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Compressibility and structural stability of two variably hydrated olivine samples ($Fo_{97}Fa_3$) to 34 GPa by X-ray diffraction and Raman spectroscopy

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Abstract

The content and transport of fluid phases such as water into the deep Earth is of great importance not only to correlate seismological models of the planet's interior with mineralogical models, but also for the understanding of the evolution of the solid Earth as well as the Earth's atmosphere. This study reports on the influence of water on the structural and physical properties of olivine, which is known to be the main constituent of the upper mantle.

Two hydrous olivines of composition $Fo_{97}Fa_3$ with water content of 4883 parts per million by weight (ppmw) (SZ0407A) and 8000 ppmw (SZ0407B) were synthesized at 1250 °C and 12 GPa. Single-crystal X-ray diffraction was used to determine unit-cell parameters of SZ0407A and SZ0407B at pressures up to 7.1 GPa at room temperature. Synchrotron powder X-ray diffraction and Raman scattering experiments were performed on sample SZ0407A in a diamond-anvil cell to 34 GPa at room temperature. For both samples, the compressibility is the largest along the **b**-axis and smallest along the **a**-axis. Using the compression (V/V_o) vs. pressure data for sample SZ0407A to 29 GPa, in conjunction with the third-order Birch-Murnaghan equation of state, we calculate the isothermal bulk modulus and its pressure derivative as $K_o = 119.2(12)$ GPa and $K_o' = 6.6(4)$. Single-crystal compression data for sample SZ0407A to 7 GPa give $K_o = 121.5(6)$ GPa and $K_o' = 5.7(2)$; and for sample SZ0407B $K_o = 122.2(12)$ GPa and $K_o' = 6.2(4)$. High-pressure Raman spectra for SZ0407A up to 34 GPa show a continuous shift of all the observed bands to higher frequency with increasing pressure; there is no indication of any first-order phase transition. However, the Raman spectra indicate subtle discontinuous changes around 22 GPa, unobserved in previously reported studies on anhydrous olivines.

Keywords: Hydrous olivine, X-ray diffraction, Raman spectroscopy, hydration mechanism, high pressure