

TEM observation in the samples of high-pressure in-situ IR experiments

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Water incorporation mechanisms in nominally anhydrous minerals in the Earth's mantle are important to understand effect of water on some physical properties (e.g. rheological properties; Hirschmann and Kohlstedt, 2012; electrical conductivity; Zhang et al., 2012, Schlechter et al., 2012). Olivine is the most consistent mineral in the upper mantle can contain small amount of water from a few wt.ppm to a few 1000 wt.ppm (e.g. Mosenfelder et al., 2006). 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. Then, we conducted to in-situ IR observation at high pressures for synthetic hydrous forsterite single crystals using DAC and KBr pressure medium. Band shift of several OH stretching bands to high wavenumber or low wavenumber with pressure were observed. In order to understand band shifts of OH stretching bands, 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. We conclude that 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. However, after in-situ IR observations, recovered sample of single crystal forsterite has some cracks. The possibility that observed band shifts occurred by deviatoric stress through KBr pressure medium still remains. Therefore, we conducted TEM observation to estimate deviatoric stress of single crystal forsterite during in-situ IR observation at high pressure. The dislocations in hydrous forsterite, whose direction is perpendicular to (010) plane, were observed. Dislocations in (010) planes are dominant slip systems of deformation involving dislocations. Amount of these dislocations were not significant large. We will discuss deviatoric stress during in-situ IR observations and effect of deviatoric stress on band shift of OH stretching bands based on dislocation density.

Keywords: FT-IR, Nominally Anhydrous Minerals, In-situ IR observation, TEM