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Structural phase transition near 825 K in titanite: Evidence from infrared spectroscopic observations

MING ZHANG,[1] EKHARD SALJE,[1,2] AND ULRICH BISMAYER[3,4]

[1]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.
[2]Interdisciplinary Research Centre in Superconductivity, Madingley Road, Cambridge, CB3 0HE, U.K.
[3]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany
[4]SFB 173, Universität Hannover, D-30060 Hanover, Germany

ABSTRACT

We report the direct experimental observation of a structural anomaly near 825 K in synthetic and natural titanite samples by high-temperature, hard-mode infrared spectroscopy. The anomaly in titanite, $CaTiSiO_5$, is characterized by a break of the temperature dependence of the 562 cm^{-1} Si-O bending mode, the 675 cm^{-1} Ti-O band, and the 900 cm^{-1} Si-O stretching modes, and the rapid decrease of the IR signal at 873 cm^{-1}. The order parameter, as determined from the temperature evolution of the frequencies of the absorption bands in the middle infrared (MIR) region follows a second-order Landau behavior with an order-parameter exponent $\beta = \frac{1}{2}$. At $T > 825$ K, the Ti-O band shows further softening, whereas the Si-O bands at 562 and 900 cm^{-1} show hardening with increasing temperature. In natural samples, the effects of impurities on the high-temperature transition are weak. For pure titanite, the transition temperature, T_c, is about 825 K and increases with increasing impurity concentration.