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Contrasting behavior of intermediate-range order structures in jadeite glass and melt

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ABSTRACT

Structures of jadeite glasses and melt are studied by the multi-angle energy-dispersive X-ray diffraction technique under high pressures and temperatures. The temperature dependence of X-ray structure factors, $S(Q)$, is obtained at experimental conditions from 4.5 GPa and 300 K to 6.3 GPa and 2173 K. When the glass sample is heated at high pressures, the first sharp diffraction peak (FSDP) in the structure factor becomes sharper and shifts to higher- Q with increasing temperature to 473 K. At higher temperatures to 873 K, both shape and position of the FSDP change only slightly. The structure factor of jadeite melt at 2173 K and 6.3 GPa clearly differs from that of the glass at 873 K (just below melting). The FSDP of the melt is broader and located at lower- Q (corresponding to higher real-space atomic distance). In addition, a small peak (second sharp diffraction peak – SSDP) appears in the $S(Q)$ of the melt between 3.0 and 3.2 \AA^{-1} , which is known to be a sign for change of short-range ordering. Although the pressure drops to 3.7 GPa upon quenching from the melt, the quenched glass exhibits densified features in the structure factor, with the FSDP located at a higher- Q than that of glass before melting at 873 K and 5.3 GPa. This implies that the intermediate-range order structure of the quenched glass (300 K, 3.7 GPa) is more densified by thermally-induced modification, although this quenched glass does not show clear SSDP in its $S(Q)$. Similar to previous studies, the glass decompressed to ambient condition remains denser than the glass before compression and heating. The FSDP position changes from 2.02 \AA^{-1} in the starting material to 2.17 \AA^{-1} in the recovered glass, suggesting that the volume of recovered glass decreases about 20% in volume. The present result implies that glasses quenched under ambient pressure do not accurately represent structural behavior of melts under high pressure, while glasses quenched under high pressure can be treated as good analogs to melts at corresponding high pressure ranges, at least from the structural behavior point of view.

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1. Introduction

Structural properties of silicate melts are closely correlated to their physical, chemical, and thermal properties (e.g., Mysen et al., 1982, 1985; Kushiro and Mysen, 2002). Our understanding of the formation and evolution of magma in the Earth and terrestrial planets, igneous processes, as well as volcanism depends critically on the knowledge of these properties (e.g., Ohtani, 1985; Kushiro, 1976). Because of technical difficulties in directly studying structure and properties of silicate melts, many researchers have made efforts in obtaining insights by studying glasses quenched from melts. For example, silica glass (SiO_2) has been well studied for pressure-induced structural changes using various approaches (e.g., Raman: McMillan et al., 1984; Devine and Arndt, 1987;

XRD: Meade et al., 1992; Inamura et al., 2001, 2004; MD: Jin et al., 1994; Trachenko and Dove, 2002, 2003). Silica glass densifies permanently when compressed to above 10 GPa at room temperature and at lower pressures when heated (McMillan et al., 1984; Devine and Arndt, 1987; Susman et al., 1991). An approximately 20% increase in density can be achieved by treatment at 7.4 GPa and 973 K (Inamura et al., 2001). In spite of the large variation in density, changes in the short-range order of the densified silica glass are small (Inamura et al., 2001; Jin et al., 1994; Trachenko and Dove, 2002, 2003). The large increase of density is attributed to a significant modification in the intermediate-range order (IRO), as represented by a drastic change in the first sharp diffraction peak (FSDP) in the structure factor (Elliott, 1991; Susman et al., 1991; Inamura et al., 2001; Trachenko and Dove, 2002). The FSDP has been observed in numerous types of glasses (e.g., Meade et al., 1992) and is generally accepted to be related to IRO of the network at separations around 2–10 Å (i.e. $\sim 2\pi/Q_{\text{FSDP}}$), originated from features such as rings of TO_4 tetrahedra (Inamura et al.,

