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Table S1: Predicted glass structures expressed in terms of coordination environments, $C_{\alpha\beta}$'s where α and β represent atomic species under consideration, and average bond lengths λ (Å) at the ambient volume and at 300 K obtained by quenching liquid $MgSiO_3$ from 3000 K and 5000 K. The numbers are presented within three significant figures. (FO: free oxygen, NBO: non-bridging oxygen, BO: bridging oxygen, O3: oxygen tri-cluster).

	640 atoms Quench rate = 0.5K/fs			
	quench from 3000 K		quench from 5000 K	
C_{SiO} (3-, 4-, 5-fold)	4.05 (0.00, 95, 5.0)	λ = 1.64	4.05 (0.00, 96, 4.00)	λ = 1.64
C_{OSi} (FO, NBO, BO, O3)	1.35 (1.6, 62, 37, 0.00)		1.35 (1.0, 63, 36, 0.00)	
C_{MgO} (3-, 4-, 5-, 6-fold)	4.60 (3.0, 42, 49, 6.0)	λ = 2.05	4.53 (1.0, 50, 44, 5.0)	λ = 2.05
C_{OMg} (0-, 1-, 2-, 3-, 4-fold)	1.53 (20, 20, 50, 9.3, 1.6)		1.51 (17, 23, 51, 8.0, 1.0)	

Table S2: Pressure variations of three elastic constants (c_{11}, c_{12}, c'_{44})) with pressure for the cold (top) and hot (bottom) compressed glasses. Root mean square deviations are shown in the parentheses. Here $c'_{44} = \frac{1}{9}\sum_{mm} c_{mm}$, where m = 4, 5, 6. See equation 8 and the related text for more details of the calculations. The uncertainties were estimated based on the different values obtained with different strains.

P (GPa)	c_{11} (GPa)	c_{12} (GPa)	(c_{11}-c_{12})/2 (GPa)	c'_{44} (GPa)
-1.1	80 (6)	24 (2)	28	29 (1)
4.7	116 (11)	51 (9)	33	34 (2)
5.3	116 (2)	57 (4)	29	35 (1)
16	238 (7)	126 (2)	56	50 (2)
38	380 (10)	234 (7)	73	73 (4)
66	509 (7)	325 (6)	92	92 (5)
109	656 (25)	446 (20)	105	126 (5)
170	908 (29)	698 (30)	105	154 (11)

P (GPa)	c_{11} (GPa)	c_{12} (GPa)	(c_{11}-c_{12})/2 (GPa)	c'_{44} (GPa)
0.8	99 (4)	41 (4)	29	33 (1)
1.9	126 (3)	54 (2)	36	39 (2)
12	206 (8)	97 (4)	55	51 (2)
37	385 (9)	215 (4)	85	76 (4)
62	516 (10)	297 (9)	109	108 (3)
105	714 (7.0)	467 (10)	123	130 (9)
169	960 (39)	629 (15)	165	167 (10)

Figure S1: Time convergences of the enthalpies of the $MgSiO_3$ glass structure. Upper, middle and lower panels depict three different volumes.

