Supporting Information

Atomistic insight into the ferroelastic post-stishovite transition by high-pressure single-crystal X-ray diffraction refinements

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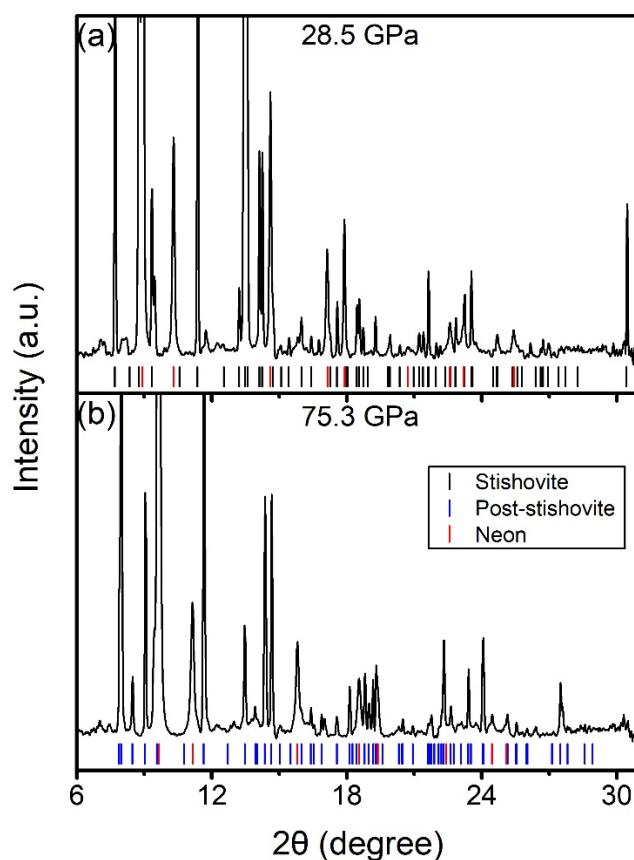
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FIGURE S1. Integrated two-dimensional x-ray diffraction patterns at high pressure. (a) Stishovite at 28.5 GPa; (b) post-stishovite at 75.3 GPa. The wavelength of X-ray beam is 0.2952 Å. Diffraction peaks of stishovite, post-stishovite, and neon are marked with black, blue, and red ticks, respectively.
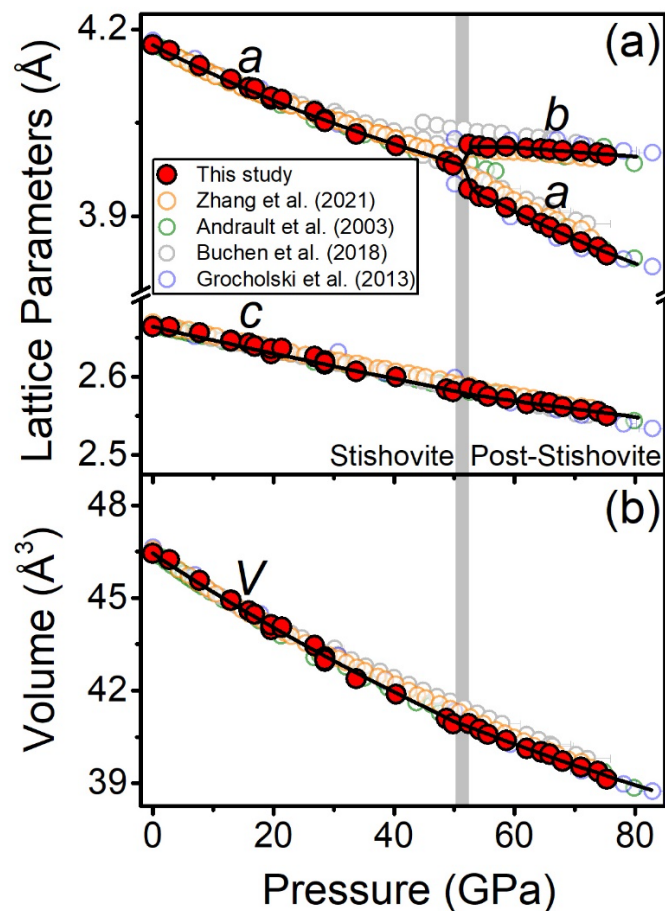
FIGURE S2. Lattice parameters and unit-cell volume of stishovite and post-stishovite at high pressure. (a) Axial length of *a*, *b*, and *c* axis; (b) unit-cell volume *V*. Lines show the best fits using the axial incompressibility or the Birch-Murnaghan equation of state (Birch, 1947). The gray vertical band shows the transition pressure. Literature results are also plotted for comparison (Andrault et al., 2003; Buchen et al., 2018; Grocholski et al., 2013; Zhang et al., 2021).