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2004), where T stands for tetrahedrally coordinated cations. Here, Q_{FSDP} is the momentum transfer (Q) of the FSDP, expressed as $Q = 4\pi \sin \theta / \lambda = 4\pi E \sin \theta / hc$, where λ , E , θ , h and c are the wavelength, energy of the X-rays, diffraction angle, Planck's constant and the speed of light in vacuum, respectively. Note that here we use the “pre-peak” definition of FSDP as discussed by Elliott (1995). This definition includes the possibility that the FSDP may be absent (as is the case for most metallic liquids), but for the glass and melt studied here the first peak in the $S_X(Q)$ is an FSDP, consistent with its structural role, and its broadening and shift to larger Q with increasing pressure. The positive pressure dependence of FSDP in Q -space represents a decrease in the intermediate correlation distances in real space with pressure. For silica glass, FSDP appears at $Q = 1.55 \text{ \AA}^{-1}$ at ambient pressure, corresponding to real-space components of period $\sim 4 \text{ \AA}$, suggesting the involvement of distance between neighboring SiO_4 tetrahedra (Si–Si distance). With increasing pressure, the position of FSDP moves almost linearly to higher Q as the density increased (Inamura et al., 2001).

Inamura et al. (2004) conducted in situ X-ray diffraction experiments on silica glass at elevated temperatures up to 19.2 GPa. They report that the position of FSDP moves to higher Q as temperature is increased in certain pressure–temperature range. The direction of the temperature-induced shift indicates a decrease in average atomic spacings in the intermediate range, suggesting that IRO is thermally relaxed to reach a denser arrangement. Around 7 GPa, the temperature-induced FSDP shift reaches saturation and crystallization temperature increases drastically. These results support the existence of a relatively stable high-pressure form of silica glass. A sudden transformation corresponding to large decrease of volume is not observed.

Aluminum is one of the major elements in the Earth and an important element in the silicate network in melts and glasses. A marked decrease in viscosity with increasing pressure has been observed in aluminosilicate melts (e.g., Kushiro, 1976, 1978; Kushiro et al., 1976). It is suggested that a change in aluminum coordination in the melt from fourfold to sixfold, with an accompanying decrease in the degree of polymerization of the melt, is responsible for this anomalous behavior (Kushiro, 1976). Since these reports, glass and melt structures of aluminosilicates, of which jadeite composition ($\text{NaAlSi}_2\text{O}_6$) is a typical example, have been investigated at high pressures to understand the mechanism of the viscosity change. A study using Raman spectra does not support Kushiro's conclusion (Sharma et al., 1979). By comparing Raman spectrum of jadeite glass at 1 atm with that of quenched glass from 4.0 GPa, these latter authors concluded that Al remains tetrahedrally coordinated throughout the pressure range. The structure of jadeite glass quenched from 1.0 GPa is studied using radial distribution analysis; no evidence of increased coordination number in aluminum is found (Hochella and Brown, 1985). Recently, structure of jadeite melt is measured up to 4.9 GPa using the multi-angle energy-dispersive X-ray diffraction technique (Sakamaki et al., 2012). It is reported that dominant structural changes are in the IRO. The changes in T–O–T angle (and T–T length) appear to correlate with the viscosity anomaly in the pressure range.

Ideally, studies for silicate melts should be performed by in situ measurements under high pressure and temperature. However, experiments based on quenched glasses recovered from high temperature and pressure are still important because of the well-known difficulties in conducting in situ melt experiments under pressure. At this juncture, it is important to recognize differences and similarities between glasses and melts. In particular, structures and properties of glasses are often strongly related to their pressure–temperature paths in synthesis processes. The contrasting behavior of glasses synthesized at different conditions will provide crucial information in understanding the relations between glasses and melts. Here we report results on the X-ray structure

factor, $S(Q)$, of jadeite glasses synthesized at different conditions and jadeite melt obtained by in situ multi-angle energy-dispersive X-ray diffraction in a Paris–Edinburgh press at elevated pressures and temperatures up to 6.3 GPa and 2173 K, respectively. We examine temperature- and pressure-induced changes in the IRO structure, and discuss the correlation and differences among the glasses and between the glasses and the melt.

2. Experimental method

Starting material was prepared from reagent-grade oxides and carbonates. Reagent-grade oxides (SiO_2 , Al_2O_3) and crystalline powder of $\text{Na}_2\text{Si}_2\text{O}_5$, previously synthesized from Na_2CO_3 and SiO_2 , were mixed in jadeite ($\text{NaAlSi}_2\text{O}_6$) composition in an agate mortar with acetone for 2 h, respectively. The mixed powder was melted at 1673 K for 5 min. Crushing and fusing were repeated three times in order to homogenize the starting materials.

