

## The thermally induced stepwise structural transformation of radiation damaged titanite

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Minerals can become metamict over geological time as a result of structural damage induced by  $\alpha$ -decay of incorporated radiogenic elements. The structural states and the thermally induced recrystallization behaviour of metamict titanite were studied by Raman spectroscopy, synchrotron single-crystal X-ray diffraction, nanoindentation and complementary high-resolution transmission electron microscopy.

Results of the Raman spectroscopic measurements show that radiation-induced periodic faults in the crystalline matrix are related to the disturbance of  $\text{SiO}_4\text{-TiO}_6\text{-SiO}_4\text{-TiO}_6$  rings comprising  $\text{TiO}_6$  octahedra from different chains. The radiation-induced amorphization includes partial change of Ti coordination from octahedral to pyramidal and/or tetrahedral, which leads to a rising Ti-O bond strength. [1]

The elastic material properties of metamict titanite during the thermally induced stepwise recrystallization were measured using nanoindentation. Changes of the elastic modulus (E) and the hardness (H) are related to increasing long-range order and vanishing amorphous interface areas. Metamict titanite shows H and E values close to titanite glass. The hardness of virgin metamict material decreases on annealing until ca. 950 K and increases at higher temperatures, while E increases continuously on annealing. For comparison crystalline titanite from Rauris and titanite glass were also measured. Rauris titanite shows strong anisotropy and H and E values are clearly larger than those of the metamict titanite sample. Synchrotron experiments confirm the recrystallization of the metamict titanite samples when the FWHM values of Bragg reflexions decrease on annealing following a linear trend from RT to 1220 K. [2]

### References

- [1] Beirau et al. Structural anisotropy and annealing-induced nanoscale atomic rearrangements in metamict titanite. *American Mineralogist* (in print 2012).
- [2] Beirau et al. Interfaces in metamict titanite: the macroscopic mechanical properties after stepwise annealing. *Phase Transitions* (in print 2012).