High-Pressure Transformation of SiO_2 Glass from a Tetrahedral to an Octahedral Network: A Joint Approach Using Neutron Diffraction and Molecular Dynamics

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A combination of *in situ* high-pressure neutron diffraction at pressures up to 17.5(5) GPa and molecular dynamics simulations employing a many-body interatomic potential model is used to investigate the structure of cold-compressed silica glass. The simulations give a good account of the neutron diffraction results and of existing x-ray diffraction results at pressures up to ~60 GPa. On the basis of the molecular dynamics results, an atomistic model for densification is proposed in which rings are "zipped" by a pairing of five- and/or sixfold coordinated Si sites. The model gives an accurate description for the dependence of the mean primitive ring size $\langle n \rangle$ on the mean Si-O coordination number, thereby linking a parameter that is sensitive to ordering on multiple length scales to a readily measurable parameter that describes the local coordination environment.

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Silica is the fundamental network glass-forming material whose behavior under pressure is of long-standing interest, partly because it acts as a reference for geophysically relevant silicates [1–12]. For the glass, the primary densification mechanisms identified by experiment are associated with a reduction of the Si-O-Si bond angle between SiO_4 tetrahedra at pressures $p \lesssim 10$ GPa and with an increase in the mean Si-O coordination number $\bar{n}_{Si}^{O}$ from four to six at higher pressures [3–5,7–11]. These simple metrics are, however, insufficient to establish the precise atomistic mechanisms of network collapse, which may evolve over multiple length scales and be dependent on the pathway used to form the high-pressure glass [13–19]. Such information is a prerequisite for understanding the density-driven changes in material properties.

Ring statistics offer insight into glass structure over multiple length scales, where this scale depends on the total number of atoms in a ring, and provide a natural language for the density-driven structural evolution of silica glass [20]. There is a need, however, for accurate experimental information to validate the particular approach taken. For example, models in which SiO_4 tetrahedra are preserved predict a rise in the mean ring size with pressure as observed for crystalline structures [20–22], whereas models with more adaptable nearest-neighbor coordination environments suggest a more complex evolution [16–18] in which fivefold coordinated Si sites can promote the formation of smaller rings [23]. X-ray diffraction (XRD) is a key structural probe of densified silica [5–7,10,11] but it is not possible to solve the structure using this technique alone [24]. Information from other structural probes is therefore necessary in order to constrain models of silica glass under pressure, thereby helping to differentiate between the various models that can be constructed on the basis of XRD results alone.

In this Letter, we employ *in situ* high-pressure neutron diffraction (ND) to measure the structure of cold-compressed silica glass at pressures up to 17.5(5) GPa, the maximum pressure that can be reliably achieved by using the ND method [25], using an experimental approach that overcomes the major difficulties found in previous work [26]. ND is sensitive to the oxygen atom correlations and therefore provides complementary information to XRD: the weighting factors for the Si-Si, Si-O and O-O correlations in the total structure factors measured in a diffraction experiment are 0.0694:0.3880:0.5427 for ND versus 0.2178:0.4978:0.2844 for XRD at a scattering vector $k = 0$. Molecular dynamics (MD) simulations using the Tangney-Scandolo [27] (TS) interatomic potentials, which incorporate anion (dipole) polarization terms [28], are found to give a good account of *both* the ND (present work) and XRD results [6,10,11,29], as well as the

