Strong hydrogen-bond generation in dense hydrous magnesium silicate phase E observed by single-crystal neutron diffraction

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Dense hydrous magnesium silicates (DHMS) are considered as the most major water transporters in cold subducting slabs, which are descending into the deep mantle. Phase E [$Mg_2SiH_4O_6$ –ideal] is one of the most important DHMS phases which is stable at conditions between 13 –17 GPa and 800 –1200 ˚C [1]. Besides its stability at such high temperatures, it stores up to 18 wt.% of water within its crystal structure, which is one of the largest among DHMS phases. Thus phase E is one of the most important carriers and transporter of water in the subducting slabs. The crystal structure of phase E was first investigated by single crystal x-ray diffraction except for its hydrogen position [2]. Its structure has brucite-like layers of MgO6 octahedra which are crosslinked by SiO4 tetrahedra [2]. The hydrogen atoms were expected to be located between these MgO6 octahedra layers like those in brucite, $Mg(OH)_2$. The previous expectation on the structure of phase E was recently confirmed by our powder neutron diffraction study [3]. In contrast, present single-crystal neutron diffraction is conducted to investigate hydrogen bonding geometry in phase E structure, including the Debye-Waller factor of the hydrogen, for which we utilize much higher spatial resolution of the single crystal method. The method has been well confirmed to be very sensitive for investigating such properties of the hydrogen atoms within a series of hydrous minerals [4, 5].
We expect that such information is helpful to understand the reason of stability of phase E at the high-temperature condition. A deuterated phase E single crystal was measured by neutron time-of-flight single-crystal Laue diffraction at Spallation Neutron Source, Oak Ridge National Laboratory. From preliminary structure refinement results, we found that the covalent bond O-D was inclined and displaced from the three-fold axis. Such O-D inclination should occur due to interlayer strong hydrogen-bond generation in the phase E structure. The details of the results will be given in the presentation.

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