Supporting Information

Enhanced optical anisotropy of six-coordinated silica polymorphs via high-pressure hydrothermal treatment

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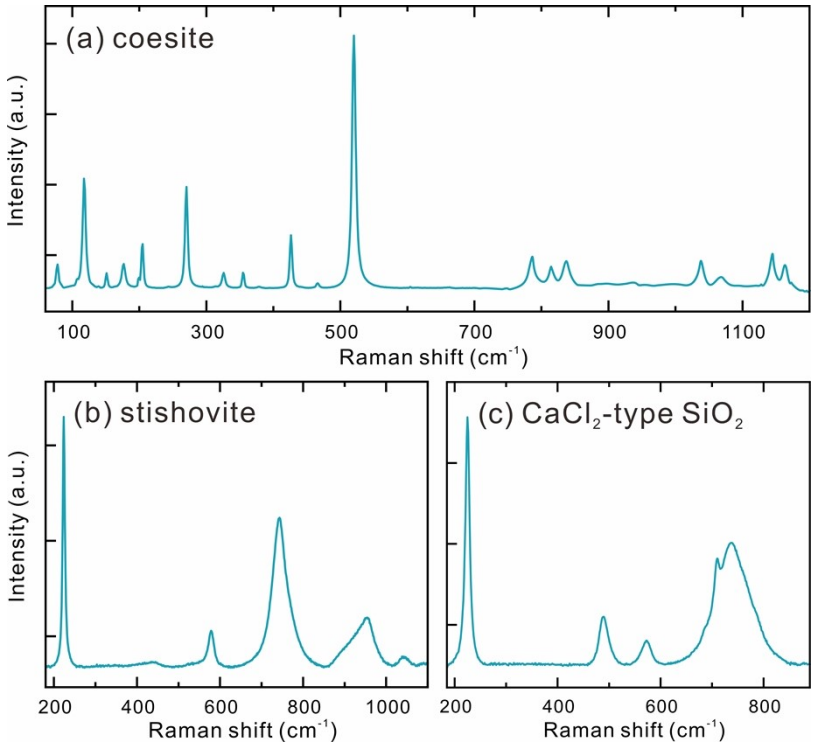

Figure S1. Raman spectra of coesite (a), stishovite (b) and $CaCl_2$-type SiO_2 (c) single crystals at ambient conditions.

