



Breaking the Barrier between Silica and Water in the Deep Interiors of Water-World Exoplanets

S.-H. Dan Shim (1), Carole Nisr (1), Huawei Chen (1), Kurt Leinenweber (1), Andrew V. G. Chizmeshya (1), Vitali B. Prakapenka (2), Clemens Prescher (3), Sergey Tkachev (2), Yue Meng (4), and Zhenxian Liu (5)

(1) Arizona State University, Tempe, Arizona, USA (shdshim@asu.edu), (2) University of Chicago, Chicago, Illinois, USA, (3) DESY, Hamburg, Germany, (4) Argonne National Lab, Illinois, USA, (5) George Washington University, Washington, DC, USA

Abstract

Studies have shown that water-world planets are common in our galaxy. Models have assumed separate layers for ice and rock for the internal structure of these planets because of the large differences in chemistry and density of rock and ice. Our new experiments found a dramatic increase in the solubility of H₂O in dense silica polymorphs at pressures above ~20 GPa, reaching a SiO₂:H₂O molar ratio of 3:1. Such large solubility of H₂O in silica can alter the mass-radius relations. The large solubility should be also considered in modeling the dynamo, the geochemical cycle, and the dynamics of water-world planets.

1. Introduction

Recent mineral physics studies have shown that some high-pressure (P) silicate phases can contain a large amount of H₂O in their crystal structures [1, 2]. It is of interest if pressure can enhance the solubility of H₂O in silicates under H₂O saturated conditions of water-world planet's deep interior. Because the Si–O bonding builds silicates and H₂O is the dominant form of planetary ice, chemical reactions between SiO₂ and H₂O at high pressure-temperature (P – T) provide important insights for such a fundamental question. It is also striking that many of the recently discovered dense hydrous phases (phase H, ϵ -FeOOH, and δ -AlOOH) [1, 3, 4] have the CaCl₂-type structure which is also stable in SiO₂ at pressures above 80 GPa and high temperature [5].

2. Experimental Methods

We conducted laser-heated diamond-anvil cell experiments to understand chemical reaction between SiO₂ and H₂O at 7–110 GPa and 700–2000 K. We measured X-ray diffraction patterns during high-pressure exper-

iments at the GSECARS sector of Advanced Photon Source. We recovered the samples after the experiments and measured infrared spectra for the quenched samples. We also conducted density functional theory calculations (DFT) to understand the effects of H₂O incorporation on the crystal structure of CaCl₂-type SiO₂.

3. Results

Silica is known to undergo a phase transition from rutile-type (i.e., stishovite) to CaCl₂-type structure at 80 GPa and high temperatures [5]. However, with a presence of H₂O, we found that the transition occurs at much lower pressure, ~20 GPa. A line of evidence supports H₂O incorporation in crystal structure of CaCl₂-type SiO₂ at high pressure: (1) Degree of orthorhombic distortion was much higher than what was found in dry system. (2) The recovered samples showed anomalously expanded volumes (up to 4%) at 1 bar. Our DFT calculations indicated that such large volume expansion is consistent with n up to 0.25 for (1– n)SiO₂– n H₂O. (3) The infrared spectra of the recovered samples found strong OH vibrational modes.

At pressures above 60 GPa, H₂O changes the structural behavior of silica, stabilizing a NiAs-type structure. Our data suggest that the NiAs-type phase can store a similar amount of H₂O as the CaCl₂-type phase. The NiAs-type hydrous silica is much more compressible than anhydrous dense silica polymorphs.

4. Implications

If H₂O is more soluble in silica in the interiors of water-world planets, as supported by our high-pressure experiments, this type of planets could have a single high metallicity layer where H₂O ice at shallower depths undergoes a gradual change to hydrous silica at greater depths, instead of separate layers of

ice and rock (Fig. 1). However, silicates in the deep interiors of water-world planets likely contain other elements, most notably Mg and Fe. Therefore, future studies should further investigate the effects of these elements under H_2O saturated conditions. On the other hand, some exoplanet hosting stars have sufficiently low Mg/Si ratios and therefore water-world planets around those stars would have rocks with sufficient SiO_2 to form free silica phases [6]. In this case, our results can be directly applicable.