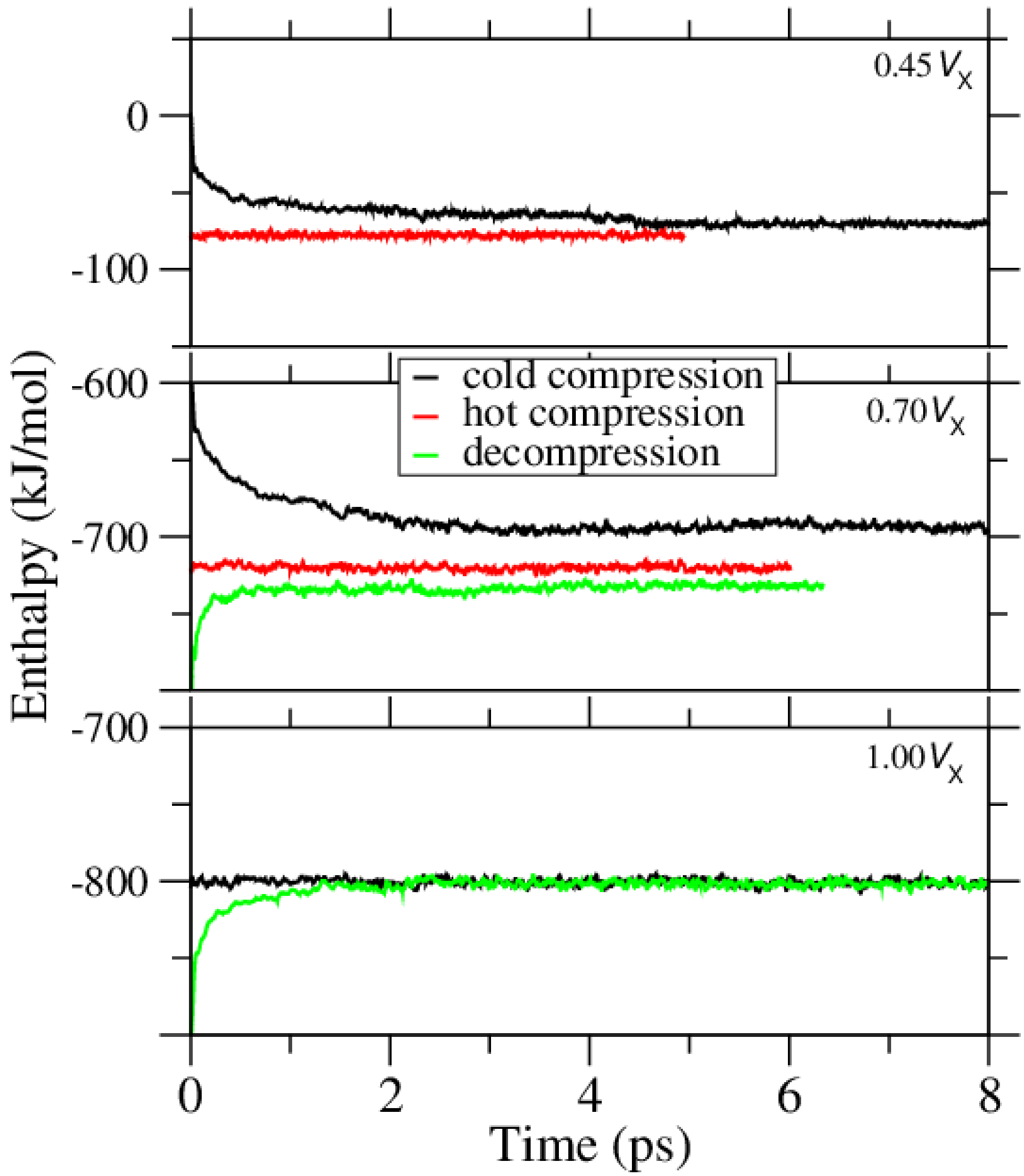

Figure S2. Temperature vs. enthalpy for 160 atom simulation cells. The equilibrated liquid at 3000 K was quenched at 0.5 K/fs with step sizes of 150 K (red) and 300 K (black). Each of the state points was equilibrated for 5 ps before quenching to the next state point. The intersection of the two regimes corresponds to the estimated glass transition temperature. (red: ~2030 K; black: ~2090 K). Note that considering the equilibration time, the effective cooling rate [150/(5000+150*2) = 0.0283 K/fs] is lower in case of 150 K quench step size (red) in comparison to the 300 K quench step size (0.0536 K/fs). This is consistent with the fact that slower cooling rate leads to lower glass transition temperature.

