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Supporting information for article:

Using powder XRD and pair distribution function to determine anisotropic atomic displacement parameters of orthorhombic tridymite and tetragonal cristobalite

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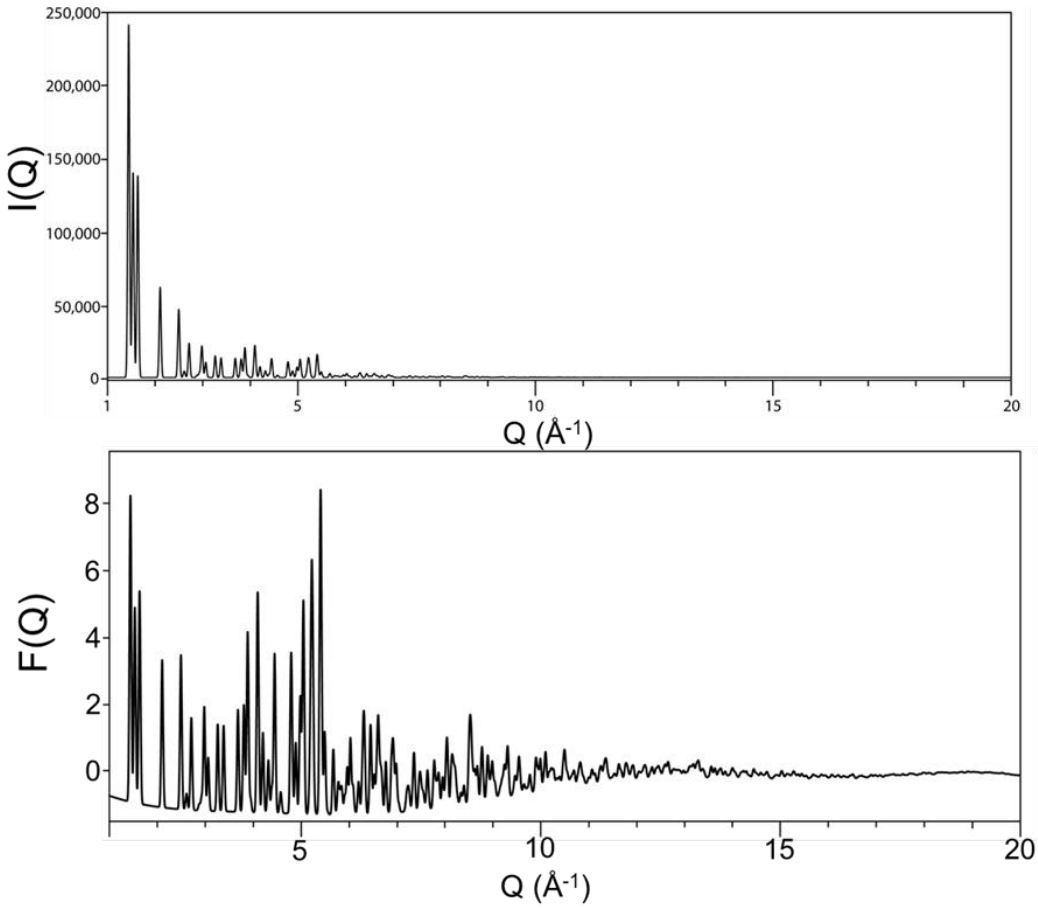

Figure S1 Synchrotron radiation XRD patterns I(Q) with reduced structure factor F(Q) of orthorhombic tridymite.

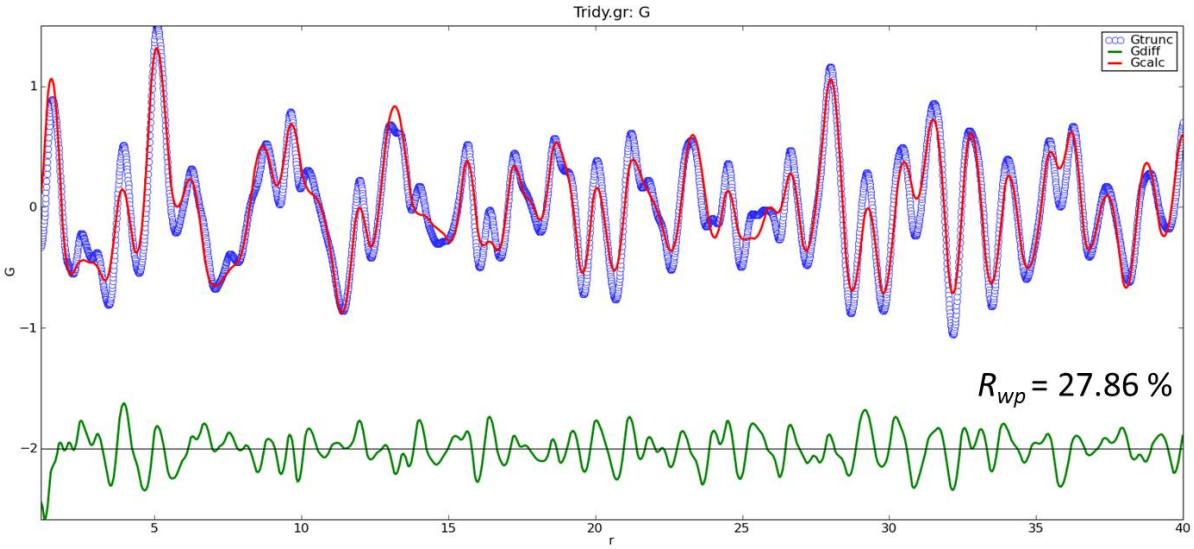

Figure S2 PDF fitting of synthetic tridymite using the structure model with ADPs from Kihara *et al*., (1986).

