Geophysical Research Abstracts
Vol. 19, EGU2017-11722, 2017
EGU General Assembly 2017

First principles investigation of the vibrational properties of hydrous wadsleyite

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Wadsleyite is the primary constituent mineral in the upper part of the Earth's transition zone and this phase can be a significant water reservoir in the Earth. There have been large numbers of reports about the structure, stability, and physical properties of hydrous wadsleyite. The vibrational measurements such as FTIR and Raman are the most commonly used for investigating the OH defects in wadsleyite. There are major and minor doublets of OH stretching bands in hydrous wadsleyite, the former exist around 3300 cm^{-1} with $d\nu/dP \sim$-10 cm^{-1} and the latter around 3600 cm^{-1} with almost no pressure dependence. There is a broad consensus that main absorption band is interpreted as the OH stretching modes existing in the M3 vacancy. On the other hand, the minor OH band is not well constrained so far. Since the stable hydrogen defects are usually less mobile in wadsleyite crystal, the determination of minor and metastable hydrogen defects are more important for investigating the transport properties including the electrical conductivity and the deformation properties. Here I investigated the structural and vibrational properties of hydrous wadsleyite using first principles techniques in order to clarify the minor metastable hydrogen positions under high-pressure.