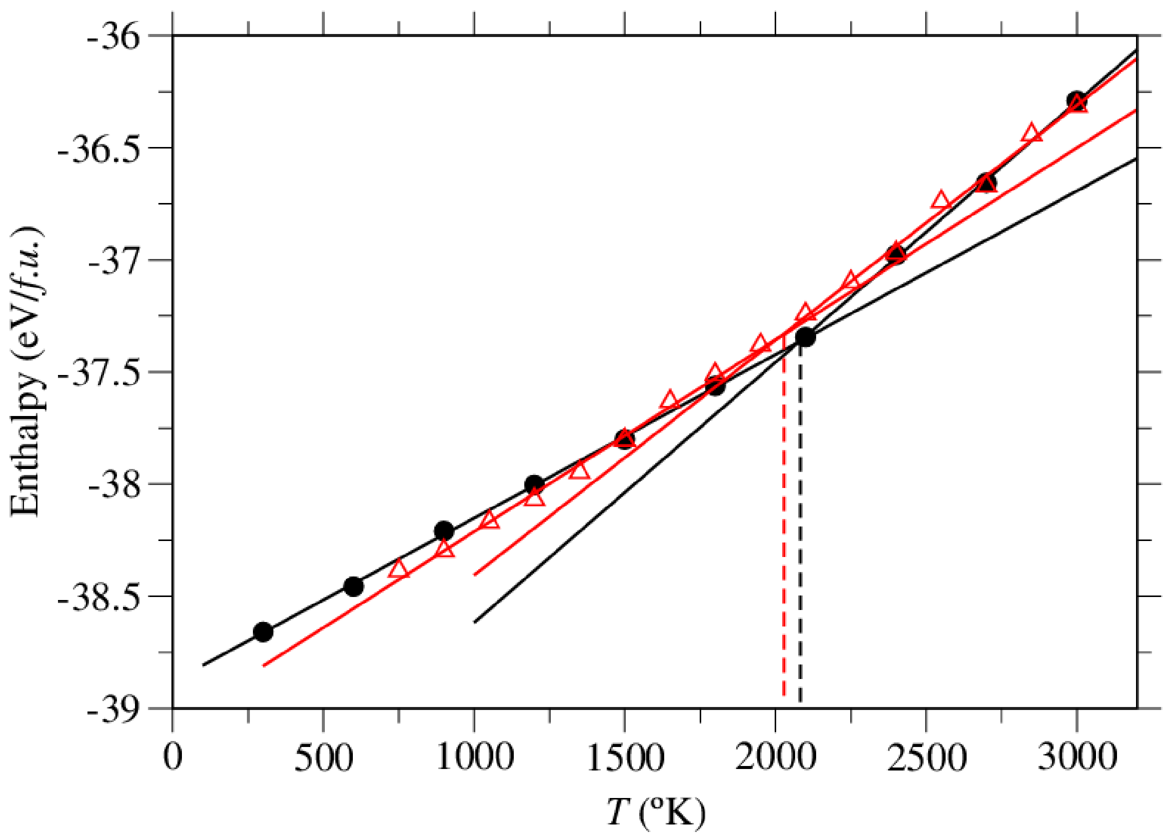

Figure S3. Total structure factors, neutron (left) and X-ray (right), at different volumes for compression (cold and hot) and decompression. Also shown for comparison are the experimental structure factors at ambient pressure (Wilding et. al., 2004). For the clarity, plots for $0.70V_x$ and $0.45V_x$ are shifted upward in *y*-direction by 1 and 2 units, respectively.

