Water Incorporation in Wadsleyite and its Effect on the Depth of the 410 km Discontinuity

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Wadsleyite (wads), the high pressure polymorph of olivine (ol), belongs to the group of NAMs, nominally anhydrous minerals. Several authors showed that it may incorporate up to 3.3 wt. % water as hydroxyl in its structure. The phase transition from ol to wads is considered to be responsible for the 410-km discontinuity. Controversial results exist about the influence of water on the depth of the ol-wads phase boundary (Chen et al., 2002; Frost & Dolejs, 2007). In order to understand the incorporation of hydrogen in Mg-end member wads quali - and quantitatively and its influence on the depth of the 410-km discontinuity experiments were performed at 1200 °C in the pressure range 11.8 – 13.8 GPa as dry and hydrous runs using a rotating multi-anvil press. The syntheses products were investigated by electron microprobe (EMPA), FTIR-spectroscopy in the OH stretching region at ambient conditions as well as insitu in a diamond anvil cell (DAC), single-crystal X-ray diffraction (SC-XRD) and transmission electron microscopy (TEM). The water content of wads synthesized at 13.8 GPa and 1200 °C was determined by secondary ion mass spectrometry (SIMS) and confirmed by Raman spectroscopy. Preliminary results yield to 8000 1000 wt ppm water in wads. We calculated a molar absorption coefficient, ε for water in wads as 64000 8000 (l mol $_{\rm H2O} \rm cm^{-2}$). This is the first direct calibration for water quantification in wads, showing again, as in case of ol, that the frequently used Paterson (1984) method underestimates the water concentration in NAMs. Jacobsen et al. (2005) suggested two different O1-O4 edges to be the best possible hydrogen sites for the most intense absorbance band around 3340 cm^{-1} but he could not distinguish between them. On the base of the EMPA, SC-XRD- and TEM-analyses as well as our polarized and mainly based on our in-situ high-pressure FTIR spectra we suggest that the OH dipole is oriented along the O1...O4 direction (3.09 Å), i.e. along an unshared edge of a vacant M3 site. According to our experiments at 1200 °C the phase boundary between ol and wads is shifted of about 0.5 GPa to lower pressures, which is half of the value observed by Frost & Dolejs (2007). They did not quantify their water content and we assume that the discrepancy between their and our results can be explained by different water contents of the coexisting phases in rotating versus static experiments. We also performed experiments by adding iron to the system and will present the first results related to the boundary shift and the water partitioning between ol and wads in the system (Mg,Fe)₂SiO₄. References

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Abs. No. **216** Meeting: **DMG 2008** submitted by: **Deon, Fiorenza** email: **fdeon@gfz-potsdam.de** date: **0000-00-00** Req. presentation: **Vortrag** Req. session: **S04**