Experimental Observations on Water-Rock Interaction at High Pressures and their Implications for the Interiors of Uranus and Neptune. S.-H. Shim¹, C. Nisr¹, T. Kim², Y. Lee², H. Chen¹, K. Leinenweber¹, A. V. G. Chizmeshya¹, S. Speziale³, V. B. Prakapenka⁴, C. Prescher⁵, S. Tkachev⁵, Y. Meng⁵, and Z. Liu⁶, ¹Arizona State University, Tempe, Arizona, USA (shds shim@asu.edu), ²Yonsei University, Seoul, Korea, ³Helmholtz-Zentrum Potsdam, Germany, ⁴University of Chicago, Chicago, IL, USA, ⁵Argonne National Lab, IL, USA, ⁶George Washington University, Washington, DC, USA.

**Introduction:** Uranus and Neptune have a thick ice layer above the rocky core. Recent studies have suggested that the ice layer may contain significant amounts of heavier elements and possibly develop a compositional gradient [1, 2]. Although studies have used simple mechanical mixtures of H₂O and silicates, the state of materials remains uncertain in such H₂O rich conditions. Understanding water-rock interaction at high pressure-temperature is also important for water-rich exoplanetary bodies, such as waterworlds and sub-Neptunes which are common in our galaxy [3].

Recent high-pressure experiments have discovered oxides and silicates which can contain a few wt% of H₂O in their crystal structures [4]. However, these experiments are designed mostly for simulating H₂O undersaturated conditions of Earth’s interior. In order to understand the water-rock interaction at high pressure and temperature conditions of the water-rich planets, we have conducted a series of experiments in laser-heated diamond-anvil cell combined with synchrotron X-ray diffraction and electron microscopy. In this abstract, we present experimental observations for H₂O-SiO₂. Our MgO-FeO-H₂O experiments are reported in T. Kim et al. in this meeting. We also discuss implications of these experimental results for the internal structure and dynamics of water-rich planets.

**Experimental Methods:** We loaded pure silica together with H₂O in diamond-anvil cells. Experiments were conducted at 7-110 GPa and 700-2000 K in laser-heated diamond-anvil cell. We have measured X-ray diffraction patterns during high-pressure experiments at the GSECARS sector of Advanced Photon Source. We measured infrared spectra and chemical compositions for the recovered samples. We also have conducted density functional theory calculations (DFT).

**Results:** Our data support large solubility of H₂O in the crystal structures of dense polymorphs of SiO₂ at high pressure and high temperature. (1) The recovered samples show anomalously expanded volumes (up to 4%) at 1 bar. Our DFT calculations indicate that such large volume expansion is consistent with H₂O incorporation up to x = 0.2 in (Siₓ,Hₓ)O₂. (2) The infrared measurements of the recovered samples found strong OH vibrational modes.

We also found that H₂O alters the phase behavior of SiO₂. For example, CaCl₂-type structure (distorted stishovite) appears at much lower pressures ~20 GPa in hydrous system. At pressures above 60 GPa, H₂O stabilizes a NiAs-type structure in hydrous system, which is not thermodynamically stable in dry SiO₂.

![Figure 1: The internal structure of the water-rich planets. (Left) Conventional view. (Right) Proposed structure based on inter-solubility of rock and ice.](Image 364x394 to 497x538)

**Discussion and Implications:** Our experimental observations provide a possible explanation for the compositional gradient in the outer layer of water-rich planets. At shallower depths, because of low mutual solubility, nearly pure H₂O would be dominant. Because pressure would enhance the mutual solubility, hydrous silica may become dominant at greater depths, instead of separate layers of ice and rock (Fig. 1). Our experiments on (Mg,Fe)O + H₂O found a large solubility of Mg²⁺ in H₂O at high pressure-temperature. Such an effect would also contribute to the compositional gradient proposed for Uranus and Neptune.

Because H₂O incorporation increases the compressibility of silica, the solubility of H₂O in silica could alter the mass-radius relations of water-world planets. Our initial result suggests that the conventional mass-radius relation based on separate ice and rock layers could underestimate the amount of H₂O, while the uncertainties in the current astrophysical measurements are too large to distinguish such an effect.

The large solubility of Mg²⁺ in H₂O suggests that the deep rocky layer in the water-rich planet would...
have silica-rich composition because of preferential leaching of Mg to the H$_2$O-rich layer.

It has been believed that the phase changes in H$_2$O play an important role for the observed magnetic field of Uranus and Neptune [5]. If significant amounts of rock components are dissolved in the H$_2$O layer as shown in our experiments, the properties of the ice layer can be altered. If the solubility of H$_2$O in SiO$_2$ and Mg$^{++}$ solubility in H$_2$O gradually increases with pressure, materials transported by convection would undergo mixing and de-mixing in the interiors of 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 (DOE, DE-FG02-94ER14466).