

High-pressure structural investigations for hydrous sodium silicate melts

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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. Particularly, the H₂O content significantly affects the properties, such as density (e.g., Sakamaki et al., 2006) and viscosity (e.g., Suzuki et al., 2011; Poe et al., 2006). Since such macroscopic properties are known to be largely determined by the microscopic structure, there are considerable interests in revealing how the structure changes with increasing pressure.

Here, structures of hydrous Na₂O-8/3SiO₂ melts with 5 wt% (NS8/3_H5) and with 9 wt% H₂O (NS8/3_H9) were determined under high pressure and temperature by the in-situ X-ray diffraction (XRD). The in-situ XRD study was carried out using a cubic-type multi-anvil apparatus MAX80, which is installed at the AR-NE5C beamline of PF-AR at Tsukuba, Japan. The experimental *P-T* conditions were about 1.5–3.0 GPa and 550–970 °C, respectively.

The obtained total structure factors, $S(Q)$ of both liquids show that the position of the first sharp diffraction peaks (FSDP) shift to higher- Q with pressure. This positional shift indicates the intermediate-range order structure of present melts become compact. The reduced radial distribution functions, $G(r)$ indicate different pressure evolutions in the average Si-O bond lengths ($r_{\text{Si-O}}$) depending on their water contents. The $r_{\text{Si-O}}$ in the NS8/3_H9 melt shows the monotonic decrease with increasing pressure, however, the $r_{\text{Si-O}}$ of the NS8/3_H5 melt hardly changes after its contraction below 1.6 GPa. The structure of the NS8/3_H9 melt is assumed to be slightly more depolymerized than the NS8/3_H5 melt at ambient pressure (Zotov and Keppler, 1998). This difference might be due to a phenomenon that the number of strongly hydrogen-bonded SiOH groups, which are favored in sodium silicate glasses and melts (Xue and Kanzaki, 2004), increase more significantly during pressure-induced depolymerization in the NS8/3_H9 melt than in the NS8/3_H5 melt. This raises Si(-NBO)/Si(-BO) (NBO: non-bridging oxygen, BO: bridging oxygen) ratio, and hence, the $r_{\text{Si-O}}$ becomes shorter.

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