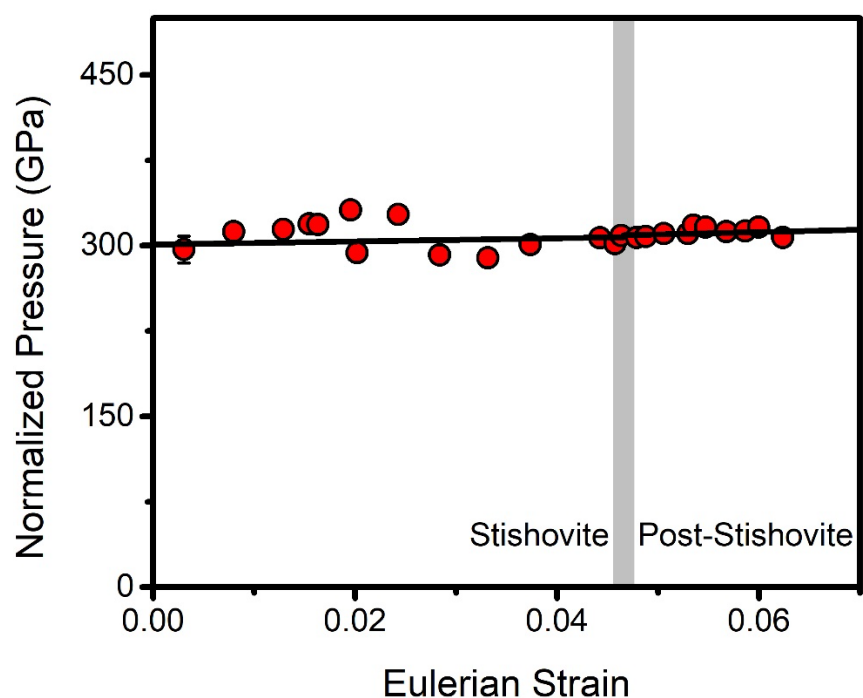
FIGURE S3. Normalized pressure as a function of Eulerian strain (*F-f* plot) for stishovite and post-stishovite phases at high pressure. Based on the Birch-Murnaghan equation of state, f and F are defined as $f = [(V_0/V)^{2/3}-1]/2$ and $F = P/[3f(2f+1)^{5/2}]$, respectively, where V_0 is the unit-cell volume at ambient pressure, V is the volume at high pressure, and P is the pressure (Angel, 2000; Birch, 1947). Lines are the best linear fits to the experimental data. The gray vertical band shows the transition region.
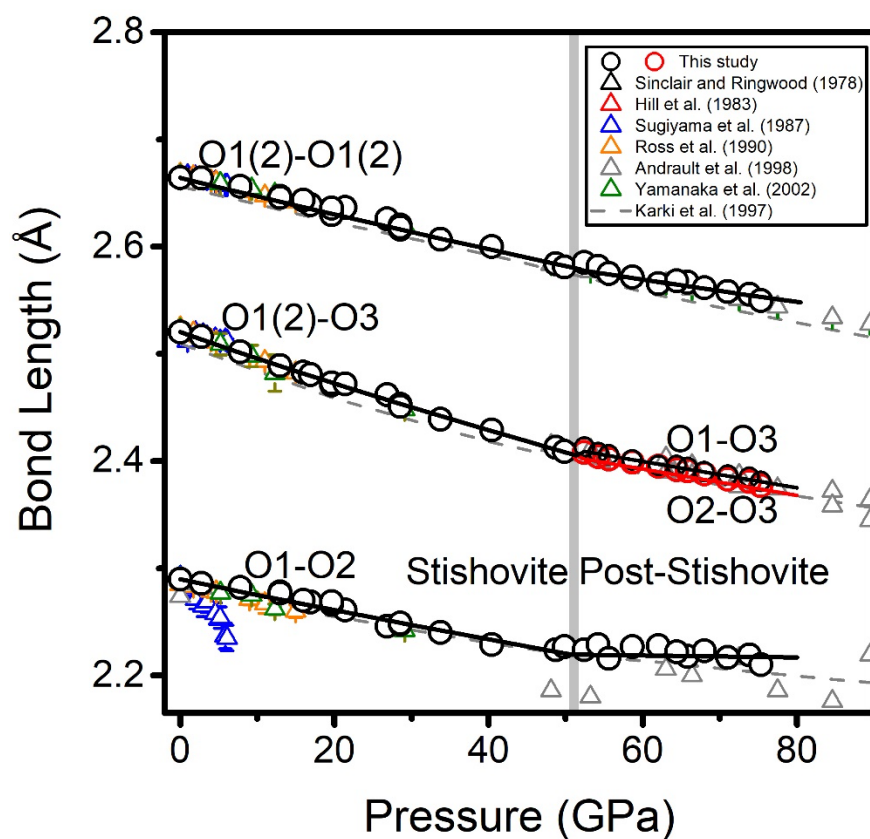
FIGURE S4. O-O interatomic distances in stishovite and post-stishovite at high pressure. Black solid lines show the best fits using the axial incompressibility (Birch, 1947). Please refer to Figure 2 for the meaning of the atom symbols next to the data. Literature data are shown for comparison (Andrault et al., 1998; Hill et al., 1983; Karki et al., 1997; Ross et al., 1990; Sinclair & Ringwood, 1978; Sugiyama et al., 1987; Yamanaka et al., 2002).
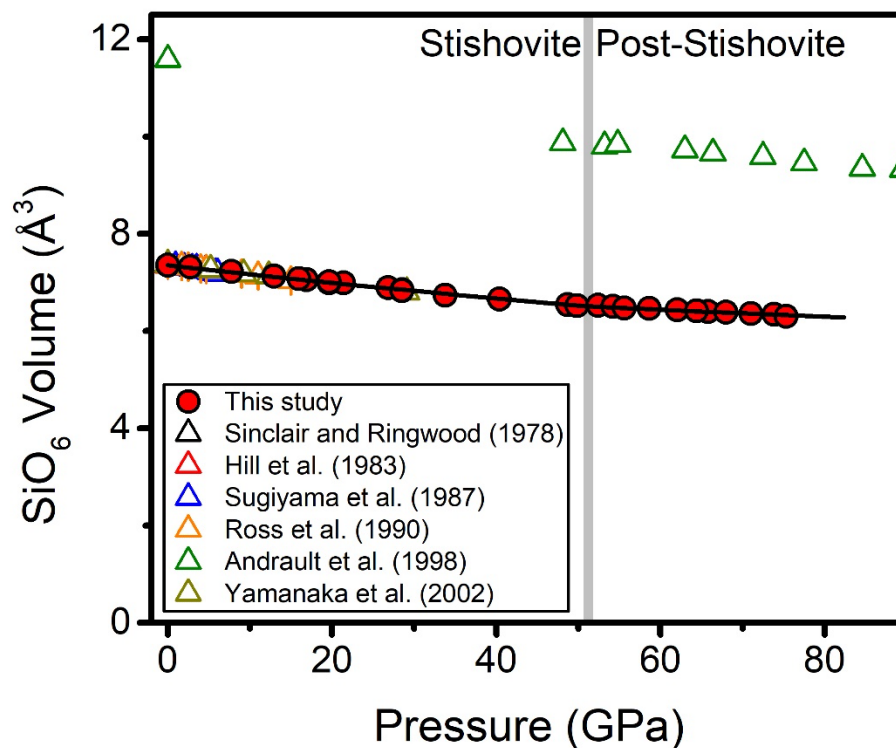