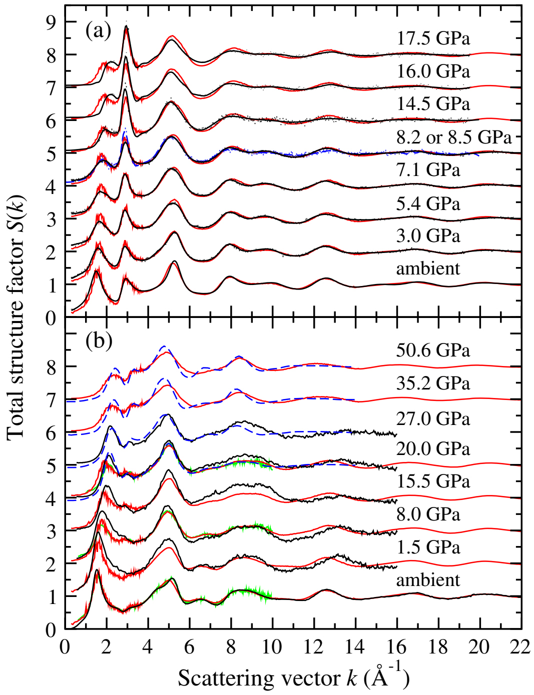

FIG. 1 (color online). The pressure dependence of the (a) neutron and (b) x-ray $S(k)$ functions. In (a), the broken (blue) curve ($p = 8.5$ GPa) and solid (black) curves (all other pressures) give spline fits to the measured data represented by the points with vertical error bars. For the experiments in the pressure range 8.5–17.5 GPa, the region $k \leq 1.55$ Å^{-1} was not accessible and the curves in this region are fitted Lorentzian functions [25]. In (b), the XRD results are from Refs. [6] [solid light (green) curves at ambient, 8.0 and 20.0 GPa], [29] [solid (black) curve at ambient], [10] [solid (black) curves at high p] and [11] [broken (blue) curves]. In (a) and (b), the solid light (red) curves show the TS MD results for the same or comparable pressures.

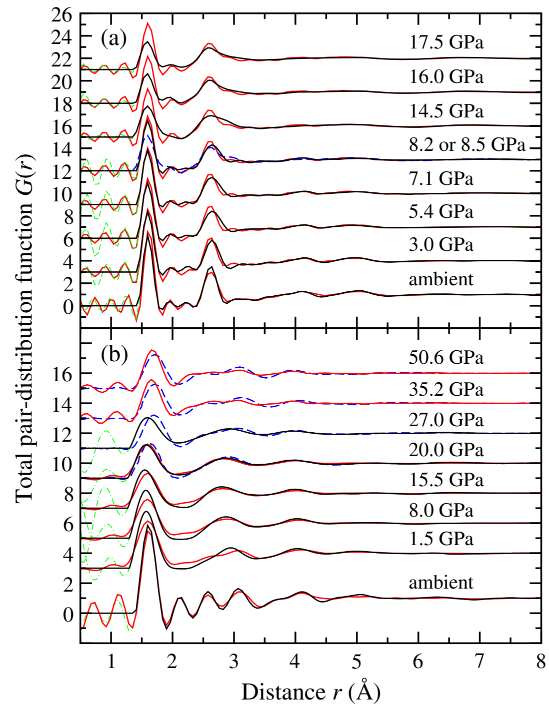

FIG. 2 (color online). The pressure dependence of the (a) neutron and (b) x-ray $G(r)$ functions. In (a), the broken (blue) curve ($p = 8.5$ GPa) and solid (black) curves (all other pressures) are the Fourier transforms of the spline fitted measured $S(k)$ functions shown in Fig. 1(a), and the broken light (green) curves show the unphysical small-r oscillations. In (b), the solid (black) curves are the Fourier transforms of the measured $S(k)$ functions shown in Fig. 1(b) from Refs. [10,29] with a cutoff $k_{\max} = 15$ Å^{-1} (and also with a Lorch [47] modification function for the Ref. [10] data), and the chained (green) curves show the unphysical small-r oscillations. The broken (blue) curves are the measured $G(r)$ functions from Ref. [11]. In (a) and (b), the solid light (red) curves are the Fourier transforms of the TS MD results given in Fig. 1, where the same modification functions were used as in experiment.

measured equation of state (see Supplemental Material [30], Fig. S1), at pressures up to ~60 GPa. A ring closure model is developed in which rings are "zipped" by a pairing of fivefold and/or sixfold coordinated Si sites. The model is in agreement with the MD results, thereby relating the pressure dependence of a parameter that is sensitive to ordering on multiple length scales to the local coordination environment in the glass.

