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Compressional behavior of hydrous SiO_2 glass

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1 Introduction

Water changes the properties of silicate melts such as viscosity, density, and sound velocity, when it is dissolved into melts. It is important to study how water dissolves in silicate melts, and many studies have been performed. Here, we focus our attention on the water-bearing vitreous silica and we have studied the structure of hydrous SiO_2 glass by the X-ray diffraction analysis using synchrotron radiation under pressure.

2 Experiment

Hydrous SiO_2 glass was synthesized using the internally heated gas pressure vessel installed at ISEI, Okayama University. Crystalline SiO_2 enclosed in Pt capsule with 3.6 wt% D_2O had been fused at 200 MPa and 1500 C for 3h, then it was quenched into glass. Unfortunately, part of deuterium was substituted by hydrogen by exchange reaction with the gas in the pressure vessel through Pt capsule. Raman spectroscopy showed the quenched hydrous glass contained Si-OH(D) as well as $H(D)_2O$ molecules.

Compression of hydrous SiO_2 glass was performed using the MAX80 system at AR-NE5C up to about 7 GPa. X-ray diffraction profiles were collected by energy dispersive method.

3 Results and Discussion

Interference function $Qi(Q)$ for hydrous SiO_2 glass at 0.1 MPa is almost the same as that of dry SiO_2 glass, except for the FSDP. The position of the FSDP of hydrous glass is at the higher Q side than that of dry one, indicating shrinkage of the intermediate range order by addition of water.

$Qi(Q)$ of hydrous glass changed gradually with pressure up to 7 GPa at 300 K (Fig. 1). Pressure variations in $Qi(Q)$ is the same as those of dry SiO_2 glass [1]. MD simulations showed that the Si-Si correlation changes with pressure and accounts for the variations of $Qi(Q)$. The radial distribution function $D(r)$ also shows the decrease of Si-Si distance with pressure without any change in Si-O and Si-Si distances. The FSDP of hydrous SiO_2 glass shift toward higher Q with pressure (Fig. 1), as shown in dry one [2]. Thus, in the hydrous SiO_2 glass, the network topology of SiO_4 tetrahedra changes with pressure.

Although hydrous SiO_2 glass takes a similar short range structure to dry one, comprising a SiO_4 tetrahedron, the medium range order of hydrous glass is smaller than dry glass. Unfortunately, we could not find how water works in structure changes of the hydrous SiO_2 glass under pressure. Compressional behavior of hydrous SiO_2 glass agrees with dry glass; the intermediate range order shrinks with increasing pressure.

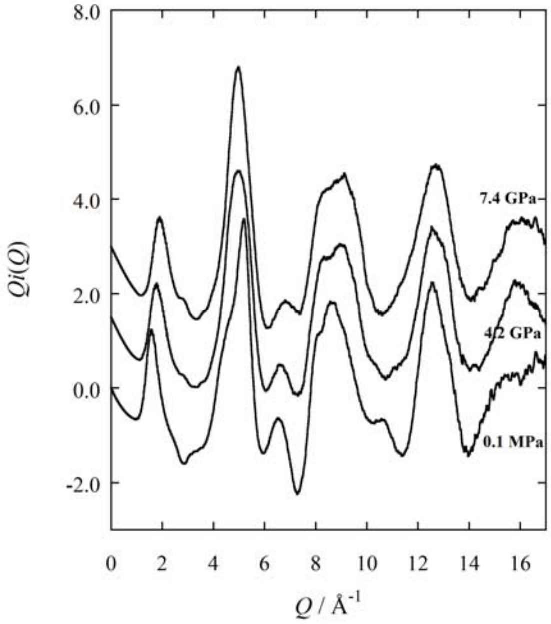

Fig. 1: Variation of interference function $Qi(Q)$ for hydrous SiO_2 glass during compression.

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