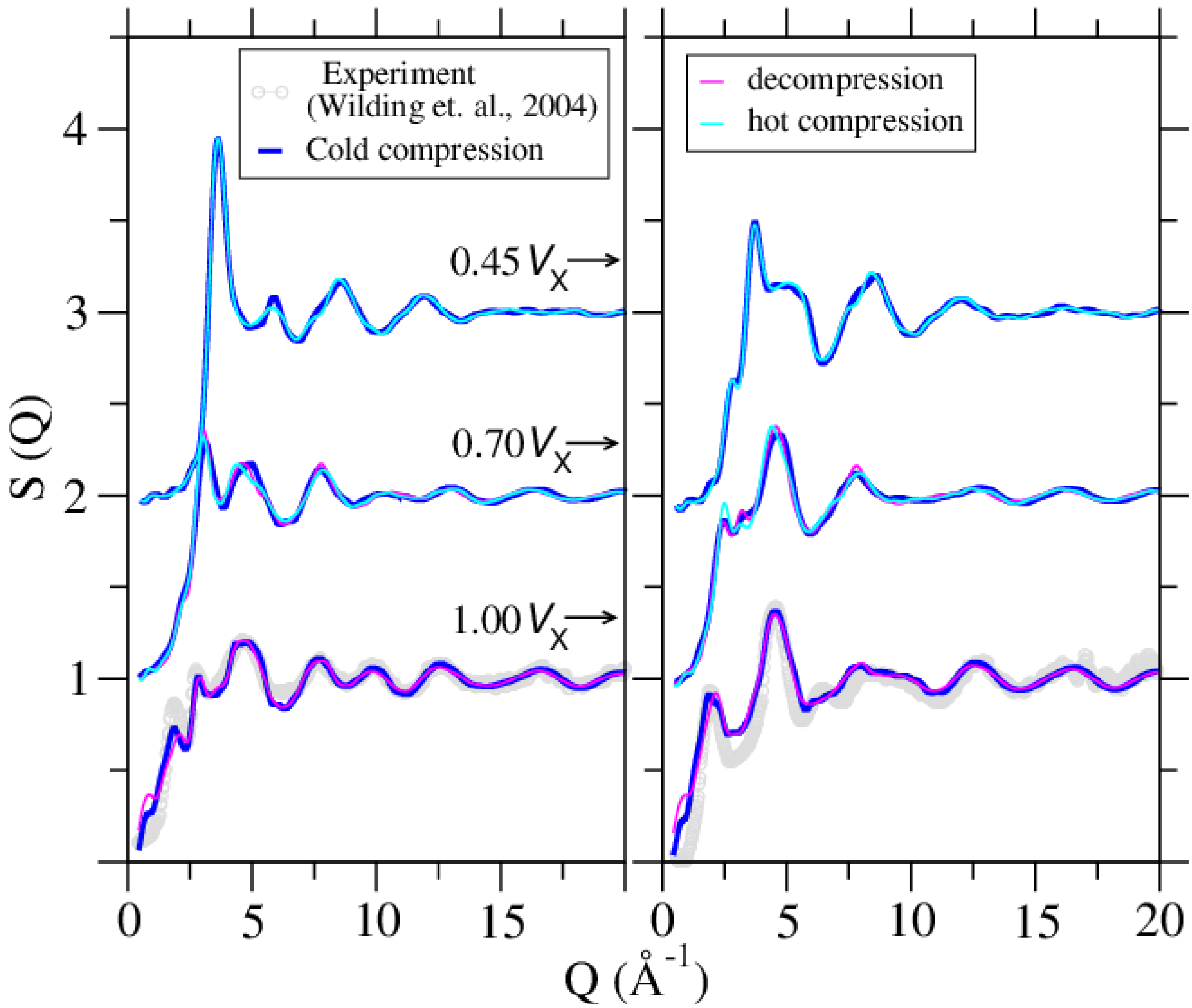

Figure S4. The pressure variations of the average inter-atomic distances along the cold (solid lines) and hot (dashed lines) compression.