Figures 1 and 2 compare the measured total structure factors $S(k)$ and pair-distribution functions $G(r)$ from ND (present work) and XRD with the cold-compression MD results. The XRD experiments used no pressure apparatus [29], a cubic-type multianvil press [6], or a diamond anvil cell [10,11]. Details of the ND [25,44,45] and MD work are given in the Supplemental Material [30], Sec. S2. The simulations reproduce all of the main features in the measured ND and XRD patterns at pressures up to 60 GPa, although there is a shift in position of the first sharp diffraction peak at ~2.2 Å^{-1} in the $p \sim 15$–20 GPa range, and the highest pressure ND $G(r)$ functions are damped relative to simulation (Supplemental Material [30], Sec. S3). Many of the discrepancies are comparable to those found between the different experiments, and originate from the challenges associated with experiments under extreme conditions, e.g., from the difficulty in correcting for diamond Compton scattering [46] and radiation induced annealing [11].

Figures 3(a)–3(b) show the pressure dependence of $\bar{n}_{Si}^{O}$ and the mean Si-O bond distance $\bar{r}_{SiO}$ for silica glass under cold compression as obtained from ND and XRD [5,10,11], from MD simulations using either the TS (present work) or Beest-Kramer-Santen (BKS) [48,49] interatomic potentials, and from first-principles MD simulations [50]. In the present ND and MD work, $\bar{r}_{SiO}$ was taken from the first peak position in $G(r)$, and $\bar{n}_{Si}^{O}$ was obtained by integrating over this peak to the first minimum where, if necessary, a Lorch [47] function was used to suppress Fourier transform artifacts. The ND results show an increase in $\bar{n}_{Si}^{O}$ above four at a pressure > 14.5(5) GPa, and are consistent with the

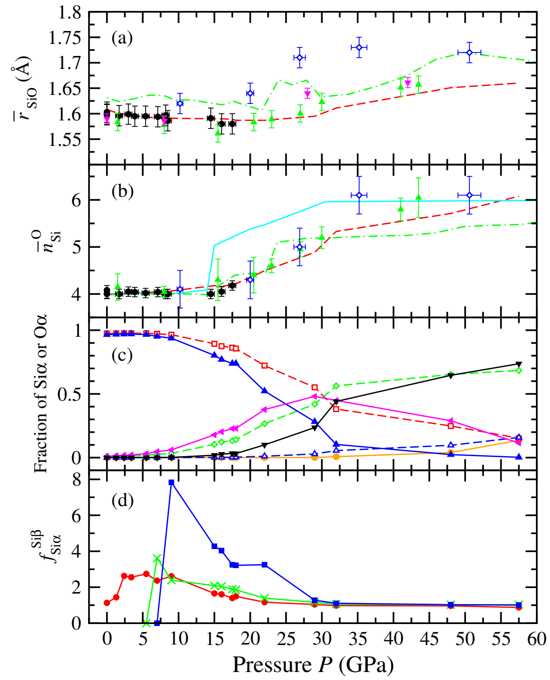

FIG. 3 (color online). The pressure dependence of the mean Si-O (a) bond distance $\bar{r}_{SiO}$ and (b) coordination number $\bar{n}_{Si}^{O}$ as measured by ND (present work) [(black) filled circle] or by XRD in the work from Refs. [5] [(magenta) filled downward triangle], [10] [(green) filled upward triangle] and [11] [(blue) open diamond]. The results are compared to MD simulations using the TS [present work, broken (red) curves] or BKS [49] [solid (cyan) curve] potentials, and to first-principles MD simulations [50] [chained (green) curves]. (c) The pressure dependence of the fractions of Si4 [(blue) filled upward triangle], Si5 [(magenta) filled backward triangle], Si6 [(black) filled downward triangle] and Si7 [(orange) filled circle] sites and of O2 [(red) open square], O3 [(green) open diamond] and O4 [(blue) open upward triangle] sites from the TS MD simulations (present work). (d) The pressure dependence of the preference factors f_{Si5}^{Si5} [(red) filled circle], f_{Si5}^{Si6} [(green) ×] and f_{Si6}^{Si6} [(blue) filled square] from the TS MD model (present work).

