First principles investigation of the vibrational properties of hydrous wadsleyite and hydrous ringwoodite

*Jun Tsuchiya[1]

1. Geodynamics Research Center, Ehime University

Wadsleyite and ringwoodite are the primary constituent minerals in the Earth's transition zone. Since these minerals are known to be able to retain up to about 3 wt% H_2O in the crystal structures, these phases are known to be the most important water reservoir in the Earth. There have been large numbers of reports about the structure, stability, and physical properties of hydrous wadsleyite and ringwoodite. The vibrational measurements such as FTIR and Raman are the most commonly used for investigating the OH defects in these minerals.
In the case of hydrous wadsleyite, there are major and minor doublets of OH stretching bands, the former exist around 3300 cm^{-1} with dn/dP~-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.
Hydrous ringwoodite, on the other hand, shows very broad OH stretching band around 3200 cm^{-1} at ambient conditions and there is no consensus about the structural explanation of these OH bands nor its high capacity of water storage.
Here I investigated the structural and vibrational properties of hydrous wadsleyite and hydrous ringwoodite using first principles techniques using several different hydrogen defects structures in order to clarify the minor metastable hydrogen positions in wadsleyite and also to shed light on the stability of hydrogen defects in hydrous ringwoodite.

Keywords: hydrous wadsleyite, hydrous ringwoodite, first principles calculation, vibrational property

