Quenchable water-rich aluminous post-stishovite: implications for water and seismic scatterers in the lower mantle

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Abstract

Seismic scatterers

ULVZs by seifertite formation?

Geochemistry

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1. Introduction

The stishovite structure (tetragonal, $P4_2/mnm$, no. 136) undergoes a weak first-order transition (Andrault et al., 1998; Hemley et al., 2000) with second-order characteristics of Landau/ferroelastic type (Tsuchida and Yagi, 1989; Carpenter et al., 2000) to the $CaCl_2$-type structure (orthorhombic, Pnnm, no. 58). This transition occurs at pressures of ∼50 GPa at room temperature (Kingma et al., 1995; Andrault et al., 1998), increasing with temperature to ∼70 GPa at 2200 K (Hirose et al., 2005; Nomura et al., 2010). A somewhat higher dT/dP was observed by Ono et al. (2002). The nature of this transition means that the shear modulus C_{11} - C_{12} decreases with increasing pressure and vanishes at the transition pressure, as observed in spectroscopic and high pressure diffraction

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studies (Kingma et al., 1995; Shieh et al., 2002). The stishovite-post-stishovite transition is therefore of interest to seismologists, as it should produce zones of low shear wave velocity which act as scatterers in the deep mantle.

Deviatoric stresses in the diamond anvil cell can cause large variations in the pressure of the stishovite to post-stishovite transition. Nonhydrostaticity greatly decreases the transition pressure from 60 GPa (Andrault et al., 2003; Hemley et al., 2000) to 40 GPa (Kingma et al., 1996; Singh et al., 2012). Molecular and lattice dynamic studies suggest that only 1.5–2.5 GPa differential stress is required to cause this decrease in pressure (Dubrovinsky and Belonoshko, 1996).

Aluminium has a profound effect on the stability of the post-stishovite phase. Al_2O_3 can be incorporated into stishovite by the substitution of Si by Al with the formation of oxygen vacancies (Smyth et al., 1995; Hirose et al., 2005; Bromiley et al., 2006; Lakshtanov et al., 2007a):

$$2Si_{Si}^{x} + O_{O}^{x} + Al_2O_3 \rightarrow 2Al_{Si}^{/} + V_{\ddot{O}} + 2SiO_2 \quad (1)$$

An alternative mechanism, where charge balance is accomplished by Al occupying the large interstitial sites is probably minor Smyth et al. (1995):

$$3Si_{Si}^{x} + 2Al_2O_3 \rightarrow 3Al_{Si}^{/} + Al_{i}^{\cdot\cdot\cdot} + 3SiO_2 \quad (2)$$

It has been argued that the addition of 4 wt% Al_2O_3 in the absence of any other components causes the transition to shift from 50 to 23 GPa at room temperature by inducing a 'chemical pressure' (Bolfan-Casanova et al., 2009). In stishovite, there is one octahedral cation position (Wyckoff notation 2a) located at the origin and the body center of the tetragonal cell. One oxygen at position 4f creates a moderately distorted octahedron with point symmetry mmm. The addition of Al *decreases* distortion of this octahedron (Smyth et al., 1995). The addition of Al should therefore have little effect on the stishovite-post-stishovite transition (Panero, 2006). The results of Bolfan-Casanova et al. (2009) are therefore unexpected; it seems possible that another component (such as H_2O) or deviatoric stress acted to stabilise the $CaCl_2$ structure.

