American Mineralogist, Volume 104, pages 857–868, 2019

Estimation of radiation damage in titanites using Raman spectroscopy

Beatrix Muriel Heller[1,*], Nils Keno Lünsdorf[1], István Dunkl[1], Ferenc Molnár[2], and Hilmar von Eynatten[1]

[1]Geoscience Center, Sedimentology and Environmental Geology, University of Göttingen, Goldschmidtstrasse 3, 37077 Göttingen, Germany
[2]Geological Survey of Finland, P.O. Box 96, FI-02151 Espoo, Finland

Abstract

Recent studies have shown that α-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 α-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 α-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^{-1} show a good correlation of full-width at half maximum (FWHM) and position with the α-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 α-dose. A simplified fitting approach considering 15 peaks is sufficient to describe the accumulated α-dose. For α-doses below 5×10^{16}α/g the iw-FWHM is independent of α-dose and ranges from 25 to 50 cm^{-1}. Above this value the iw-FWHM increases linearly with increasing α-dose up to 3×10^{18}α/g. The linear correlation can be described as iw-FWHM[cm^{-1}] ≈ 39(±1.2)[cm^{-1}] + 3.84(+0.61,–0.26) × 10^{-17}[cm^{-1}/(α/g)] × α-dose[α/g]. The approach provides a pre-selection method to optimize the range of α-doses of titanite crystals to be dated by (U-Th)/He thermochronology.

Keywords: Titanite, (U-Th)/He, metamictization, radiation damage, α-dose, Raman spectroscopy, thermochronology