Structural compression of hydrous forsterite, part II

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Forsterite is the magnesium endmember of olivine, $(Mg,Fe)_2SiO_4$, which is the major component of the Earth's mantle. The influence of the incorporation of hydrogen in the forsterite structure on the elastic properties was recently investigated [1]. Infrared spectroscopic results showed that the incorporation of hydrogen can be achieved by the hydrogarnet substitution, $SiO_4 \leftrightarrow O_4H_4$ [2,3], or as OH replacing oxygen in the octahedral magnesium coordination, either of the Mg1 or the Mg2 site, i.e. by protonation of the magnesium octahedral edges [4]. In this project we are interested in the effect of hydrogen incorporation on the structural compression, which is studied by a combination of infrared spectroscopy and single-crystal X-ray diffraction. For a detailed description of the bond compression in wet forsterite, which was described in a previous report, i.e. in part I, a comparison with the bond compression in dry forsterite is necessary by analysing data being collected with the same experimental conditions.

Single crystals of dry Mg_2SiO_4 were grown from the melt by the Institute of Crystal Growth, IKZ in Berlin-Adlershof. Intensity data were collected at 0.7(2), 5.4(2), and 9.3(2) GPa using synchrotron X-ray diffraction at beamline D3 at DORIS III, HASYLAB. The single-crystal with a size of 120 x 100 x 50 μm^3 was loaded together with a ruby ball for pressure determination into an ETH-type diamond anvil cell used for pressure generation. A methanol-ethanol (4:1) mixture was used as a pressure-transmitting medium. Intensity data were collected in fixed-phi mode on a HUBER four-circle diffractometer using a point detector and a wavelength of 0.45 Å. These data were corrected for beam drifts and for absorption by the crystal and the diamond-anvil cell components [5,6,7]. The high-pressure structures were refined with 18 parameters and about 180 non-symmetry equivalent reflections with $I > 4s(I)$ using the program SHELXL-97 [8]. The preliminary refinements converged to residual values of $R1$ ($I > 4s(I)$) = 0.038-0.044 and $wR2$ = 0.101 - 0.117. Structure refinements were carried out with isotropic displacement parameters for all atoms.

A first analysis of the data indicates a difference in the Si–O2 bond distances between wet and dry forsterite, with the Si–O bond length being larger in wet forsterite. In which way this is associated with the H incorporation will be clarified by infrared spectroscopy and the full data analysis.

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