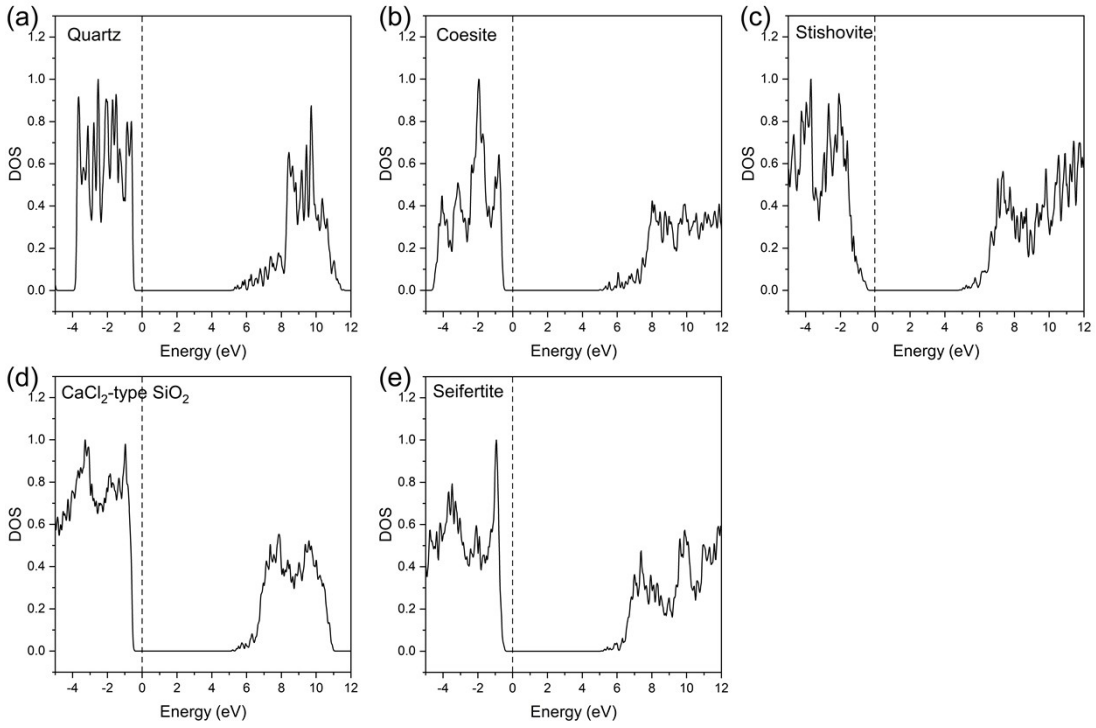

Figure S2. DOS of quartz (a), coesite (b), stishovite (c), $CaCl_2$-type SiO_2 (d) and seifertite (e) at 1 atmosphere and static conditions. The structure of $CaCl_2$-type SiO_2 is obtained from a previous study and free of Al.

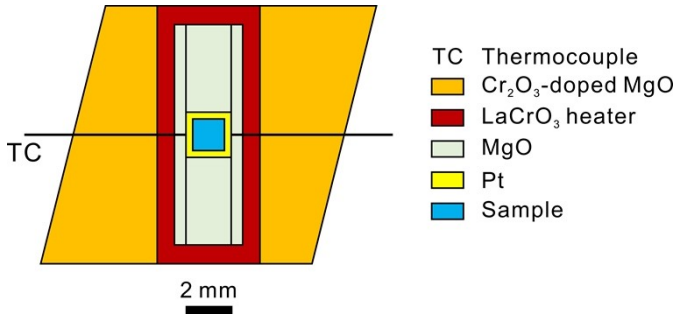

Figure S3. Schematic drawing of the cell assembly used for synthesizing coesite in this study. The cell assembly used for synthesizing stishovite is similar, but with smaller size.

Table S1. Chemical compositions of recovered products determined by electron probe microanalysis.

Phase	SiO_2 (wt %)	Al_2O_3 (wt %)	Total (wt %)
Coesite	99.03(42)	0.21(13)	99.23(58)
Stishovite	98.19(35)	0.30(11)	98.51(47)
$CaCl_2$-type silica	89.29(68)	8.90(16)	98.20(70)

Table S2. Crystal data and structure refinements for coesite, stishovite and $CaCl_2$-type silica.

Phase	Coesite	Stishovite	$CaCl_2$-type silica
Synthesis conditions	9 GPa, 1000 ℃	23 GPa, 1600 ℃	24 GPa, 1900 ℃
Water content	200 ppm	0.62(15) wt %	1.08(5) wt %
Crystal system	Monoclinic	Tetragonal	Orthorhombic
Space group	*C*2/*c*	$P4_2/mnm$	*Pnnm*
a (Å)	7.141(2)	4.1998(3)	4.2573(7)
b (Å)	12.383(4)	4.1998(3)	4.1844(7)
c (Å)	7.118(2)	2.6741(3)	2.6828(10)
α (°)	90	90	90
β (°)	119.553(9)	90	90
γ (°)	90	90	90
V (Å^3)	547.5(3)	47.167(9)	44.79(2)
Z	16	2	2
Temperature (K)	296(2)	296(2)	293(2)
F (000)	240	60	60
θ_{max} (°)	22.150	32.836	40.327
Index ranges	$-7\leq h\leq 6$; $-12\leq k\leq 13$; $-7\leq l\leq 6$	$-3\leq h\leq 5$; $-5\leq k\leq 5$; $-3\leq l\leq 4$	$-7\leq h\leq 7$; $-7\leq k\leq 7$; $-3\leq l\leq 4$
Reflections collected	864	256	928
Independent reflections/ R_{int}	224 / 0.0494	49 / 0.0122	169 / 0.0309
Number of parameters	24	8	11
Goodness of fit on F^2	1.181	1.249	1.185
Final *R* indices [I > 2σ(I)]	R_1 = 0.0437, wR_2 = 0.1024	R_1 = 0.0254, wR_2 = 0.0680	R_1 = 0.0344
R indices (all data)	R_1 = 0.0770, wR_2 = 0.1224	R_1 = 0.0268, wR_2 = 0.0695	R_1 = 0.0339, wR_2 = 0.09