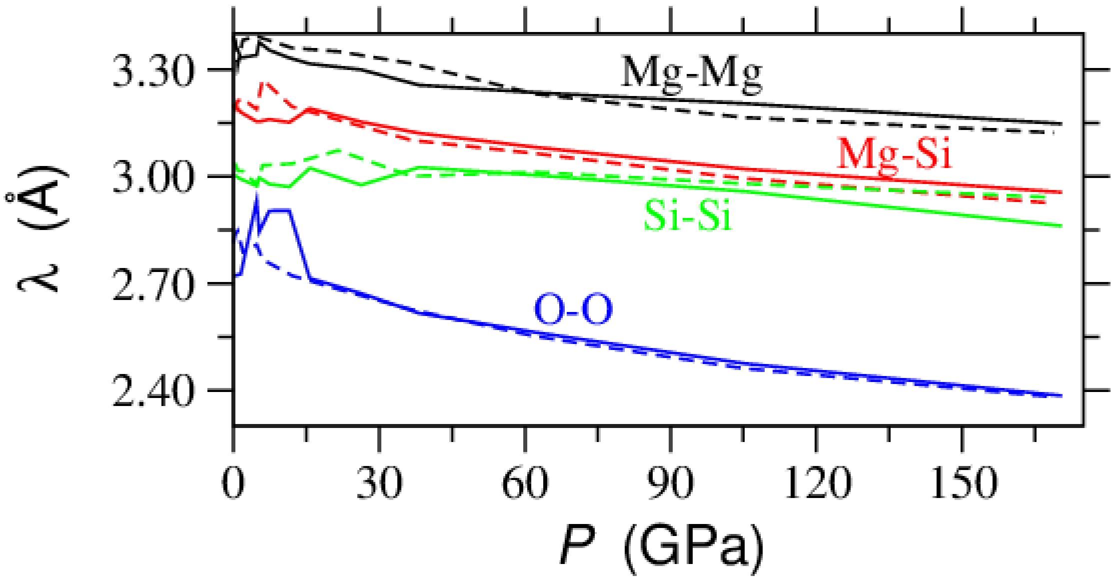

Figure S5. The mean coordination numbers as a function of pressure along the cold (solid lines) and hot (dashed lines) compression.

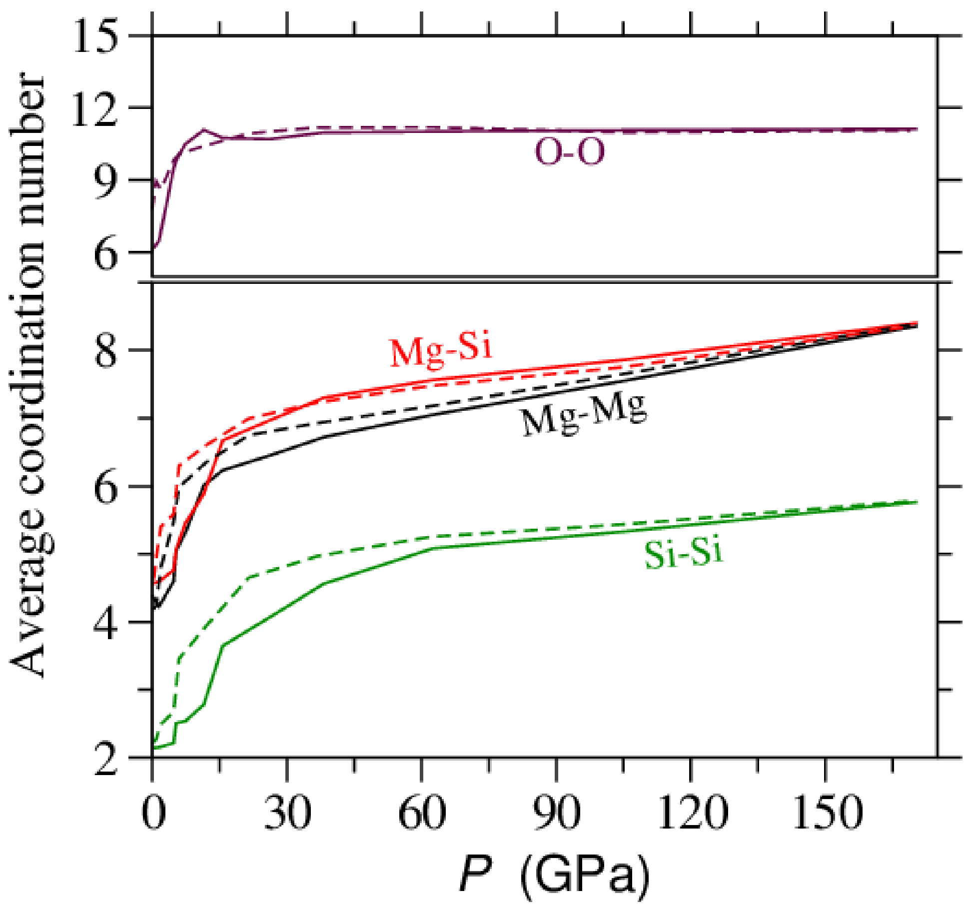

Figure S6. Calculated bond angle distributions for the 160 atom simulation cells. Decompression from different peak pressures: 6 GPa (red), 27 GPa (magenta) and 174 GPa (blue). Gray curves correspond to the distribution for the uncompressed (V_X) case. Individual curves are shifted in *y*-direction for the clarity.