Another important factor to consider is temperature. Because the degree of hydration can increase at lower temperatures [7], the H_2O solubility in silica should be more significant in the interiors of cooler water-world planets [8]. For Uranus and Neptune in our solar system, studies have estimated temperatures higher than 2000 K for the high metallicity layer [9], which is higher than temperature of our experiments and therefore the solubility could be less severe. However, if internal temperature is sufficiently high, because SiO_2 and H_2O can form a single fluid even at very low pressures [10], the mutual solubility could be much more extensive.

Because H_2O incorporation increases the compressibility of silica, the solubility of H_2O in silica could alter the mass-radius relations of water-world planets. Our initial result suggests that the conventional relation based on separate ice and rock layers could underestimate the amount of H_2O , although the uncertainties in the current astrophysical data need to improve to convincingly resolving such an effect. It has been believed that the phase changes in H_2O play an important role for the observed magnetic field of Uranus and Neptune [11]. If a significant amount of silicate is dissolved in the H_2O layer, the properties of ice layer can be altered. If the solubility of H_2O in SiO_2 gradually increases with pressure, materials transported by convection would undergo mixing and de-mixing at different depths in water-world planets, affecting the geochemical cycle.

Acknowledgements

The work has been supported by NASA (80NSSC18K0353) and NSF (EAR1338810). The results reported herein benefit from NASA's Nexus for Exoplanet System Science (NExSS) research coordination network. S.-H.S. and H.C. were supported by the Keck foundation. The synchrotron experiments were conducted at GSECARS, Advanced Photon Source (APS) (NSF, EAR-1128799) and

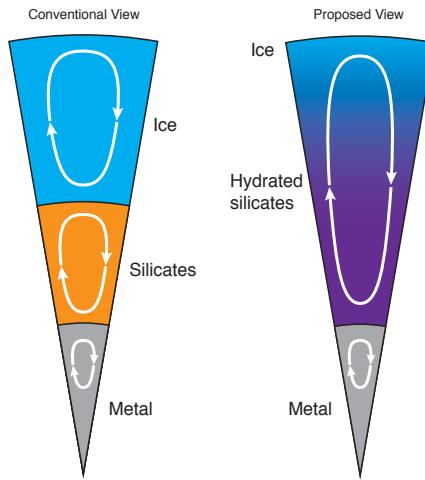


Figure 1: The internal structure of the water-world planets. (Left) Conventional view. (Right) Proposed structure based on inter-solubility of rock and ice.

(DOE, DE-FG02-94ER14466).

References

- [1] Nishi M, et al. *Nature Geoscience*, 7(3):224–227, 2014.
- [2] Ohira I, et al. *Earth and Planetary Science Letters*, 401:12–17, 2014.
- [3] Sano-Furukawa A, et al. *American Mineralogist*, 93(10):1558–1567, 2008.
- [4] Gleason A, et al. *Earth and Planetary Science Letters*, 379:49–55, 2013.
- [5] Ono S, et al. *Earth and Planetary Science Letters*, 197(3):187–192, 2002.
- [6] Bond J C, et al. *The Astrophysical Journal*, 715(2):1050, 2010.
- [7] Spektor K, et al. *Proceedings of the National Academy of Sciences*, 108(52):20918–20922, 2011.
- [8] Unterborn C T, et al. *arXiv preprint arXiv:1706.02689*, 2017.
- [9] Helled R, et al. *The Astrophysical Journal*, 726(1):15, 2010.
- [10] Newton R C and Manning C E. *Earth and Planetary Science Letters*, 274(1-2):241–249, 2008.
- [11] Redmer R, et al. *Icarus*, 211(1):798–803, 2011.