It has also been suggested that the coupled substitution of Al and H may have a significant effect on the transition pressure. Lakshtanov et al. (2007b) have shown that the addition of 6 wt% Al_2O_3 and 0.24 wt% H_2O reduces the transition pressure to 24 GPa at room temperature. The substitution mechanism in this case is probably

$$2Si_{Si}^{x} + Al_2O_3 + H_2O \rightarrow 2Al_{Si}^{/} + 2H_i^{\cdot} + 2SiO_2 \quad (3)$$

Given that high pressure δ-AlOOH is isostructural with the post-stishovite phase above ca. 19 GPa (Sano-Furukawa et al., 2008; Kuribayashi et al., 2014), after transforming from the $P2_1nm$ structure (no. 31) (Suzuki et al., 2000; Komatsu et al., 2006; Vanpeteghem et al., 2007), it seems sensible to suggest that addition of an AlOOH component lowers the transition pressure. Ab initio calculations support this suggestion (Umemoto et al., 2015). The equilibrium transition for 6.25 mol% AlOOH is at ca. 15 GPa at room temperature, implying an even more marked reduction than observed in the experimental data (Lakshtanov et al., 2007b). This could be due to inaccuracies in the ab-initio data, or metastable preservation of the tetragonal phase in the experiments. Umemoto et al. (2015) also suggest that the larger number of hydrogen sites stabilises the tetragonal structure at high temperatures, changing the slope of the transition. The tetragonal $\rightarrow$ orthorhombic transition in their simulations is associated with splitting of the hydrogen sites on the equatorial oxygens into two groups, one occupied and the other unoccupied. Additionally, the redistribution of hydrogens among equatorial oxygens in the tetragonal $\rightarrow$ orthorhombic transition implies that it is now first order and no longer ferroelastic. Anelasticity by hydrogen hopping seems a plausible alternative to reduce seismic body wave speeds.

Despite this, H_2O contents in tetragonal stishovite measured using the FTIR calibration of Pawley et al. (1993) are less than 20% of that expected from an AlOOH component (Panero et al., 2003; Bromiley et al., 2006; Litasov et al., 2007) and in MORB compositions (Chung and Kagi, 2002).

This study was designed to investigate water solubility in Al-rich stishovite by synthesising crystals at relatively high temperature (Ono, 1999). In doing so, we created and quenched an Al-H rich post-stishovite phase.

1.1. Hysteresis vs. stabilisation

(Umemoto et al., 2015)

1.2. Mechanism of shear wave velocity reduction

Ferroelasticity (Carpenter et al., 2000) Snoek relaxation (anelasticity via H mobility) (Snoek, 1941; Nowick and Berry, 1972; McKnight et al., 2007).

1.3. Mechanisms of Al-, H incorporation

We found that hydrogen was most stable when bonded to the apical oxygen of the Al-octahedron, with the hydroxyl bond along ⟨110⟩ and co-planar with Al (Panero and Stixrude, 2004).

The relatively short O-O distance and correspondingly long O-H distance in the stishovite-AlOOH solid solution would lead one to expect a low OH stretching frequency compared to other nominally anhydrous minerals, consistent with the value of 3111 cm^{-1} observed by Pawley et al. (1993).

Symmetric bonding (Panero and Stixrude, 2004)

1.4. Water concentrations in stishovite

Pawley et al. (1993) calibration Panero et al. (2003) Bromiley et al. (2006), Litasov et al. (2007), MORB Chung and Kagi (2002),

1.5. Elastic properties

Andrault et al. (2003) Lakshtanov et al. (2005) Ono et al. (2002) Sano-Furukawa et al. (2009)

1.6. Phase relations in the lower mantle

Irifune and Ringwood (1993) Wood (2000) Hirose (2002) Walter et al. (2015) Litasov and Ohtani (2005)

1.7. Datasets and modelling

Holland and Powell (2011) Stixrude and Lithgow-Bertelloni (2011) Cottaar et al. (2014)

1.7.1. Elastic properties AlOOH

Suzuki (2009) (Sano-Furukawa et al., 2008) Vanpeteghem et al. (2002) Tsuchiya and Tsuchiya (2009) Li et al. (2006)

2. The solid solution (MgSi, $Fe^{2+}Si$, Fe_2^{3+}, Al_2)O_4H_2

2.1. Endmembers

2.1.1. SiO_2

2.1.2. δ-AlOOH

2.1.3. δ-FeOOH

Pnma (no.62 α) to $P2_1nm$ (no. 31, ε) (Gleason et al., 2008) to Pnnm (no. 58, high spin) to Pnnm (no. 58, low spin) (Gleason et al., 2013)

2.1.4. "Phase H"

The addition of an $MgSiO_4H_2$ component also stabilises the Pnnm structure in stishovite (Komatsu et al., 2011). A previous candidate space group (Pnn2; no. 34 Kudoh et al., 2004) is now thought to be unlikely.

