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Venue: Zoom

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Recent developments in structural measurement of amorphous materials under pressure

Knowledge of pressure-induced structural changes in amorphous silicates are among the most important issues in understanding the behavior of silicate magmas in the Earth's interior. However, in contrast to wide range of high-pressure studies on the structural changes in silicate minerals, experimental investigation of structure of silicate magmas at high pressure conditions has still remain challenging. Although silicate and oxide glasses have been studied as an alternate approach to understand the pressure-induced structural changes of silicate magmas at high pressures, because of similarities in the pressure-induced structural changes in silicate melts and glasses, structural investigations of the previous high-pressure experimental studies were still limited mainly on the nearest neighbor Si-O distance and coordination number, and/or fast sharp diffraction peak of the structure factor (S(Q)), due to experimental difficulties of structural analysis beyond the nearest neighbor distance at in situ high pressure conditions. Recently, ambient pressure study has enabled precise structural analysis of SiO, glass beyond the nearest neighbor distances by utilizing high-energy X-ray and neutron diffraction measurements combined with the reverse Monte Carlo (RMC) modelling. Such detailed structural analysis may open a new way to understand pressure-induced structural behaviors in silicate and oxide glasses.

In order to overcome current technical difficulties in the structural measurement of amorphous materials under pressure, we developed in situ high-pressure pair distribution function measurement by utilizing high flux and high energy X-rays from undulator sources at BL37XU and BL05XU beamlines in SPring-8. In particular, a double multilayer monochromator with a wide energy band width was employed at BL05XU, enabling enhancement of the X-ray flux by three orders of magnitude, compared with that of a conventional beamline using a double crystal monochromator of silicon. The substantial leap in X-ray flux enabled precise determination of a structure factor (S(Q)) of SiO₂ glass at in situ high-pressure conditions up to 6.0 GPa over an extended momentum transfer (Q) range up to 19-20 Å⁻¹, which is almost two times larger than that in conventional high-pressure angle-dispersive X-ray diffraction measurements using monochromatic X-ray. The high-quality S(Q) data, in conjunction with the RMC modelling, opens new way to understand structural behavior of SiO₂ glass at in situ high pressure conditions.