The high pressure behaviour of 10 Å phase: a spectroscopic and diffractometric study up to 42 GPa

P. Comodi (1), F. Cera (1), L. Dubrovinsky (2) and S. Nazzareni (1)

(1) Dipartimento di Scienze della Terra, Università di Perugia, I-06100 Perugia, Italy, (2) Bayerisches Geoinstitut, Universitat Bayreuth, D-95440 Bayreuth, Germany (comodip@unipg.it/ Fax: +39 075 5852603)

10 Å phase, $Mg_3Si_4O_{10}(OH)_2H_2O$, represents an important phase for storage, transport, and release of water in subducting slabs to depths exceeding the stability field of talc. Moreover the occurrence of this phase is not restricted to the ternary MgO-SiO_2-H_2O system, but an aluminous 10 Å phase was found in peridotitic systems. Recently the crystal structure of 10 Å phase was resolved by single-crystal X-ray diffraction and one water molecule was localized in the interlayer of a phlogopite stacking sequence, in the site occupied in mica by potassium. At room condition water molecule disorder with six weak hydrogen bonds pointing toward the upper basal ring and six pointing toward the lower ring was found.

X-ray powder diffraction data and Raman spectra of 10 Å phase were collected under high pressure condition to determine the equation of state and investigated the evolution of hydrogen bonding. The phase remained stable up to 42 GPa at room temperature, indeed in the-quasi hydrostatic experiments with compression and decompression paths, the behaviour was completely reversible. The equation of state of 10 Å phase was obtained by using diamond anvil cell, and collecting powder X-ray diffraction measurements at pressures up to 42 GPa. Fitting with a third-order Birch-Murnghan equation of state the P-V data yields values of $V_0 = 492.9(3)$, $K_0 = 39 (3)$ GPa and K' = 12.5 (8). No significant differences are obtained if the Vinet EoS is used instead. The linear compressibility coefficients of a and b and β parameters are 1.20(16) 10^{-3} GPa $^{-1}$, 1.72(9) 10^{-3} GPa^{-1}, 3.6(7) 10^{-4} GPa^{-1}respectively. For c lattice parameter an exponential decay is used to describe the evolution with P: $c/c_0 = 0\ 0.876\ (2) + 0.116\,e^{-P/6.7(5)}$.

The Raman frequencies of all lattice modes (low frequency region <1200 cm^{-1}) are observed to increase monotonically with increasing pressure and decrease with decompression as well the OH stretching vibration modes of hydroxyl, at 3626 cm^{-1}. On the other hand the stretching bands of the water molecules in 10 Å phase (at 3596.9 and 3672.5 cm^{-1}) were found to shift in opposite directions as a result of the different degree of intermolecular hydrogen-bonding between non-equivalent water H atoms and the oxygen of the tetrahedral layer.

The different evolution of the two OH stretching bands of the water molecules together with the lattice parameters compressibility was interpreted by a rotation of water with pressure that led to an hydrogen bond formation due to the tetrahedral distortion. This distortion was a consequence of the larger compressibility of the octahedral layer with respect to tetrahedral layer, as observed in several phyllosilicates when pressure increase. This mechanism could explain how the pressure should stabilize this phase and give a rationale to the paucity of the natural finding under ambient conditions compared with usually production by synthesis in laboratory under high P/T gradients.