Stability (Ohtani et al., 2014) Ab initio P2/m (no. 10) (Tsuchiya, 2013) Pnnm (no. 58) (Bindi et al., 2014) $P2_1nm$ (no. 31) (Nishi et al., 2014)

Kudoh et al. (2004) suggested a hypothetical high pressure form of $Mg(OH)_2$ also in the space group Pnnm from Mg incorporation. Importance of the AlOOH - phase H solid solution Ohira et al. (2014)

3. Other phases

Ohtani (2015)

3.1. Water in seifertite

Post-stishovite undergoes a phase transition to the mineral seifertite with the scrutinyite (α-PbO_2) structure (orthorhombic, Pbcn, no. 60 or Pb2n) at about 120-140 GPa and 2000-2500 K (Murakami et al., 2003; Grocholski et al., 2013). The addition of aluminium under dry conditions may stabilise seifertite to 110 GPa at 2000 K (Hirose et al., 2005), although this remains controversial (Grocholski et al., 2013). The effect of hydrogen on the structure is currently unknown. As there are no hydrous phases known with the seifertite structure, the addition of water probably destabilises seifertite relative to post-stishovite. This supposition is supported by the lack of water in the isostructural TiO_2 (II) phase, which contains negligible water (Bromiley et al., 2004).

δ-AlOOH remains stable throughout the lower mantle, and probably transforms to a cubic structure ($Pa\bar{3}$) at core pressures (Tsuchiya and Tsuchiya, 2011).

3.2. δ-Al(OH)$_3$

$P2_12_12_1$ (no. 19) to Pnma (no. 62) at ∼67 GPa Matsui et al. (2011). Xue and Kanzaki (2007)

3.3. Ca-perovskite

Tetragonal (probably P4/mmm, no. 123) (Shim et al., 2002) → Cubic (Pm3m) for low Al contents. For pure $CaSiO_3$, transition occurs at ca. 580 K at 50 GPa (Kurashina et al., 2004; Komabayashi et al., 2007)

Orthorhombic (Pbnm) → Cubic (Pm3m) for Al-rich $CaSiO_3$ (Kurashina et al., 2004). At 5.9 wt%, transition occurs at ca. 1840 K at 50 GPa (Kurashina et al., 2004).

In a pyrolitic mantle composition, the $CaSiO_3$ perovskite contains 1.0–2.3 wt.% Al_2O_3 at upper mantle pressures and somewhat less (0.7–1.6 wt.%) at lower mantle pressures (Kesson et al., 1998; Wood, 2000; Hirose, 2002)

In a MORB composition, 2.0–4.8 wt.% and 1.2–4.5 wt.% Al_2O_3 are included in $CaSiO_3$-rich perovskite in garnetite and perovskitite lithologies, respectively (Kesson et al., 1994; Irifune and Ringwood, 1993; Hirose and Fei, 2002).

3.4. Reaction with metal

(Terasaki et al., 2012)

4. Lower mantle scatterers

Deuss et al. (2013) Kaneshima and Helffrich (1998, 2003) Niu et al. (2003) Krüger et al. (2001) Kaneshima (2009) Bina et al. (2010) Kaneshima et al. (2010) Bentham and Rost (2014) Asahara et al. (2013) Mookherjee (2011)

5. Experimental and analytical techniques

6. Chemical composition

Figure 1: Single crystal XRD spectra of post-stishovite

7. Conclusions

References

Andrault, D., Angel, R.J., Mosenfelder, J.L., Le Bihan, T., 2003. Equation of state of stishovite to lower mantle pressures. American Mineralogist 88, 301–307.

