

Behavior and origin of hydrogen defects in natural orthopyroxene during high-temperature processes

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ABSTRACT

Spectral features of hydrogen defects in natural mantle minerals derive from physico-chemical conditions of the lithosphere. Although hydrogen defects in synthetic orthopyroxene have been well investigated, their complex spectral features in natural orthopyroxenes are still difficult to decipher. To clarify this issue, it is indispensable to reveal what happens to hydrogen defects during high-temperature processes, thereby fingerprinting the origins of hydrogen defects observed in natural orthopyroxene. Here, we carry out Fourier transform infrared spectroscopic studies on hydrogen defects of three natural orthopyroxenes at elevated temperatures to 1000 °C. Hydrogen defects display reversible disordering at temperatures above 700 °C, which is different from those at ambient conditions. Moreover, hydrogen diffusivities are significantly different between the orthopyroxene samples from different tectonic settings despite their similar iron contents. Even for the same crystal, different hydrogen defects display different diffusion behaviors. Hydrogen defects corresponding to the 3420 cm⁻¹ band have the fastest diffusivity relative to the other hydrogen defects. Most importantly, hydrogen defects can redistribute in the crystal, with new hydrogen defects produced at the cost of the initial hydrogen defects rather than involving a reaction with an external hydrogen source. Combining these findings with previously reported hydrogen defects in natural olivine and clinopyroxene at high temperatures, we propose that: (1) to correctly relate hydrogen defects features to geological processes, it is imperative to understand their behavior and origin, and (2) hydrogen disordering should be taken into account when predicting and extrapolating data on physical properties of the mantle from room-temperature measurements.

Keywords: Hydrogen defect, diffusivity, redistribution, orthopyroxene, high temperature, FTIR