Structural investigations of basaltic glass under high pressure using X-ray and neutron diffraction techniques

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Structure determinations of basaltic glass have been conducted under high pressure using X-ray diffraction (XRD) and neutron diffraction (ND) techniques. The total structure factor, $S(Q)$ suggests that the position of the first sharp diffraction peak (FSDP) shifts to higher-Q region with increasing pressure. This shift indicates the intermediate-range structure of glass becomes compact. The radial distribution function, $G(r)$ shows the shrinkage of the average T-T length, and no detectable change of the average T-O length with increasing pressure (T means tetrahedrally coordinated cations, such as Si^{4+} and Al^{3+}). This result implies that drastic shrinkage of network structure involving a decrease in the mean T-O-T angle is the dominant structural evolution under experimental pressure conditions. Moreover, the second sharp diffraction peak, SSDP (Elliot, 1995) was observed in $S(Q)$ from the ND experiment. The intensity of SSDP enhanced, while that of FSDP weakened with increasing pressure. These trends indicate the disordering of the intermediate-range order (Salmon, 1994) and the ordering of the extended-range order (Salmon et al., 2005), respectively. $G(r)$ of ND also indicates no extension of the T-O bond in the present study. Considering the T-O extension reported in basaltic liquid (Sakamaki et al., 2013), this difference seems to be due to thermal effect. Also, $G(r)$ of ND represents the Mg-O and Fe-O distances show increase two times at about 2.0 and 6.0–6.9 GPa. These changes might be caused by the increase in their coordination numbers due to the polymerization of TO_4 tetrahedron. On the other hand, Ca-O and Na-O distances are less sensitive to the pressure. Since the Mg/Fe-O distance is shorter than the Ca/Na-O distance, the Coulomb force between Mg/Fe and O ions is larger than that of Ca/Na and O ions. Hence, Mg and Fe cations are easier to combine with non-bridging or isolated O anions than Ca and Na cations.

Keywords: silicate glass, X-ray diffraction, neutron diffraction, amorphous structure

