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Elastic softening of metamict titanite $CaTiSiO_5$: Radiation damage and annealing

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Abstract

We have measured the elastic response of radiation-damaged titanite, $CaTiSiO_5$, as a function of thermal annealing. We estimate the bulk modulus of the damaged samples (~24% amorphous) to be 85 GPa, which is much softer than for undamaged crystalline titanite [131.4 GPa; Angel et al. (1999)]. Conversely, the lowest shear modulus of the radiation-damaged material is 52–58 GPa, which is harder that of the undamaged titanite, 46–52 GPa. The bulk and shear moduli of the radiation-damaged materials are close to those of thermal titanite glass, $B_{glass} \approx 75$ GPa and $G_{glass} \approx 47$ GPa, and are much smaller than expected based on other radiation-damaged materials such as zircon ($ZrSiO_4$). Surprisingly, annealing of the damaged titanite in the range $600 < T < 1000$ K leads to additional massive softening of the shear moduli. During annealing the shear modulus of titanite sample 1 softened from 58 to 29 GPa, and sample 2 softened from 52 to 19 GPa. The temperature range for the softening coincides with that found for crystallization of the amorphous regions, as measured previously by diffraction and spectroscopic methods. In contrast to the huge softening of the ultrasonically measured shear modulus, the calorimetrically measured Debye temperature θ_D increases by ~5%, suggesting a small intrinsic hardening of the acoustic shear modes. Additional heating to 1473 K leads, in one titanite sample, to a steep increase of the shear modulus to values much larger than that of the initial, radiation-damaged material. Theoretical models are discussed to rationalize the massive softening due to both radiation damage and subsequent anneal.

Keywords: Titanite, resonant ultrasound spectroscopy, elastic moduli, metamict, Kramers-Kronig, heat capacity