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Metamictization and recrystallization of titanite: An infrared spectroscopic study

MING ZHANG,[1,*] EKHARD K.H. SALJE,[1] ULRICH BISMAYER,[2] LEE A. GROAT,[3] AND THOMAS MALCHEREK[4]

[1]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB2 3EQ, U.K.
[2]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany
[3]Department of Earth and Ocean Sciences, University of British Columbia Vancouver, British Columbia, V6T 1Z4, Canada
[4]Institut für Mineralogie, Westfälische Wilhelms-Universität Münster Corrensstr. 24, D-48149 Münster, Germany

ABSTRACT

Radiation damage and the recrystallization of natural titanite ($CaTiSiO_5$) were studied using infrared spectroscopy in the spectral range from 50 to 7500 cm^{-1}. The results show that radiation damage leads to systematic changes in spectral features: decreasing absorption and reflectivity, line broadening, and loss of orientational dependence. Strongly damaged titanite shows hydroxylate bands between 2200 and 3500 cm^{-1}. The band most affected by radiation damage is the Ti-O stretching band near 670 cm^{-1}. It shifts to 710 cm^{-1} in the most damaged samples, possibly indicating the presence of TiO_5 complexes in metamict titanite. Titanite glasses (quenched melts of $CaTiSiO_5$) show spectral features different from those of radiation-damaged titanite, especially in the Ti-O and Si-O stretching regions.

Annealing radiation-damaged titanites at high temperatures results in the recovery of damaged crystalline regions. Recrystallization near 900 K is characterized by an increase in reflectivity, integrated absorbance, and line sharpening. Different infrared bands show recovery at different temperatures. The restoration of the Ti-O stretching band near 670 cm^{-1} and an infrared band near 285 cm^{-1} took place at temperatures of 1200–1400 K. Temperature-induced changes of the OH-absorption bands could be responsible for the previously reported differences in the temperature evolution of infrared spectra of OH species between in situ and quench experiments.