XRD results of Refs. [10,11] within the experimental error. The pressure dependence of $\bar{r}_{SiO}$ from the work of Ref. [11] is, however, systematically different from that found from ND and from the XRD results of Refs. [5,10], which may originate from radiation induced annealing [11]. With the exception of these $\bar{r}_{SiO}$ values [11], the TS model gives a good account of the measured changes in $\bar{n}_{Si}^{O}$ and $\bar{r}_{SiO}$ over a wide pressure range extending to 60 GPa. When $\bar{n}_{Si}^{O}$ first increases above four, the MD simulations do not show an increase in $\bar{r}_{SiO}$ but reveal an asymmetric broadening of the first peak in the Si-O partial pair-distribution function $g_{SiO}(r)$ as additional oxygen atoms approach a central Si atom (Supplemental Material [30], Fig. S4). The ND results at pressures above 14.5 GPa also show this behavior as indicated by the shoulder on the high-r side of the first peak in $G(r)$ [Fig. 2(a)] and by the parameters shown in Figs. 3(a)–3(b).

The TS MD results show that, at pressures up to ~10 GPa, the network is dominated by Si4 and O2 sites [Fig. 3(c)], where the Siα and Oα notation refers to α-fold coordinated Si and O atoms, respectively. Structural changes are primarily associated with a reduction of the Si-O-Si bond angle which increases the packing fraction of SiO_4 tetrahedra. At higher pressures, the Si-O-Si bond angle reaches a minimal value of ~90° and $\bar{n}_{Si}^{O}$ increases via the formation of higher coordinated Si sites, where Si5 sites dominate over a window $p \sim 25$–32 GPa and Si6 sites dominate when $p \gtrsim 32$ GPa [Fig. 3(c)]. A small number of Si7 sites form when $p > 40$ GPa. To respect the glass stoichiometry, O2 sites convert to higher coordinated sites, with O3 sites becoming dominant when $p \gtrsim 30$ GPa [Fig. 3(c)].

To establish the atomistic mechanisms of network collapse under cold compression, we first consider the evolution in identity of the Si sites by finding the probability $P(\alpha, p_i \text{ and } \beta, p_j)$ that a given Si atom is α-fold coordinated at pressure p_i and β-fold coordinated at the next highest pressure p_j. As shown in Fig. 4(a), the dominant Si-O coordination number changes are $4 \to 5$ and $5 \to 6$. Few direct $4 \to 6$ changes occur (~6% at $p \sim 30$ GPa), supporting the key role played by Si5 sites as intermediaries in the transformation of silica from a low-pressure tetrahedral to a high-pressure octahedral glass.

The pressure dependence of the mean primitive ring size $\langle n \rangle \equiv \sum n\ell_n / \sum \ell_n$ is given in Fig. 4(b), where ℓ_n is the number of rings comprising a total number of n atoms. A ring is primitive if it cannot be decomposed into smaller rings [20]. The corresponding dependence of $\langle n \rangle$ on $\bar{n}_{Si}^{O}$ is given in the inset to Fig. 4(b). For the cold-compressed material, there is a near-linear dependence between $\langle n \rangle$ and $\bar{n}_{Si}^{O}$. As will be shown, this dependence can be rationalized by a densification mechanism based on successive ring-closure events, where these events result from the formation of Siα sites with $\alpha > 4$.

On cold compression, a single closure event will convert a ring of mean size $\langle n_0 \rangle$ into two rings of mean size $(\langle n_0 \rangle/2) + 1$, thereby increasing the total number of rings from N_0 to $N_0 + 1$. For m such events, it follows that $(N_0 + m)\langle n \rangle = (N_0 - m)\langle n_0 \rangle + 2m[(\langle n_0 \rangle/2) + 1] = N_0\langle n_0 \rangle + 2m$ where $\langle n \rangle$ is the mean ring size after m closures, and it is assumed that these rings remain primitive. An illustration of this process is given in the Supplemental Material [30], Fig. S6.

