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OH species, U ions, and CO/CO_2 in thermally annealed metamict zircon ($ZrSiO_4$)

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Abstract

Metamict zircon crystals have been thermally annealed between 500 and 1800 K and analyzed using infrared and optical spectroscopy in the spectral region of 1400–7000 cm^{-1}. Recrystallization and dehydroxylation via complex proton/OH diffusion, redistribution, and incorporations of additional hydrogen-related species within the crystal structure of zircon occur at temperatures above 700 K in partially metamict zircon and above 1200 K in heavily amorphized material. Thermally induced changes in O-H stretching spectra are different between $\boldsymbol{E} \parallel \mathbf{c}$ and $\boldsymbol{E} \perp \mathbf{c}$ in weakly metamict zircon. The O-H stretching band near 3342 cm^{-1} (with $\boldsymbol{E} \perp \mathbf{c}$) in an untreated sample shifts to 3277 cm^{-1} at 1200 K, where the frequency of O-H stretching bands with $\boldsymbol{E} \parallel \mathbf{c}$ increases. Conversions of hydrogen-related species were observed and extra OH bands were found at temperatures between 1200 and 1600 K. A dramatic change of OH spectra was recorded between 1600 and 1800 K in partially metamict crystals, resulting in additional absorption features (near 3098 and 2998 cm^{-1} along $\boldsymbol{E} \perp \mathbf{c}$). U^{4+} and U^{5+} related spectra are also affected by high-temperature annealing. For highly metamict zircon, the U^{4+} band near 4830 cm^{-1} shows an increase in intensity above 1200 K. Additional IR bands at 2146 and 2344 cm^{-1} appear in the spectra of metamict zircon annealed at high temperatures. Their frequencies are consistent with stretching vibrations of CO and CO_2.

Keywords: Infrared spectroscopy, zircon, high temperature, hydroxyl species, metamictization, uranium, CO, CO_2, dehydroxylation and recrystallization