Andrault, D., Angel, R.J., Mosenfelder, J.L., Le Bihan, T., 2003. Equation of state of stishovite to lower mantle pressures. American Mineralogist 88, 301–307.

Andrault, D., Fiquet, G., Guyot, F., Hanfland, M., 1998. Pressure-Induced Landau-Type Transition in Stishovite. Science 282, 720.

Asahara, Y., Hirose, K., Ohishi, Y., Hirao, N., Ozawa, H., Murakami, M., 2013. Acoustic velocity measurements for stishovite across the post-stishovite phase transition under deviatoric stress: Implications for the seismic features of subducting slabs in the mid-mantle. American Mineralogist 98, 2053–2062.

Bentham, H.L.M., Rost, S., 2014. Scattering beneath Western Pacific subduction zones: evidence for oceanic crust in the mid-mantle. Geophysical Journal International 197, 1627–1641.

Bina, C.R., Suetsugu, D., Bina, C., Inoue, T., Wiens, D., Jellinek, M., 2010. Scale limits of free-silica seismic scatterers in the lower mantle. Physics of the Earth and Planetary Interiors 183, 110–114.

Bindi, L., Nishi, M., Tsuchiya, J., Irifune, T., 2014. Crystal chemistry of dense hydrous magnesium silicates: The structure of phase H, $MgSiH_2O_4$, synthesized at 45 GPa and 1000 °C. American Mineralogist 99, 1802–1805.

Bolfan-Casanova, N., Andrault, D., Amiguet, E., Guignot, N., 2009. Equation of state and post-stishovite transformation of Al-bearing silica up to 100 GPa and 3000 K. Physics of the Earth and Planetary Interiors 174, 70–77.

Bromiley, G., Hilaret, N., McCammon, C., 2004. Solubility of hydrogen and ferric iron in rutile and TiO2 (II): Implications for phase assemblages during

ultrahigh-pressure metamorphism and for the stability of silica polymorphs in the lower mantle. Geophysical Research Letters 31.

Bromiley, G.D., Bromiley, F.A., Bromiley, D.W., 2006. On the mechanisms for H and Al incorporation in stishovite. Physics and Chemistry of Minerals 33, 613–621.

Carpenter, M.A., Hemley, R.J., Mao, H.K., 2000. High-pressure elasticity of stishovite and the $P4_2/mnm \rightarrow Pnnm$ phase transition. Journal of Geophysical Research 105, 10807.

Chung, J.I., Kagi, H., 2002. High concentration of water in stishovite in the MORB system. Geophysical Research Letters 29, 16–1–16–4. 2020.

Cottaar, S., Heister, T., Rose, I., Unterborn, C., 2014. BurnMan: A lower mantle mineral physics toolkit. Geochemistry, Geophysics, Geosystems 15, 1164–1179.

Deuss, A., Andrews, J., Day, E., 2013. Seismic Observations of Mantle Discontinuities and Their Mineralogical and Dynamical Interpretation. pp. 295–323.

Dubrovinsky, L.S., Belonoshko, A.B., 1996. Pressure-induced phase transition and structural changes under deviatoric stress of stishovite to $CaCl_2$-like structure. Geochimica et Cosmochimica Acta 60, 3657–3663.

Gleason, A., Jeanloz, R., Kunz, M., 2008. Pressure-temperature stability studies of feooh using x-ray diffraction. American Mineralogist 93, 1882–1885.

Gleason, A., Quiroga, C., Suzuki, A., Pentcheva, R., Mao, W., 2013. Symmetrization driven spin transition in ε-FeOOH at high pressure. Earth and Planetary Science Letters 379, 49 – 55.

