

Effect of water on the structure of sodium silicate melts under pressure

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Behavior of high-pressure silicate melts, which is controlled by their physico-chemical properties, is crucial to understand the magmatism in the deep Earth. Particularly, the H₂O content significantly affects the properties, such as density (e.g., Matsukage et al. 2005; Sakamaki et al. 2006) and viscosity (e.g., Poe et al. 2006; Suzuki et al. 2011). Since such physical properties can be largely determined by the atomic structure, there are considerable interests in revealing how the structure changes with increasing pressure.

Here, structures of dry Na₂O-8/3SiO₂ (NS8/3) melts and hydrous ones with 5 wt% (NS8/3-H5) and with 9 wt% H₂O (NS8/3-H9) were determined under high pressure and temperature by means of 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 Photon Factory, KEK at Tsukuba, Japan. The experimental *P*-*T* conditions were about 1.4–6.7 GPa and 900–1060 °C, respectively.

The obtained total structure factors, *S*(*Q*) of dry NS8/3 and NS8/3-H5 melts show that the position of the first sharp diffraction peaks (FSDP) monotonically shift to higher-*Q* with pressure. In contrast, the pressure dependence of the FSDP for NS8/3-H9 melt has a minimum around 4 GPa. This minimum indicates the intermediate-range order structure of the melt extends up to 4 GPa and shrinks at higher pressure. The reduced radial distribution functions, *G*(*r*) of NS8/3-H9 melt indicate different pressure evolutions in the average Na-O bond lengths, showing a sharp elongation between 3 and 4 GPa. This implies an enlargement of the -Na-O-Na- domain (Greaves 1985; Noritake 2017), and so this elongation can explain the decrease of the FSDP position up to 4 GPa. With increasing pressure, the O-O and Si-Si lengths in NS8/3-H9 melt remains constant, whereas these lengths in dry NS8/3 melt monotonically decrease. The difference in this behavior to the pressure increase can be explained that the Si-O-Si angle dominantly bends in polymerized melts with increasing pressure, while modifier cations mainly work as a cushion and the Si-O-Si angle does not shrink accordingly in depolymerized melts (Wang et al. 2014).

Keywords: hydrous silicate melt, liquid structure, synchrotron X-ray diffraction, high pressure and temperature