FIGURE S5. Volume of the SiO_6 octahedron in stishovite and post-stishovite at high pressure. The black solid line represents the best fit to the data using the Birch-Murnaghan equation of state (Birch, 1947). Previous studies are plotted as open triangles for comparison (Andrault et al., 1998; Hill et al., 1983; Ross et al., 1990; Sinclair & Ringwood, 1978; Sugiyama et al., 1987; Yamanaka et al., 2002).

TABLE S1. Equation of state parameters of stishovite and post-stishovite phases

References	Stishovite			Post-stishovite		
	V_0	K_{T0}	K_T'	V_0	K_{T0}	K_T'
This study	46.6(2)	301.2(18)	4.1(2)	47.54(33)	259.1(61)	4.1(3)
Andrault et al. (2003)	46.5	309.9(11)	4.59(23)	46.31(15)	334(7)	4 (fixed)
Buchen et al. (2018)	46.4(1)	344(25)	6.0(11)	48.22(44)	241(18)	4.72(4)
Fischer et al. (2018)	46.6	302	5.24(9)	46.6	341(4)	3.20(16)
Nisr et al. (2017)	46.569	312(2)	4.59 (fixed)			

Note: V_0, K_{T0}, and K_T' are unit-cell volume, isothermal bulk modulus, and its pressure derivative at ambient conditions, respectively. Numbers in parentheses represent $\pm 1\sigma$ uncertainties.