X-ray diffraction measurements on aluminosilicate glasses at ultrahigh-pressure conditions

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Knowledge about the pressure-induced structural changes in magmas, natural silicate melts, near the pressure conditions of the Earth’ s core-mantle boundary (CMB) region is important in understanding the buoyancy and motion of magmas at the CMB. However, such knowledge is still scarce due to challenges in the experiments on silicate melts at the extreme pressure and temperature conditions of the CMB. Investigation of structures of silicate glasses, considered analogues of silicate melts, is one of the ways to address this issue. Efforts have been made to understand the structures at >100 GPa in silicate glasses using the diamond anvil cell (DAC) by using Brillouin scattering (e.g., Murakami and Bass, 2010) and X-ray diffraction methods (e.g., Prescher *et al.*, 2017). However, there are still challenges to collect structural information of amorphous materials inside DAC because the sample volume of DAC is normally very small.

The opposed type double-stage large volume cell developed in Paris–Edinburgh (PE) press can provide a capability of ultrahigh-pressure generation using a large volume sample (~100 times larger than DAC sample) with a wide solid angle access for X-ray diffraction ($2\theta_{max} = 35°$). This advanced capability makes an advantage in measuring structure factor $S(Q)$ of glass under ultrahigh-pressures. The maximum pressure generation by the double-stage cell depends on the culet sizes of the 2nd-stage diamond anvils (e.g., Kono *et al.*, 2020). Using the 0.5 mm culet anvil design, we succeeded in generating pressure of 131 GPa, comparable to the pressure of the CMB (Ohira *et al.*, 2019).

We have investigated ultrahigh-pressure structural changes in aluminosilicate glasses using the opposed type double-stage cell combined with a multi-angle energy-dispersive X-ray diffraction technique. A 60 mol% Al_2O_3–40 mol% SiO_2 glass shows that its T–O (T = Si, Al) length starts to deviate from the linear compression trend above ~110 GPa and becomes constant at 110–121 GPa, implying the increase of average Al–O CN from 6 to >6. On the other hand, a basaltic glass does not show a plateau of T–O length under compression, while there are marked changes in the short and long T–T peaks in the pair distribution function $g(r)$, which is assigned as the distances between corner-sharing TO_x polyhedra and between edge-sharing polyhedra, respectively. Our results show that the basaltic glass transforms gradually from the corner-sharing dominant structure to the edge-sharing dominant structure up to 120 GPa, similar to $MgSiO_3$ glass (Kono *et al.*, 2018). Our result implies that the processes of ultrahigh-pressure structural changes in the magmas at the CMB varies depending on their chemical compositions.

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