The 518th Geodynamics Seminar

H/D partitioning between forsterite, wadsleyite and ringwoodite : ab initio free energy calculation

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Deuterium is the heavy stable isotope of hydrogen. The D/H ratio shows large variation in various astronomical bodies such as protosolar nebula ($2x10^{-5}$), Earth ($1.5x10^{-4}$) , Venus ($1.6x10^{-2}$) and carbonaceous chondrites (~$2x10^{-4}$) (e.g. Saal et al. 2013). Many studies are conducted to determine the D/H ratio in various rocks with different origins of the Earth, since this may be the key to understand the evolutional history and the origin of water of the Earth.

In this study, we determined the free energy of D and H bearing forsterite, wadsleyite and ringwoodite by ab initio calculation in order to determine the equilibrium constants of D and H isotopic exchange reactions between them. First we determined the stable structures of hydrous forsterite, wadsleyite and ringwoodite with Mg vacancy with two hydrogen atoms or Si vacancy with four hydrogen atoms based on density functional theory. Then, the phonon frequencies are calculated based on density functional perturbation theory (Baroni et al. 2001). We used quasi-harmonic approximation to calculate the free energy.

We determined the Gibbs free energy of isotopic exchange reaction between forsterite and wadsleyite, and also between wadsleyite and ringwoodite. In both cases, we found that H is preferably partitioned into higher pressure phases. The average D/H ratio in the current Earth's sea water is similar to those of carbonaceous chondrites. However, by the circulation of water in the deep interior especially including the mantle transition zone, D/H ratio may change in the evolutional history of the Earth.

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