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Effect of chemical environment on the hydrogen-related defect chemistry in wadsleyite

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ABSTRACT

The effect of chemical environment on the hydrogen-related defect chemistry in wadsleyite was investigated using Fourier-transform infrared (FTIR) spectroscopy. Samples were annealed at P = 14–16 GPa and T = 1230–1973 K using Kawai-type multi-anvil apparatus. The effect of oxygen fugacity (f_{O_2}) was investigated using three metal-oxide buffers (Mo-MoO_2, Ni-NiO, and Re-ReO_2). The effect of water fugacity (f_{H_2O}) was studied using two different capsule assemblies ("nominally dry" and "dry" assemblies). A range of total OH concentration ($C_{OH,Total}$) of studied wadsleyeites varies between <50 H/10^6Si (<3 wt ppm H_2O) and 23 000 H/10^6Si (1400 wt ppm H_2O). The observed FTIR spectra were classified into four different classes, i.e., peaks at 3620 ("3620"), 3480 ("3480"), and 3205 cm^{-1} ("3205") and the others (Group O), where the Group O includes peaks at 3270, 3330, and 3580 cm^{-1}. The variation in OH concentration corresponding to each peak was analyzed separately. The OH concentrations correspond to "3620," "3480," and "3205" were found to be highly dependent on both f_{H_2O} and f_{O_2}. Assuming $C_{OH,Group\ O} = 2[(2H)_M^x]$ ($C_{OH,Group\ O}$ is OH concentration of Group O), present data were analyzed by using thermodynamic model for concentration of hydrogen-related defects. Based on analytical results, OH concentration of "3620" and "3480" was found to be reasonably explained by q = 1/2 and r = 1/12 (q and r are f_{H_2O} and f_{O_2} exponents, respectively), whereas that of "3205" was consistent with q = 1/2 and r = –1/12. These results suggest that "3620" and "3480" correspond to $H_M^{\prime}$ whereas "3205" corresponds to $H^{\bullet}$, respectively, under the charge neutrality condition of $[Fe_M^{\prime}] = 2[V_M^{\prime\prime}]$.

Keywords: Wadsleyite, water, hydrogen-related defect, oxygen fugacity, mantle transition zone