Grocholski, B., Shim, S.H., Prakapenka, V.B., 2013. Stability, metastability, and elastic properties of a dense silica polymorph, seifertite. Journal of Geophysical Research: Solid Earth 118, 4745–4757.

Hemley, R.J., Shu, J., Carpenter, M.A., Hu, J., Mao, H.K., Kingma, K.J., 2000. Strain/order parameter coupling in the ferroelastic transition in dense SiO_2. Solid State Communications 114, 527–532.

Hirose, K., 2002. Phase transitions in pyrolitic mantle around 670-km depth: Implications for upwelling of plumes from the lower mantle. Journal of Geophysical Research (Solid Earth) 107, 2078.

Hirose, K., Fei, Y., 2002. Subsolidus and melting phase relations of basaltic composition in the uppermost lower mantle. Geochimica et Cosmochimica Acta 66, 2099–2108.

Hirose, K., Takafuji, N., Sata, N., Ohishi, Y., 2005. Phase transition and density of subducted MORB crust in the lower mantle. Earth and Planetary Science Letters 237, 239–251.

Holland, T.J.B., Powell, R., 2011. An improved and extended internally consistent thermodynamic dataset for phases of petrological interest, involving a new equation of state for solids. Journal of Metamorphic Geology 29, 333–383.

Irifune, T., Ringwood, A.E., 1993. Phase transformations in subducted oceanic crust and buoyancy relationships at depths of 600-800 km in the mantle. Earth and Planetary Science Letters 117, 101–110.

Kaneshima, S., 2009. Seismic scatterers at the shallowest lower mantle beneath subducted slabs. Earth and Planetary Science Letters 286, 304–315.

Kaneshima, S., Helffrich, G., 1998. Detection of lower mantle scatterers northeast of the Marianna subduction zone using short-period array data. Journal of Geophysical Research 103, 4825–4838.

Kaneshima, S., Helffrich, G., 2003. Subparallel dipping heterogeneities in the mid-lower mantle. Journal of Geophysical Research (Solid Earth) 108, 2272.

Kaneshima, S., Helffrich, G., Suetsugu, D., Bina, C., Inoue, T., Wiens, D., Jellinek, M., 2010. Small scale heterogeneity in the mid-lower mantle beneath

the circum-Pacific area. Physics of the Earth and Planetary Interiors 183, 91–103.

Kesson, S.E., Fitz Gerald, J.D., Shelley, J.M., 1998. Mineralogy and dynamics of a pyrolite lower mantle. Nature 393, 252–255.

Kesson, S.E., Fitz Gerald, J.D., Shelley, J.M.G., 1994. Mineral chemistry and density of subducted basaltic crust at lower-mantle pressures. Nature 372, 767–769.

Kingma, K., Mao, H.K., Hemley, R., 1996. Synchrotron X-ray diffraction of SiO_2 to multimegabar pressures. High Pressure Research 14, 363–374.

Kingma, K.J., Cohen, R.E., Hemley, R.J., Mao, H.K., 1995. Transformation of stishovite to a denser phase at lower-mantle pressures. Nature 374, 243–245.

Komabayashi, T., Hirose, K., Sata, N., Ohishi, Y., Dubrovinsky, L.S., 2007. Phase transition in CaSiO3 perovskite. Earth and Planetary Science Letters 260, 564 – 569.

Komatsu, K., Kuribayashi, T., Sano, A., Ohtani, E., Kudoh, Y., 2006. Redetermination of the high-pressure modification of AlOOH from single-crystal synchrotron data. Acta Crystallographica Section E 62, 216–218.

Komatsu, K., Sano-Furukawa, A., Kagi, H., 2011. Effects of Mg and Si ions on the symmetry of δ-AlOOH. Physics and Chemistry of Minerals 38, 727–733.

Krüger, F., Baumann, M., Scherbaum, F., Weber, M., 2001. Mid mantle scatterers near the Mariana Slab detected with a double array method. Geophysical Research Letters 28, 667–670.