Experiments were conducted using a Paris–Edinburgh press installed at the HPCAT 16-BM-B beamline, Advanced Photon Source (APS), Argonne National Laboratory. Structure measurements were performed using the energy dispersive X-ray diffraction technique described in Yamada et al. (2011). A schematic illustration of the high-pressure cell assembly is shown in Fig. 1 (Sakamaki et al., 2012). The outer pressure media consisted of machinable zirconia (ZrO_2) pallets and sintered boron-epoxy. Machinable magnesia (MgO) in cylinder shape was placed between the boron-epoxy gasket and the graphite heater for protection, heat insulation, and X-ray transparency. Graphite capsule was used as sample container, insulated by a hexagonal boron nitride (hBN) sleeve and MgO plugs placed on top and bottom of the capsule. Pressures were determined by the equation of state of MgO (Speziale et al., 2001). Temperature was estimated using the relationship calibrated by electric power in a separate temperature calibration experiment with the same cell assembly.

The 16-BM-B is a bending magnet beamline providing white X-rays (5–120 keV) with high brightness. In our experiments, the incident X-ray was collimated by two sets of vertical (0.1 mm) and horizontal (0.1 mm) slits. The diffracted signal was collimated with a 0.1 mm gap scattering slit 80 mm downstream from the sample and a 0.1×5.0 mm receiving slit 400 mm further downstream from the scattering slit. A Ge solid-state detector (SSD)

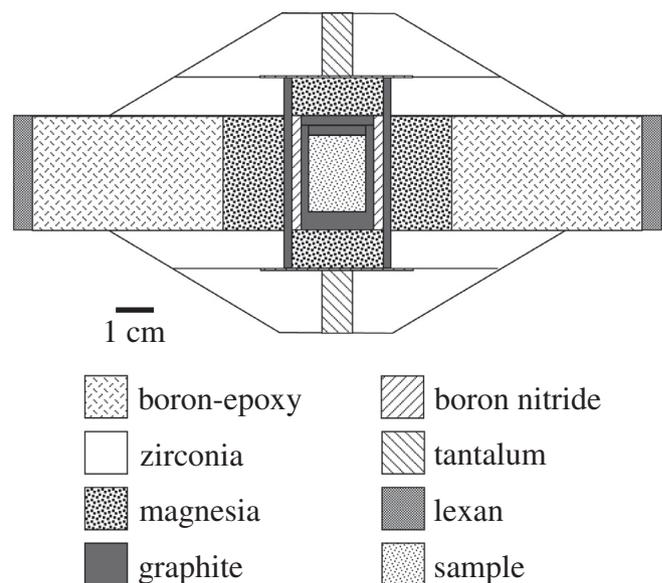


Fig. 1. A cross section of the cell assembly.

was mounted on a two-theta arm on a large Huber rotation stage, which allowed accurate control on the two-theta angle. Diffraction patterns were collected for 9 fixed diffraction angles ($2\theta = 3^\circ, 4^\circ, 5^\circ, 7^\circ, 9^\circ, 11^\circ, 15^\circ, 20^\circ$ and 25°). Collecting time varied with diffraction angles, as intensities decrease with increasing angle. All patterns were collected until the maximum intensity reached at least 2000 counts. The structure factors, $S(Q)$ s, were obtained from the measured X-ray diffraction data using an analytical program by Funakoshi (1997) according to the formula:

$$S(Q) = \left\{ I^{coh}(Q) - \sum_{j=1}^m f_j^2(Q) \right\} / \left\{ \sum_{j=1}^m f_j(Q) \right\}^2 \quad (1)$$

where $I^{coh}(Q)$ is the coherent intensity resulting from the correlations of atoms, $f_j(Q)$ is the atomic scattering factors of the j -th atom, and the summation is taken over the formula unit.