As shown in Fig. 4(a), the primary Si-O coordination number changes are $4 \to 5$ and $5 \to 6$. One ring closure is therefore necessary to form a Si5 site from a Si4 site, whereas two ring closures are necessary to form a Si6 site from a Si4 site. Thus, if f_α denotes the fraction of α-fold coordinated Si atoms and N_{Si} denotes the total number of Si atoms, then $m = N_{Si}(f_5 + 2f_6)$. If this process were to continue *ad infinitum* then $m = N_{Si}\sum_{\alpha=5}^{\infty}(\alpha - 4)f_\alpha$. Indeed, the MD results show that Si-O coordination number changes of $6 \to 7$ are common at the highest investigated

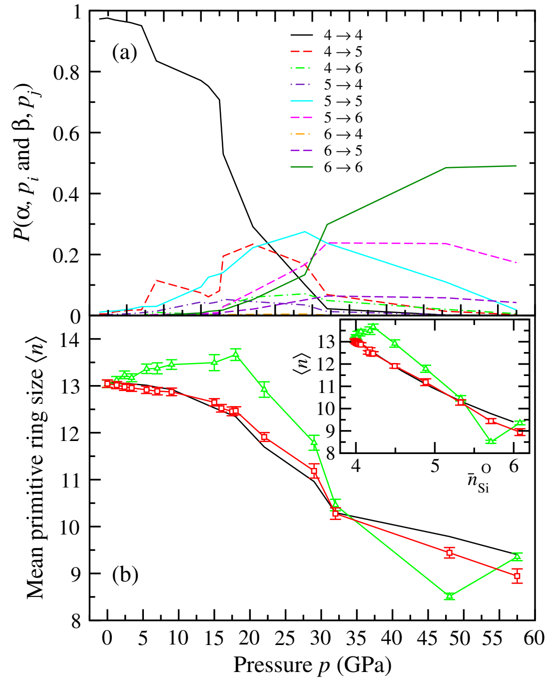

FIG. 4 (color online). (a) The pressure dependence of the probability $P(\alpha, p_i \, \text{and} \, \beta, p_j)$ from cold-compression TS MD simulations. The $\alpha \to \beta$ labels indicate a change (broken curves) or not (solid curves) in the number α of O atoms bound to a Si atom as the pressure is increased from p_i to the next-highest value p_j. (b) The pressure dependence of the mean primitive ring size $\langle n \rangle$ from cold-compression [(red) open square] and quench-from-the-melt [(green) open triangle] TS MD simulations. The inset shows the same information but as a function of $\bar{n}_{\rm Si}^{\rm O}$. In each panel the solid (black) curve gives the prediction of the ring closure model.

pressures, but that changes of $5 \to 7$ or $4 \to 7$ are rare. Provided that no Si atom has a coordination number < 4 then $\bar{n}_{\rm Si}^{\rm O} = \sum_{\alpha=4}^{\infty} \alpha f_\alpha$ or, since $\sum_{\alpha=4}^{\infty} f_\alpha = 1$, it follows that $\bar{n}_{\rm Si}^{\rm O} = 4 + \sum_{\alpha=5}^{\infty} (\alpha - 4) f_\alpha$. Thus, $\langle n \rangle = [N_0 \langle n_0 \rangle + 2N_{\rm Si}(\bar{n}_{\rm Si}^{\rm O} - 4)]\{N_0 + N_{\rm Si}(\bar{n}_{\rm Si}^{\rm O} - 4)\}^{-1}$ or, since in the case of the TS cold-compressed MD model $N_0 = 3.98(16) N_{\rm Si} \simeq 4 N_{\rm Si}$,

$$\langle n \rangle \simeq [4\langle n_0 \rangle + 2(\bar{n}_{\rm Si}^{\rm O} - 4)]/\bar{n}_{\rm Si}^{\rm O}. \quad (1)$$