Kudoh, Y., Kuribayashi, T., Suzuki, A., Ohtani, E., Kamada, T., 2004. Space group and hydrogen sites of δ-AlOOH and implications for a hypothetical high-pressure form of $Mg(OH)_2$. Physics and Chemistry of Minerals 31, 360–364.

Kurashina, T., Hirose, K., Ono, S., Sata, N., Ohishi, Y., 2004. Phase transition in Al-bearing $CaSiO_3$ perovskite: implications for seismic discontinuities in the lower mantle. Physics of the Earth and Planetary Interiors 145, 67–74.

Kuribayashi, T., Sano-Furukawa, A., Nagase, T., 2014. Observation of pressure-induced phase transition of δ-AlOOH by using single-crystal synchrotron X-ray diffraction method. Physics and Chemistry of Minerals 41, 303–312.

Lakshtanov, D.L., Litasov, K.D., Sinogeikin, S.V., Hellwig, H., Li, J., Ohtani, E., Bass, J.D., 2007a. Effect of al3+ and h+ on the elastic properties of stishovite. American Mineralogist 92, 1026–1030.

Lakshtanov, D.L., Sinogeikin, S.V., Litasov, K.D., Prakapenka, V.B., Hellwig, H., Wang, J., Sanches-Valle, C., Perrillat, J.P., Chen, B., Somayazulu, M., Li, J., Ohtani, E., Bass, J.D., 2007b. The post-stishovite phase transition in hydrous alumina-bearing SiO_2 in the lower mantle of the Earth. Proceedings of the National Academy of Sciences 104, 13588–13590.

Lakshtanov, D.L., Vanpeteghem, C.B., Jackson, J.M., Bass, J.D., Shen, G., Prakapenka, V.B., Litasov, K., Ohtani, E., 2005. The equation of state of Al,H-bearing SiO_2 stishovite to 58 GPa. Physics and Chemistry of Minerals 32, 466–470.

Li, S., Ahuja, R., Johansson, B., 2006. The elastic and optical properties of the high-pressure hydrous phase δ-AlOOH. Solid State Communications 137, 101–106.

Litasov, K.D., Kagi, H., Shatskiy, A., Ohtani, E., Lakshtanov, D.L., Bass, J.D., Ito, E., 2007. High hydrogen solubility in Al-rich stishovite and water transport in the lower mantle. Earth and Planetary Science Letters 262, 620 – 634.

Litasov, K.D., Ohtani, E., 2005. Phase relations in hydrous MORB at 18-28 GPa: implications for heterogeneity of the lower mantle. Physics of the Earth and Planetary Interiors 150, 239–263.

Matsui, M., Komatsu, K., Ikeda, E., Sano-Furukawa, A., Gotou, H., Yagi, T., 2011. The crystal structure of δ-Al(OH)$_3$: Neutron diffraction measurements and ab initio calculations. American Mineralogist 96, 854–859.

McKnight, R.E., Carpenter, M.A., Darling, T.W., Buckley, A., Taylor, P.A., 2007. Acoustic dissipation associated with phase transitions in lawsonite, caal2si2o7(oh)2h2o. American Mineralogist 92, 1665–1672.

Mookherjee, M., 2011. Mid-mantle anisotropy: Elasticity of aluminous phases in subducted MORB. Geophysical Research Letters 38, n/a–n/a. L14302.

Murakami, M., Hirose, K., Ono, S., Ohishi, Y., 2003. Stability of $CaCl_2$-type and α-PbO_2-type SiO_2 at high pressure and temperature determined by in-situ X-ray measurements. Geophysical Research Letters 30. 1207.

Nishi, M., Irifune, T., Tsuchiya, J., Tange, Y., Nishihara, Y., Fujino, K., Higo, Y., 2014. Stability of hydrous silicate at high pressures and water transport to the deep lower mantle. Nature Geoscience 7, 224–227.