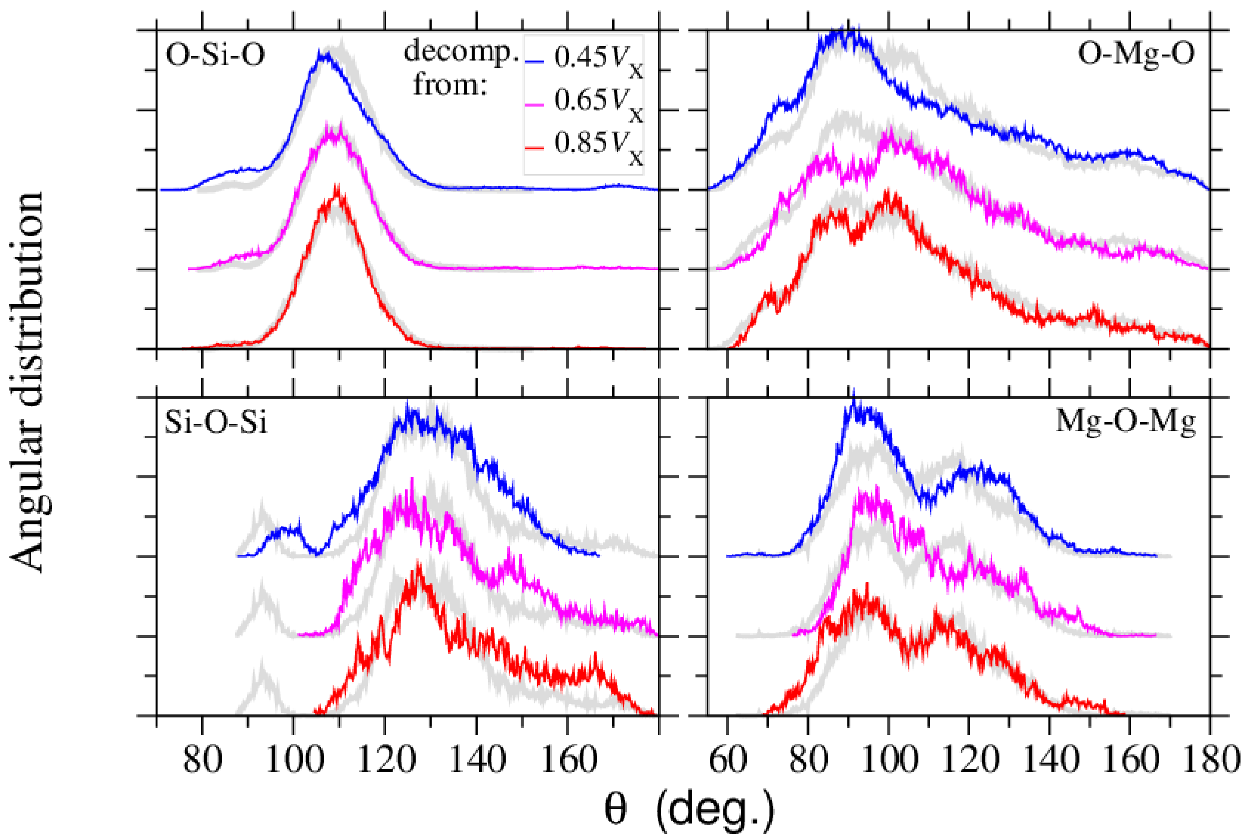

Figure S7. Calculated distributions (normalized) of O–Si–O, Si–O–Si, O–Mg–O and Mg–O–Mg angles at different volumes (V_X, 0.7V_X and 0.45V_X) along the cold compression. Also shown are the hot compressed results (gray line) at 0.7V_X. Distributions for liquid $MgSiO_3$ (3000 K) at V_X (blue) and 0.45V_X (brown) are also shown for comparison.