3. Results and discussion

3.1. Temperature-induced densification in jadeite glass

Fig. 2 displays the pressure–temperature points at which the structure measurements were performed. Pressure was first increased to 4.5 GPa at room temperature, then the sample was heated at a constant applied ram load. Typically in the PE cell, as temperature increases, pressure increases slightly. The crystallization temperature for jadeite glass is 1073 K (the appearance of the first crystalline peak), as indicated by the cross (×) in Fig. 2. Obtained structure factors are shown in Fig. 3. Table 1 indicates the experimental conditions, the position of FSDP, and the full width at half maximum (FWHM) of FSDP. The fresh, as synthesized glass (f-glass) exhibits a weak and broad FSDP. Under pressure, as temperature increases, FSDP of the glass prior to melting (pm-glass) moves to higher- Q and becomes sharper. For the rest of the peaks at $Q > 4 \text{ \AA}^{-1}$, shifts in peak positions are relatively small. Because of less sensitivity of these peaks to temperature–pressure change, TO_4 tetrahedral units remain fairly rigid. Fig. 4 is an expanded view of $S(Q)$ between 1.8 and 3.0 \AA^{-1} . Fig. 4a shows variations in the shape of FSDP of jadeite glass during heating. The largest change

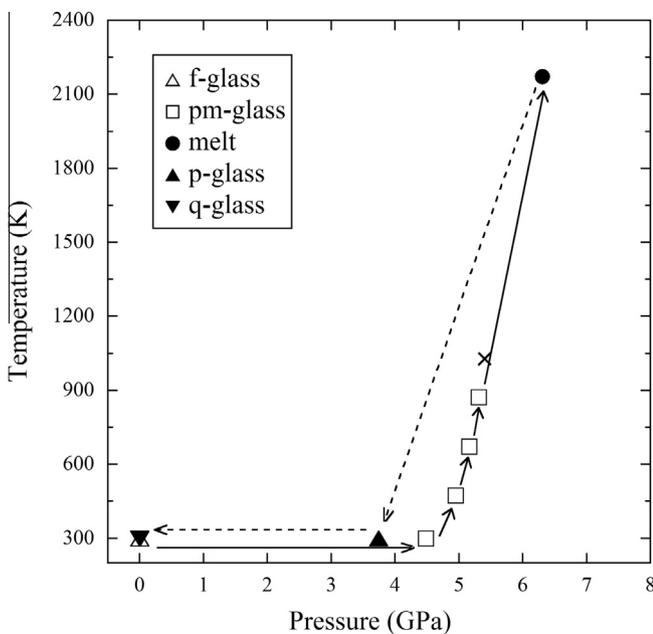


Fig. 2. Pressure–temperature diagram summarizing the experimental condition of this study. Open triangle, open squares, solid circle, solid triangle and reversed solid triangle are f-glass, pm-glass, melt, p-glass and q-glass, respectively.

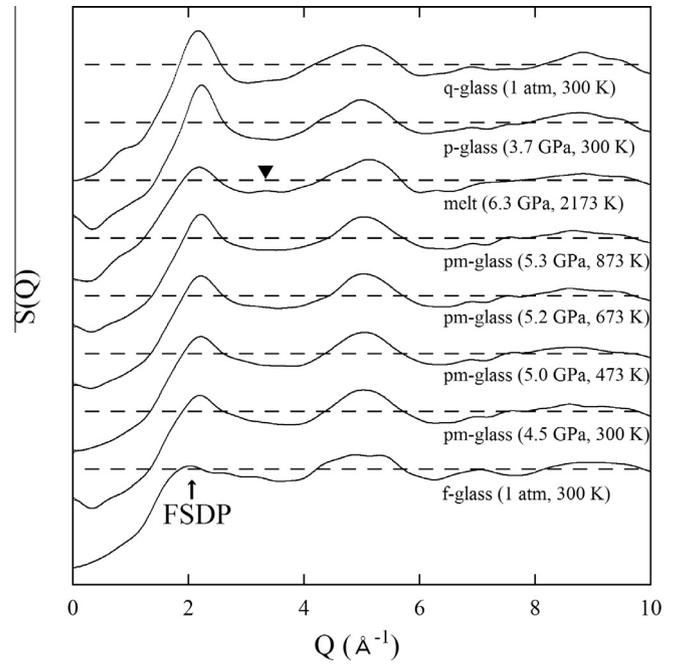


Fig. 3. Structure factors, $S(Q)$, at various pressure–temperature conditions. The arrow is the position of the FSDP, and reversed solid triangle indicates the SSDP which is observed only in $S(Q)$ of melt.