Niu, F., Kawakatsu, H., Fukao, Y., 2003. Seismic evidence for a chemical heterogeneity in the midmantle: A strong and slightly dipping seismic reflector beneath the Mariana subduction zone. Journal of Geophysical Research (Solid Earth) 108, 2419.

Nomura, R., Hirose, K., Sata, N., Ohishi, Y., Suetsugu, D., Bina, C., Inoue, T., Wiens, D., Jellinek, M., 2010. Precise determination of post-stishovite phase transition boundary and implications for seismic heterogeneities in the mid-lower mantle. Physics of the Earth and Planetary Interiors 183, 104–109.

Nowick, A., Berry, D., 1972. Anelastic relaxation in crystalline solids, acad. Press, New York .

Ohira, I., Ohtani, E., Sakai, T., Miyahara, M., Hirao, N., Ohishi, Y., Nishijima, M., 2014. Stability of a hydrous δ-phase, AlOOH-$MgSiO_2(OH)_2$, and a mechanism for water transport into the base of lower mantle. Earth and Planetary Science Letters 401, 12–17.

Ohtani, E., 2015. Hydrous minerals and the storage of water in the deep mantle. Chemical Geology , –.

Ohtani, E., Amaike, Y., Kamada, S., Sakamaki, T., Hirao, N., 2014. Stability of hydrous phase H $MgSiO_4H_2$ under lower mantle conditions. Geophysical Research Letters 41, 8283–8287. 2014GL061690.

Ono, S., 1999. High temperature stability limit of phase egg, $AlSiO_3(OH)$. Contributions to Mineralogy and Petrology 137, 83–89.

Ono, S., Hirose, K., Murakami, M., Isshiki, M., 2002. Post-stishovite phase boundary in SiO_2 determined by in situ X-ray observations. Earth and Planetary Science Letters 197, 187–192.

Ono, S., Suto, T., Hirose, K., Kuwayama, Y., Komabayashi, T., Kikegawa, T., 2002. Equation of state of Al-bearing stishovite to 40 GPa at 300 K. American Mineralogist 87, 1486–1489.

Panero, W.R., 2006. Aluminum incorporation in stishovite. Geophysical Research Letters 33, n/a–n/a. L20317.

Panero, W.R., Benedetti, L.R., Jeanloz, R., 2003. Transport of water into the lower mantle: Role of stishovite. Journal of Geophysical Research (Solid Earth) 108, 2039.

Panero, W.R., Stixrude, L.P., 2004. Hydrogen incorporation in stishovite at high pressure and symmetric hydrogen bonding in δ-AlOOH. Earth and Planetary Science Letters 221, 421 – 431.

Pawley, A.R., McMillan, P.F., Holloway, J.R., 1993. Hydrogen in Stishovite, with Implications for Mantle Water Content. Science 261, 1024–1026.

Sano-Furukawa, A., Kagi, H., Nagai, T., Nakano, S., Fukura, S., Ushijima, D., Iizuka, R., Ohtani, E., Yagi, T., 2009. Change in compressibility of δ-AlOOH and δ-AlOOD at high pressure: A study of isotope effect and hydrogen-bond symmetrization. American Mineralogist 94, 1255–1261.

Sano-Furukawa, A., Komatsu, K., Vanpeteghem, C.B., Ohtani, E., 2008. Neutron diffraction study of δ-AlOOD at high pressure and its implication for symmetrization of the hydrogen bond. American Mineralogist 93, 1558–1567.

Shieh, S.R., Duffy, T.S., Li, B., 2002. Strength and Elasticity of SiO_2 across the Stishovite-$CaCl_2$-type Structural Phase Boundary. Physical Review Letters 89, 255507.

Shim, S.H., Jeanloz, R., Duffy, T.S., 2002. Tetragonal structure of $CaSiO_3$ perovskite above 20 GPa. Geophysical Research Letters 29, 2166.

