

In-situ IR high pressure experiment on hydrous forsterite

*Moe Sakurai¹, Noriyoshi Tsujino¹, Shigehiko Tateno¹, Toshihiro Suzuki², Takashi Yoshino¹, Katsuyuki KAWAMURA³, Eiichi Takahashi²

1. Institute for Planetary Materials, Okayama University, 2. Dept of Earth and Planetary Sciences, School of Science, Tokyo Tech., 3. Graduate School of Environmental and Life Science, Okayama Univ.

The uppermost mantle is mainly composed of olivine and pyroxene. These minerals can contain small amount of water from a few wt.ppm to a few 1000 wt.ppm (e.g. Mosenfelder et al., 2006). Presence of even such small amount of water can change some physical properties (e.g. rheological properties; Hirschmann and Kohlstedt, 2012; electrical conductivity; Zhang et al., 2012, Schlechter et al., 2012). Many water incorporation mechanisms of olivine were suggested by experimental studies (e.g. Bai and Kohlstedt 1993, Berry et al., 2005) and theoretical studies (e.g. Umemoto et al., 2011) and were controversial. On the other hand, the mechanism by which water influences physical properties is not well understood. In order to study the role of water, the positions of hydrogen ions in crystal sites should be investigated at first.

FT-IR spectra are sensitive to the strength of OH covalent bond. A clue to reveal the positions can be obtained by using the FT-IR method. However, the experimental FT-IR spectra were obtained from quench polycrystalline recovered samples. Since hydrogen atom is very light, therefore, quenched recovered sample may not hold positions of original hydrogen atoms. In fact, Faust and Williams (1996) reported behavior of hydroxyl bonding of phase B at high pressure using in-situ IR spectra. Phase B, which is known as hydrous phase in the subduction zone, have the two bands of 3345 and 3404 cm^{-1} in IR spectra associated with the two hydroxyl sites. They reported the pressure dependence of the peaks. In their experiment, opposite peak shifts of the two bands of 3345 and 3404 cm^{-1} were observed and it is demonstrated that hydrogen position in phase B changes with pressure.

In this study, we performed in-situ IR observations at high pressures for forsterite (Fo) single crystals using DAC. At first I developed in-situ IR observation method at high pressure for low water content of nominally anhydrous minerals in the upper mantle. Using this technique, polarized IR spectra parallel to crystal axis of synthetic hydrous Fo were obtained under high pressure for the first time. First principle calculation (DFT calculation) for hydrogen position in Fo was carried out at various pressures. Hydrogen position in Fo was estimated based on the comparison of the vibrational frequencies measured by the FT-IR methods and simulation by the first-principles methods. The band shift observed in experiments under high pressure could be explained by the hydrogen position change in Si Site with pressure calculated by DFT.

Keywords: FT-IR, DFT calculations, nominally anhydrous minerals, in-situ IR observation, upper mantle