The similarities and differences of the compression mechanism between phase A and chondrodite structure

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The compression mechanisms of phase A, Mg7Si2H6O14 was compared with that of chondrodite, Mg5Si2O8(OH, F)2, using the X-ray diffraction data and FT-IR spectra data of both minerals under high-pressure conditions. Both minerals are kinds of the DHMS minerals, which are considered as the carrier and reservoir of water in the deep Earths interior. Although crystal structure of phase A and chondrodite are based on the hexagonal closest packed anion array, the structure of phase A is slightly different from that of chondrodite, especially in the view of the arrangements of polyhedron. The anisotropy of the compression of both minerals is very similar and the stacking direction is less compressible than another directions in both minerals. In FT-IR spectra observation of chondrodite, the peak of OH-streching vibration near 3380cm-1 was moved to the lower wave number and the peaks around 3580cm-1 moved to the higher one with increasing pressure. It is considered that the lower shift is corresponding to the formation of hydrogen bonding and the higher shift is caused by the repulsion of H-H and/or M-H. The same phenomena would be observed in phase A since the surrounding of the hydrogen positions in phase A structure is very similar to that in chondrodite. The H-H repulsion may be played a significant role in the decomposition and transition of the DHMS minerals.