Singh, A.K., Andrault, D., Bouvier, P., 2012. X-ray diffraction from stishovite under nonhydrostatic compression to 70 GPa: Strength and elasticity across the tetragonal $\rightarrow$ orthorhombic transition. Physics of the Earth and Planetary Interiors 208209, 1 – 10.

Smyth, J.R., Swope, R.J., Pawley, A.R., 1995. H in rutile-type compounds; II, Crystal chemistry of Al substitution in H-bearing stishovite. American Mineralogist 80, 454–456.

Snoek, J.L., 1941. Effect of small quantities of carbon and nitrogen on the elastic and plastic properties of iron. Physica 8, 711–733.

Stixrude, L., Lithgow-Bertelloni, C., 2011. Thermodynamics of mantle minerals - II. Phase equilibria. Geophysical Journal International 184, 1180–1213.

Suzuki, A., 2009. Compressibility of the high-pressure polymorph of AlOOH to 17 GPa. Mineralogical Magazine 73, 479–485.

Suzuki, A., Ohtani, E., Kamada, T., 2000. A new hydrous phase δ-AlOOH synthesized at 21 GPa and 1000 °C. Physics and Chemistry of Minerals 27, 689–693.

Terasaki, H., Ohtani, E., Sakai, T., Kamada, S., Asanuma, H., Shibazaki, Y., Hirao, N., Sata, N., Ohishi, Y., Sakamaki, T., Suzuki, A., ichi Funakoshi, K., 2012. Stability of FeNi hydride after the reaction between Fe-Ni alloy and

hydrous phase (δ-AlOOH) up to 1.2 Mbar: Possibility of H contribution to the core density deficit. Physics of the Earth and Planetary Interiors 194–195, 18–24.

Tsuchida, Y., Yagi, T., 1989. A new, post-stishovite high-pressure polymorph of silica. Nature 340, 217–220.

Tsuchiya, J., 2013. First principles prediction of a new high-pressure phase of dense hydrous magnesium silicates in the lower mantle. Geophysical Research Letters 40, 4570–4573.

Tsuchiya, J., Tsuchiya, T., 2009. Elastic properties of δ-AlOOH under pressure: First principles investigation. Physics of the Earth and Planetary Interiors 174, 122 – 127. Advances in High Pressure Mineral Physics: from Deep Mantle to the Core.

Tsuchiya, J., Tsuchiya, T., 2011. First-principles prediction of a high-pressure hydrous phase of AlOOH. Phys. Rev. B 83, 054115.

Umemoto, K., Kawamura, K., Hirose, K., , Revenaugh, J., Wentzcovitch, R., 2015. Post-stishovite transition in hydrous aluminous sio$_2$. PNAS -.

Vanpeteghem, C., Sano, A., Komatsu, K., Ohtani, E., Suzuki, A., 2007. Neutron diffraction study of aluminous hydroxide δ-AlOOD. Physics and Chemistry of Minerals 34, 657–661.

Vanpeteghem, C.B., Ohtani, E., Kondo, T., 2002. Equation of state of the hydrous phase δ-AlOOH at room temperature up to 22.5 GPa. Geophysical Research Letters 29, 1119.

Walter, M., Thomson, A., Wang, W., Lord, O., Ross, J., McMahon, S., Baron, M., Melekhova, E., Kleppe, A., Kohn, S., 2015. The stability of hydrous silicates in Earth's lower mantle: Experimental constraints from the systems MgO–SiO_2–H_2O and MgO–Al_2O_3–SiO_2–H_2O. Chemical Geology , –.

Wood, B.J., 2000. Phase transformations and partitioning relations in peridotite under lower mantle conditions. Earth and Planetary Science Letters 174, 341–354.

Xue, X., Kanzaki, M., 2007. High-Pressure δ-$Al(OH)_3$ and δ-AlOOH Phases and Isostructural Hydroxides/Oxyhydroxides: New Structural Insights from High-Resolution ^{1}H and ^{27}Al NMR. The Journal of Physical Chemistry B 111, 13156–13166.