occurs between 300 and 473 K, where FSDP shifts slightly to higher- Q (lower values in real space), indicating a shrinkage of the IRO structure. Between 473 and 873 K, the change of FSDP is small. Intensity of FSDP increases slightly with temperature, and its position shifts slightly to higher- Q , indicating that the characteristic distance in real space is reduced. The direction of the shift is in contrary to what is expected from normal thermal expansion behavior. This suggests that the density of jadeite glass increases with temperature due to relaxation of the IRO structure, at least between 300 and 473 K. The sharpening of the FSDP is also counter intuitive as peak broadening at high temperature is expected due to increased thermal vibration. On the contrary, the sharpening suggests an increase in the correlation length or a more ordered, homogeneous structure at high temperature, which further supports the notion that the IRO structure is thermally relaxed during heating. This sharpening continues up to 873 K, as can be seen by the decrease in peak width and increase in peak maximum.

Simulation studies have shown similar events and the resultant changes in the topology of tetrahedron connectivity in silica glass. Trachenko and Dove (2002, 2003) show that for silica the tetrahedral topology does not break below 3 GPa. Bond breaking and rebonding begin above 3 GPa at room temperature and the number of rebonding events increases markedly above 5 GPa. At elevated temperatures, the number of rebonding events increases. They report a gradual decrease of 7% in volume up to 1200 K and 3.6 GPa. The change in topology results in a change in the configuration of SiO_2 tetrahedra, with a decrease in the size of $(\text{SiO}_4)_n$ rings. Jadeite has the same NBO/T ratio (=0) as that of silica. Here NBO stands for non-bridging oxygen. Both silica and jadeite glasses have a similar polymerized network structure. The IRO modification observed in the jadeite glass with temperature may be similarly related to the changes in the topology of tetrahedral connectivity toward more efficient packing, including a decrease in $(\text{TO}_4)_n$ rings.

3.2. Comparison between jadeite glass and melt

Fig. 4b compares FSDP in $S(Q)$ between glasses and melt. The FSDP of the melt is broader and centered at lower- Q relative to

Table 1
Experimental conditions and analysis of FSDP.

	Pressure (GPa)	Temperature (K)	FSDP (\AA^{-1})	FWHM (\AA^{-1})
f-Glass	0	300	2.016	0.86
pm-Glass	4.5	300	2.202	0.64
	5.0	473	2.215	0.61
	5.2	673	2.220	0.58
	5.3	873	2.221	0.56
	6.3	2173	2.186	0.61
Melt	3.7	300	2.229	0.50
q-Glass	0	300	2.173	0.61

