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Synthesis methods and unit-cell volume of end-member titanite ($CaTiOSiO_4$)

Dimitrios Xirouchakis,[1] Martin Kunz,[1,2] John B. Parise,[1] and Donald H. Lindsley[1]

[1]Center for High Pressure Research and Department of Earth and Space Sciences, State University of New York at Stony Brook, Stony Brook, New York 11794-2100, U.S.A.

[2]European Synchotron Radiation Facility, High Pressure Group, BP 220 Avenue des Martyrs, F-38043 Grenoble Cedex, France

Abstract

Unit-cell parameters of synthetic, end-member titanite ($CaTiOSiO_4$) critically depend on the synthesis conditions, as is shown for studies reported in the literature and for new samples reported here. Our study suggests that phase-pure samples are likely to be obtained only if they are synthesized entirely below the solidus. In contrast, samples synthesized either directly from melt or by annealing of glass tend to have higher unit-cell volumes, contain Si-rich and Ca-Si–rich phase impurities, and may be nonstoichiometric. The observed variations in cell parameters among the samples strongly correlate with synthesis methods and can be explained by vacancies in the Ca or Si site or both. This result is particularly important because the thermodynamic properties currently in use for titanite are based on samples synthesized from melts of stoichiometric composition and thus are suspect even though they have been determined carefully. To establish a reference point for future studies concerned with the chemical and physical properties of this material we report our findings along with a redetermination of the unit-cell parameters [a = 7.062(1), b = 8.716(2), and c = 6.559(1) Å; β = 113.802(9)°, V=369.4(3) Å^3] from powder X-ray data of synthetic, stoichiometric titanite.