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## Estimation of radiation damage in titanites using Raman spectroscopy

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## ABSTRACT

Recent studies have shown that  $\alpha$ -damage in titanite influences He diffusivity and thus the closure temperature of the (U-Th)/He system in titanite. We compare different methods for measuring the  $\alpha$ -dose in titanite by Raman spectroscopy. Raman spectra of randomly oriented titanite fragments from the Archean Karelian domain in eastern Finland along with some well-studied young titanites and U-Pb standard reference materials were analyzed and related to the concentration of  $\alpha$ -emitting elements (U and Th) that generated damage in the respective grains. Automated curve-fitting was performed by the IFORS software and different curve-fitting protocols were tested and compared.

The Raman bands at 424 and 465 cm<sup>-1</sup> show a good correlation of full-width at half maximum (FWHM) and position with the  $\alpha$ -dose. However, these bands are not always present because titanite is highly anisotropic implying that Raman spectra are sensitive to orientation. The intensity-weighted mean FWHM (iw-FWHM) of all Raman bands of a spectrum proves to be the most robust measure of the  $\alpha$ -dose. A simplified fitting approach considering 15 peaks is sufficient to describe the accumulated  $\alpha$ -dose. For  $\alpha$ -doses below  $5 \times 10^{16} \alpha/g$  the iw-FWHM is independent of  $\alpha$ -dose and ranges from 25 to 50 cm<sup>-1</sup>. Above this value the iw-FWHM increases linearly with increasing  $\alpha$ -dose up to  $3 \times 10^{18} \alpha/g$ . The linear correlation can be described as iw-FWHM[cm<sup>-1</sup>]  $\approx 39(\pm 1.2)$ [cm<sup>-1</sup>]  $+ 3.84(\pm 0.61, -0.26) \times 10^{-17}$ [cm<sup>-1</sup>/( $\alpha/g$ ]]  $\times \alpha$ -dose[ $\alpha/g$ ]. The approach provides a pre-selection method to optimize the range of  $\alpha$ -doses of titanite crystals to be dated by (U-Th)/He thermochronology.

**Keywords:** Titanite, (U-Th)/He, metamictization, radiation damage,  $\alpha$ -dose, Raman spectroscopy, thermochronology