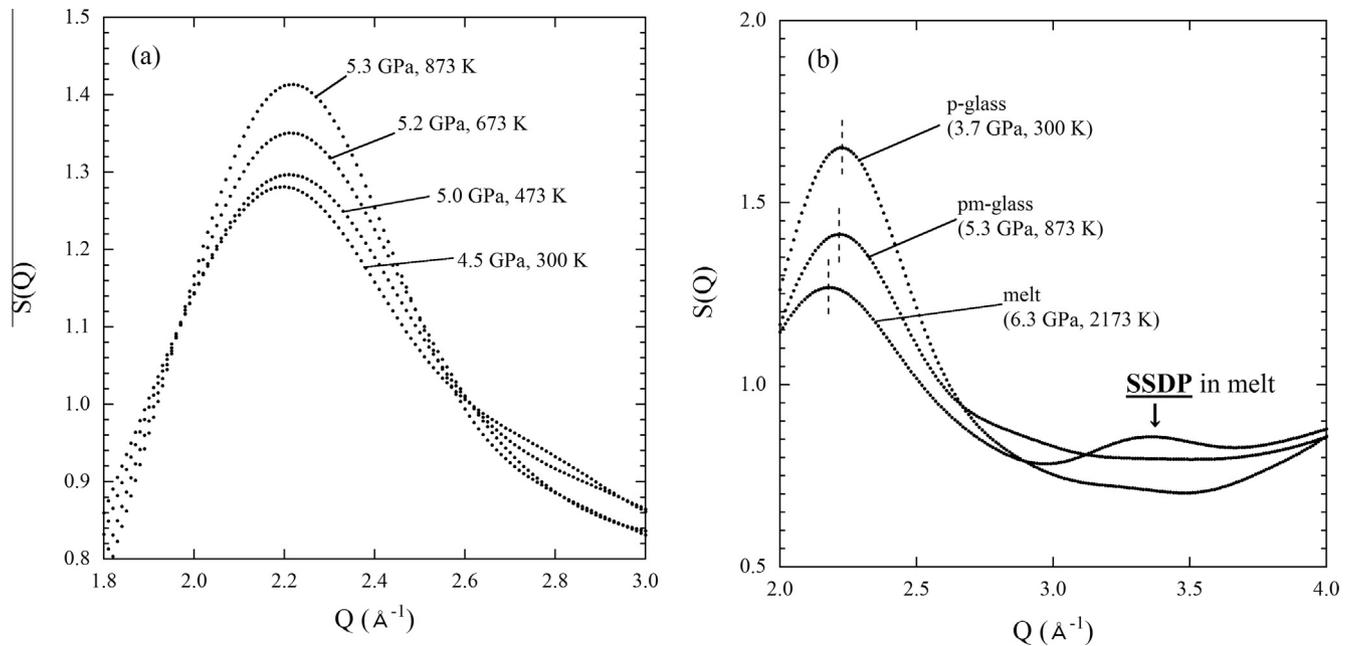


Fig. 4. Structure factors, $S(Q)$, of jadeite glass and melt. (a) $S(Q)$ of jadeite pm-glass with temperature around 5 GPa. (b) Comparison of $S(Q)$ between pm-glass, melt and p-glass. The broken line indicates each center of FSDP positions.

the peak of the pm-glass at 5.3 GPa and 873 K, while that of quenched glass remains sharper and shifts to higher- Q . These changes can be explained by effects of thermal expansion and thermal vibration. High temperature expands the tetrahedral network and causes the FSDP in $S(Q)$ broader. On the other hand, an increase in temperature from 300 to 873 K results in a contraction in the glass structure (Fig. 4a). An interesting feature in the $S(Q)$ of the melt is that a small peak appears on the right side (~ 3.0 – 3.2\AA^{-1}) of the FSDP. Elliott (1995) refers to this as the “second sharp diffraction peak (SSDP)”. The SSDP is reported in previous X-ray diffraction studies of silicate glasses (e.g., Sato and Funamori, 2010), and is attributed to a short-range ordering, such as a more densely packed structure, resulting in a diminution of the interstitial volume between the silicate network (Salmon et al., 2005).

Fig. 5a summarizes observed temperature dependence of position of the FSDP. With increasing temperature, FSDP of pm-glass (open squares: \square) shifts toward high- Q , while at 2173 K FSDP of the melt (solid circle: \bullet) is centered around a much lower- Q region. Thus, while the IRO structure in glass shrinks with temperature, that of melt expands. The quenched glass has been made from melt by shutting of power with a quench rate roughly 500 K/s. At 3.7 GPa (solid triangle: \blacktriangle) FSDP position of the quenched glass under pressure (p-glass) is different from both the melt and the pm-glass. The position of FSDP is interpreted as resulting from real-space atomic arrangements with characteristic repeated distance $2\pi/Q_{\text{FSDP}}$ (e.g., Zotov et al., 1996). Assuming that the IRO volume is proportional to $(2\pi/Q_{\text{FSDP}})^3$, the quenched glass (3.7 GPa,

$Q_{\text{FSDP}} = 2.23 \text{\AA}^{-1}$) would have a decrease in specific IRO by $\sim 4\%$ compared with the pm-glass (4.5 GPa, $Q_{\text{FSDP}} = 2.20 \text{\AA}^{-1}$) at 300 K. Clearly, thermal history plays a significant role in the structure of the glass.

Fig. 5b summarizes the FSDP position as a function of pressure. The melt structure, collected at the highest pressure condition ($P = 6.3 \text{ GPa}$), shows a FSDP position at lower- Q region. The dashed arrow indicates compression behavior of the glass before melting, from 1 atm to 4.5 GPa at 300 K, and the IRO change is about 23%. On the other hand, the dotted arrow corresponds to decompression for the quenched glass from 3.7 GPa to 1 atm at 300 K. The fact that FSDP position shifts to lower- Q indicates that the q-glass after pressure releasing could not maintain the IRO structure at high pressure. During decompression, the increase in volume is only about 8%. The difference in volume changes between compression and decompression further indicates that the structure of treated glass has changed to a denser state in the end. The FSDP position changes from 2.02\AA^{-1} for the f-glass to 2.17\AA^{-1} for the q-glass. This suggests that the IRO of the quenched glass has decreased by about 20%.

