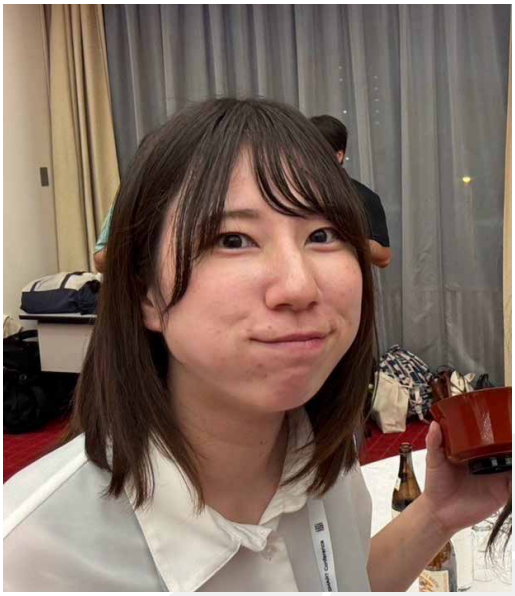
THE GEODYNAMICS SEMINAR

No 638



Ms. Kikuyo Inagaki

Master student (M1)

Geodynamics Research Center

2025.11.7 (Fri.) 16:30 ~

Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.

Ehime Univ.

Keywords

1. Stishovite
2. Structural model
3. Infrared spectra

Ab initio structural models and infrared spectra of hydrous stishovite

Understanding the chemical composition and dynamics of the Earth's interior is important for revealing how our planet formed and evolved. Hydrogen, the most abundant element in the universe, reacts easily with minerals and significantly modifies their physical properties. In the mantle, water is mainly stored in nominally anhydrous minerals (NAMs), which contain small amounts of hydrogen incorporated into their crystal structures. Hydrogen in these minerals can influence the melting temperature, viscosity, and seismic wave velocity of the mantle. Therefore, understanding the behavior of hydrogen in NAMs is essential for studying the deep Earth.

Stishovite, a high-pressure polymorph of SiO_2, is one of the major NAMs stable in the shallow lower mantle. It transforms from a tetragonal to an orthorhombic structure around 56 GPa, which may explain the seismic velocity reduction observed in subducted slabs. In this study, we performed first-principles calculations to investigate how hydrogen incorporation affects the crystal structure and vibrational properties of hydrous stishovite.

The results indicate that the configuration with hydrogen occupying the equatorial oxygen site is energetically more favorable than that with hydrogen at the apical oxygen site. One of the calculated infrared absorption peaks shows good agreement with experimental observations, supporting the reliability of our structural model. Other peaks in the experimental data do not match, and the most stable model remains unclear. Therefore, further verification is required for other potential hydrogen bonding sites. Subsequently, molecular dynamics simulations will be used to investigate hydrogen behavior at high temperatures.

Contact: Steeve Gréaux, PhD. (e-mail: greaux.steeve_georgi.me@ehime-u.ac.jp)