

# Structural study of hydrous sodium silicate melts under high pressure

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Keywords: high pressure, hydrous silicate melt, X-ray diffraction, neutron diffraction.

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The behaviors of high pressure silicate melts, which is controlled by their physico-chemical properties, are important to understand the magma activity in the deep Earth. Water strongly affects the physical properties of silicate melts, such as density [1] and viscosity [2, 3], however, the effects of water on these properties have remained poorly understood. To understand the behavior of water and its mechanism in silicate melts, it is necessary to clarify the structure of hydrous silicate melts under high pressure. In this study, we focused on a simple model magma,  $\text{Na}_2\text{O}\cdot 7/3\text{SiO}_2$  (NS7/3) melt containing water, and performed the structural investigation by X-ray diffraction and neutron diffraction measurements under high pressure.

Dry NS7/3 glass was synthesized by quenching a mixture of reagent powders of  $\text{SiO}_2$  and  $\text{Na}_2\text{CO}_3$  melted in a furnace. The starting material of hydrous NS7/3 melt was prepared by encapsulating dry NS7/3 glass in a platinum capsule and then adding 5 wt% or 9 wt% water. High pressure X-ray diffraction measurements were carried out using a cubic multianvil press at the AR-NE5C beamline of PF-AR in Japan. In addition to get the information on the bonding of hydrogen and hydroxyl, we also performed high pressure neutron diffraction measurements using a six-axis multianvil press at the BL11 beamline of J-PARC MLF in Japan.

We successfully obtained the total structure factors of hydrous NS7/3 melts containing 5 wt% water (NS7/3-5H) and 9 wt% water (NS7/3-9H) at P-T conditions of 1.5–3 GPa and 550–970 °C. The first sharp diffraction peaks (FSDP) of the total structure factors of NS7/3-5H and NS7/3-9H, associated with the intermediate-range order structures, are shifted to higher Q region with pressure. These indicate that the network structures consisting of  $\text{SiO}_4$  tetrahedra in NS7/3-5H and NS7/3-9H are gradually shrinking.

Fig. 1 shows a comparison of the radial distribution functions of NS7/3-5H and NS7/3-9H at different pressures, calculated by the Fourier transform of the total structure factors. Pressure dependences of the average Si-O distance ( $r_{\text{Si-O}}$ ,  $\sim 1.6\text{\AA}$ ) reflecting Si-O bonds in  $\text{SiO}_4$  tetrahedra are shown in Fig.2. The  $r_{\text{Si-O}}$  in NS7/3-9H decreases with increasing pressure, while the  $r_{\text{Si-O}}$  in NS7/3-5H remains constant. It has been reported that the  $r_{\text{Si-O}}$  in  $\text{SiO}_4$  tetrahedra becomes slightly shorter when depolymerization of the  $\text{SiO}_4$  network structure occurs [5]. Our results suggest that the depolymerization of the network structure in silicate melt is promoted by the increase of water ( $>5$  wt%) and pressure ( $>1.6$  GPa).

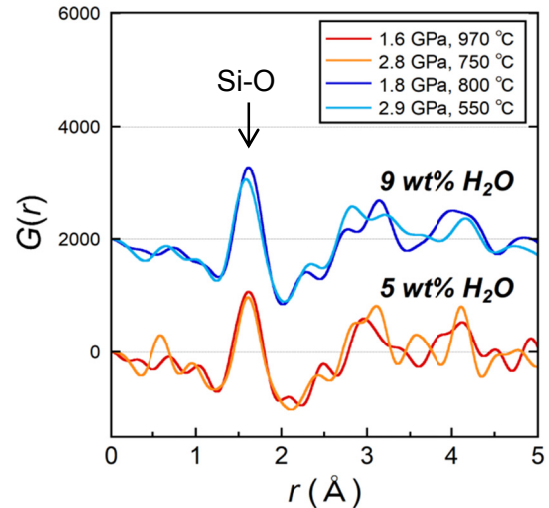


Figure 1. A comparison of the radial distribution functions of NS7/3-5H and NS7/3-9H at different pressures. The distinct peak at  $r \sim 1.6\text{\AA}$  indicates the average Si-O distance reflecting Si-O bonds in  $\text{SiO}_4$  tetrahedra.

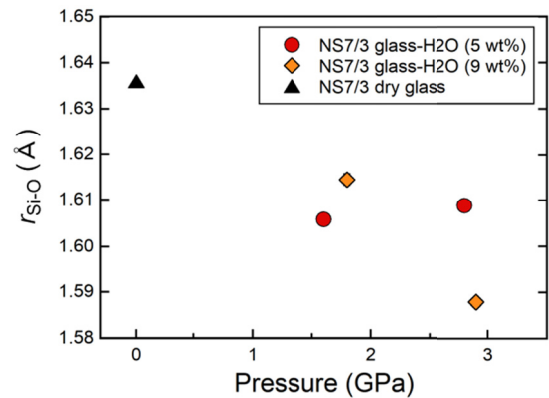


Figure 2. Pressure dependences of the average Si-O distances ( $r_{\text{Si-O}}$ ). Data for dry  $\text{Na}_2\text{O}\cdot 7/3\text{SiO}_2$  (NS7/3) glass is from C. Huang et al., 1990 [4].

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