4. Summary

The structure factors for jadeite glasses and melt are measured up to 6.3 GPa and 2173 K by means of an in situ X-ray diffraction method. The temperature dependence of FSDP position for jadeite

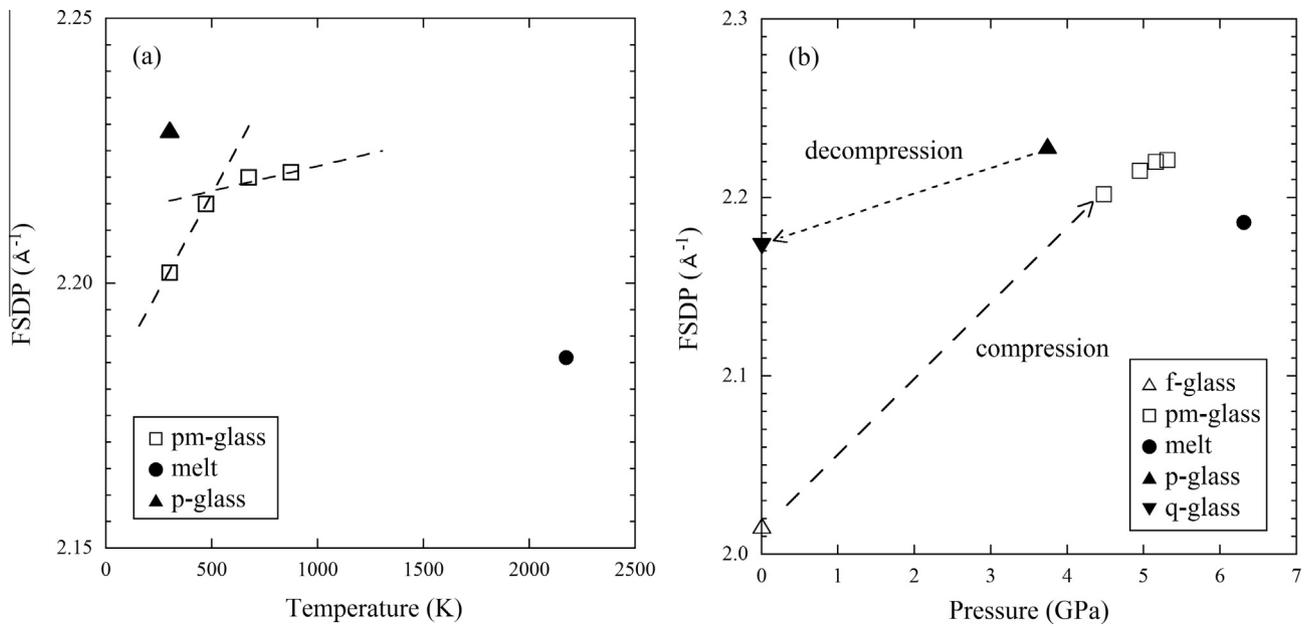


Fig. 5. FSDP positions under this experimental condition. (a) The temperature dependence of the FSDP position. Open squares, solid circle and solid triangle are pm-glass, melt and p-glass, respectively. Broken lines are guide for eyes. (b) FSDP positions of this study as a function of pressure. Open triangle, open squares, solid circle, solid triangle and reversed solid triangle are f-glass, pm-glass, melt, p-glass and q-glass, respectively.

glasses does not show a monotonous change. At temperatures up to 473 K, the shift to higher- Q is large, and between 473 and 873 K the shift is small. Compared to glasses, FSDP of the melt at 6.3 GPa and 2173 K shifts to lower- Q and becomes broader. In the higher- Q region in $S(Q)$ of the melt, SSDP is observed around $3.0\text{--}3.2 \text{\AA}^{-1}$, which is a sign of a short-range ordering (Elliott, 1995). The quenched glass from the melt exhibits a denser IRO structure, similar to that of the melt. FSDP of the quenched glass (p-glass) is at higher- Q than that of the pm-glass at 873 K without melting. This implies that glasses quenched under ambient pressure may not be good candidates to represent melt structure under high pressure. The present results suggest that glasses quenched under high pressure may be used as good analogs to melts at corresponding pressure ranges, at least from the structural behavior point of view.

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