As shown in Fig. 4(b), the ring closure model gives an accurate description of the cold-compression MD results for the dependence of $\langle n \rangle$ on $\bar{n}_{\rm Si}^{\rm O}$ and also for the dependence of $\langle n \rangle$ on p, where the p versus $\bar{n}_{\rm Si}^{\rm O}$ relationship was taken from MD simulations. It is notable that ~85% of the rings present at ambient pressure in the MD simulations are also present at the highest pressure, although they may no longer be primitive; i.e., many of the initial connections between Si atoms survive to high p. It is also notable that permanent densification in silica glass, which occurs at $p \gtrsim 10$ GPa [2,3,18], is associated with a change in $d\langle n \rangle / dp$ [Fig. 4(b)] but not initially with a substantial increase of $\bar{n}_{\rm Si}^{\rm O}$ above four [Fig. 3(b)]. The ring closure model does not give as accurate a description for the $\langle n \rangle$ versus $\bar{n}_{\rm Si}^{\rm O}$ or p dependence obtained from quench-from-the-melt TS MD simulations where, in accordance with the independent nature of successive liquid configurations, a negligible number ($< 1\%$) of ambient pressure rings are also present at higher p.

To highlight the spatial distribution of the evolving higher coordinated Si sites, we use the preference factor $f_{{\rm Si}\alpha}^{{\rm Si}\beta} \equiv c_{\rm Si} \bar{n}_{{\rm Si}\alpha}^{{\rm Si}\beta} / c_{{\rm Si}\beta} \bar{n}_{{\rm Si}\alpha}^{\rm Si}$ for the tendency of Siβ sites to cluster around Siα sites [51]. If there is no preference for β-fold coordinated Si atoms to occupy the Si sites that surround Siα then $f_{{\rm Si}\alpha}^{{\rm Si}\beta} = 1$. Otherwise, a preference or aversion for occupancy by β-fold coordinated Si atoms gives $f_{{\rm Si}\alpha}^{{\rm Si}\beta} > 1$ or $f_{{\rm Si}\alpha}^{{\rm Si}\beta} < 1$, respectively. The results [Fig. 3(d)] show that when Si5 or Si6 sites first emerge they are more likely to be linked to other Si5 or Si5/Si6 sites, respectively. The rings close, therefore, by a "zipper" mechanism in which a single ring closure event resulting from the formation of a higher-coordinated Siα ($\alpha > 4$) site promotes further closure events at neighboring sites, a process that helps to preserve local charge neutrality (see Supplemental Material [30], Sec. S4). An implication is that the system shows a separation into regions dominated either by Si5 and Si6 sites or by Si4 sites.

In summary, the MD results using the TS interatomic potentials give a good account of both the new ND results and the XRD results of Refs. [6,29] at pressures up to ~20 GPa. They also give a good account of the available XRD data at higher pressures in terms of the Si-O bond lengths from Refs. [5,10] and the Si-O coordination numbers from Refs. [10,11]. Fivefold coordinated Si atoms are found to act as important intermediaries in the transformation from a tetrahedral to an octahedral glass where Si6 sites dominate. A model in which rings are "zipped" by a pairing of higher-coordinated Si sites describes the simulated dependence on $\bar{n}_{\rm Si}^{\rm O}$ of the mean primitive ring size $\langle n \rangle$, which is a measure of structural ordering over multiple length scales. The role played by oxygen packing in the structural transformations that occur in SiO_2 and in other oxide glasses is described elsewhere [52].

The zipper model should be applicable to the cold compression of other chemically ordered glass-forming networks and thereby help in understanding phenomena such as permanent densification. The model also provides a coarse-grained reference for the $\langle n \rangle$ versus $\bar{n}_{\rm Si}^{\rm O}$ dependence obtained from quench-from-the-melt modeling [Fig. 4(b)], despite the reorganization of rings via diffusive processes, and will act as a guide in the development of ring closure models for modified silicate networks. All of this is important because network connectivity governs, e.g., the equation of state and transport properties for both silica and geophysically relevant silicates [12,16,53,54].

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[30] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.113.135501 which contains (i) the background theory, (ii) the details of the neutron diffraction and molecular dynamics methods, (iii) some supplemental results to emphasise the validity of our approach, (iv) an illustration of a stage in the "zipper" ring closure process, and (v) Refs. [31–43].
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