO₄) at high pressure and high temperature

MARTIN KUNZ,[1,]* THILO ARLT,[2,]† AND JANO STOLZ[3]

[1]Labor für Kristallographie, ETH Zentrum, Sonneggstrasse 5, CH-8092 Zürich
[2]Bayerisches Geoinstitut, Universutät Bayreuth, D-95440 Bayreuth*
[3]Labor für mineralogische und chemische Kristallographie, Freiestrasse 3, CH-3012 Bern

ABSTRACT

A set of powder diffraction data was collected for synthetic titanite (CaTiOSiO₄) at simultaneously high pressures and high temperatures in a *P-T* field between 275 K to 650 K and room pressure to 4.9 GPa, respectively. With these data it was possible to relate the *A*2/*a* high-pressure phase at >3.5 GPa (room temperature) to the *A*2/*a* high temperature phase observed above 825 K (room pressure). The slope of the phase transition is –180 K/GPa. The data also allowed the extraction of *P-V-T* equations of state with the following parameters: for $P2_1/a$: $K_{298,0} = 113.4(3)$, $(\partial K_{T,0}/\partial T)_P = -0.061(3)$ GPa/K, $V_{298,0} = 369.04(2)$ Å³, $\alpha_0 = 2.07(5)/10^5$ K. For $A2/a$: $K_{298,0} = 135.2(2)$, $(\partial K_{T,0}/\partial T)_P = -0.073(1)$ GPa/K, $V_{298,0} = 367.12(2)$ Å³, $\alpha_0 = 2.8(2) / 10^5$ K, where K is bulk modulus, V is volume, and α is thermal expansivity. A structural analysis based on Rietveld refinements revealed that the polymerized CaO₇ polyhedra dominantly affect the structural response to changing pressure and temperature. The TiO₆ octahedra rotate almost rigidly in response to the compression of the CaO₇ polyhedra with which they share edges. The SiO₄ tetrahedra show a strong angular distortion with only little change in bond lengths.