

First principles studies of hydrous wadsleyite under high pressure

Jun Tsuchiya[1]; Taku Tsuchiya[2]

[1] GRC, Ehime University; [2] GRC, Ehime Univ

Wadsleyite is thought to be a primary constituent in the upper part of the Earth's transition zone and this phase can be a significant water reservoir in the Earth. We have investigated and clarified the structural properties of hydrous wadsleyite using first principles calculation. The structural changes induced by the protonation of wadsleyite were quite consistent with those obtained by experiments. Using our structural models, we have also calculated elastic properties of this mineral. We demonstrated that the seismic velocities of hydrous wadsleyite decrease almost linearly with increasing the degree of hydration. Using these results, we can discuss the amount of water in hydrous wadsleyite and effects of water on the dynamics in the mantle transition zone.

Research supported by the Ehime Univ Project Fund and in part by JSPS.