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Thermal annealing of radiation damaged titanite

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ABSTRACT

Radiogenic impurities of 400 to 800 ppm U and Th in titanite, $CaTiSiO_5$, lead to moderate radiation damage ($\approx 1.5 \times 10^{18}$ α-decay events/g) and therefore to partial amorphization ($\approx$30%). Powder X-ray diffraction on such damaged titanite from the Cardiff locality in Canada shows that two modifications of the crystalline material coexist. Both modifications are structurally β phase but differ systematically in their lattice parameters and also in their chemical composition. One modification exhibits strong particle size broadening in X-ray diffraction patterns, whereas it is almost unstrained with respect to fully annealed titanite. The other modification shows large strain broadening and increased specific volume (about 3%) due to a high concentration of defects. The unstrained modification consists of small nucleation centers in the damaged material, and it grows when the sample is annealed. At annealing temperatures above 823 K, this modification dominates rapidly and replaces the strained titanite. The results of Rietveld refinement of the annealed samples and of the time evolution of isothermal annealing studies are discussed. The analysis of volume strain and of structural strain resulting from the peak profiles suggests a temperature-dependent activation energy for the recrystallization process, with $E_A \approx 380$ kJ/mol at $T > 873$ K and $E_A \approx 500$ kJ/mol at temperatures 773 K $< T <$ 873 K.