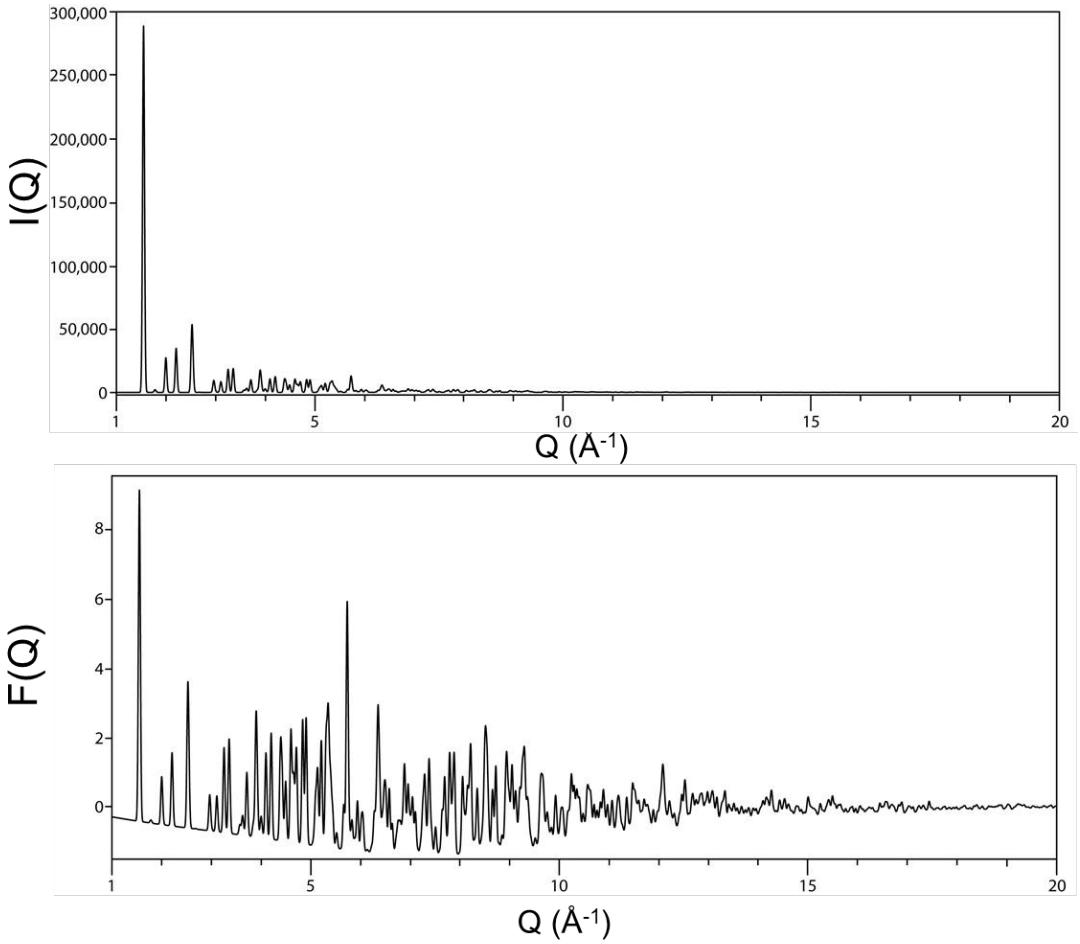

Figure S3 Synchrotron radiation XRD patterns I(Q) with reduced structure factor F(Q) of tetragonal tridymite.

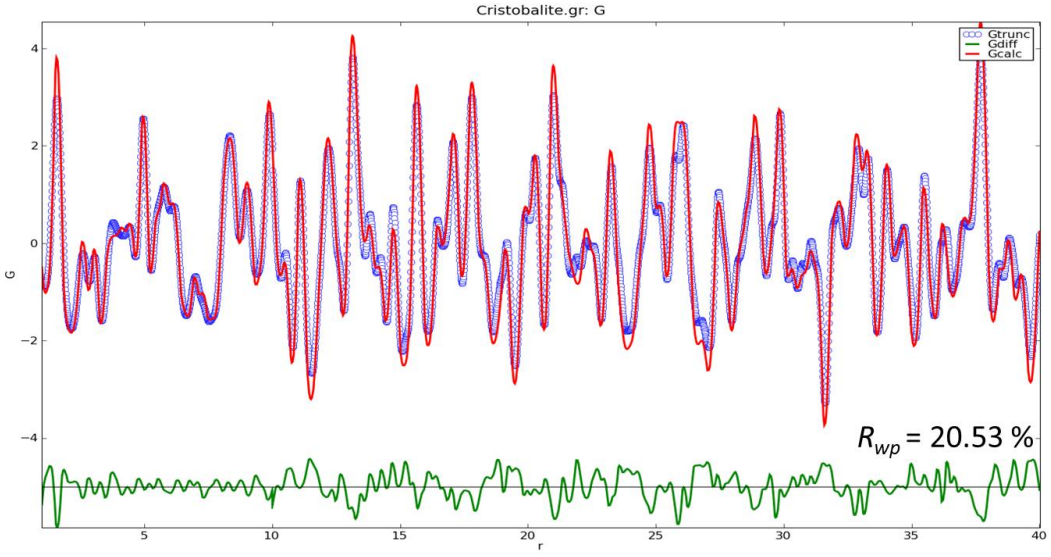

Figure S4 PDF fitting of natural tetragonal cristobalite using structure model with ADPs from Downs & Palmer (1994).

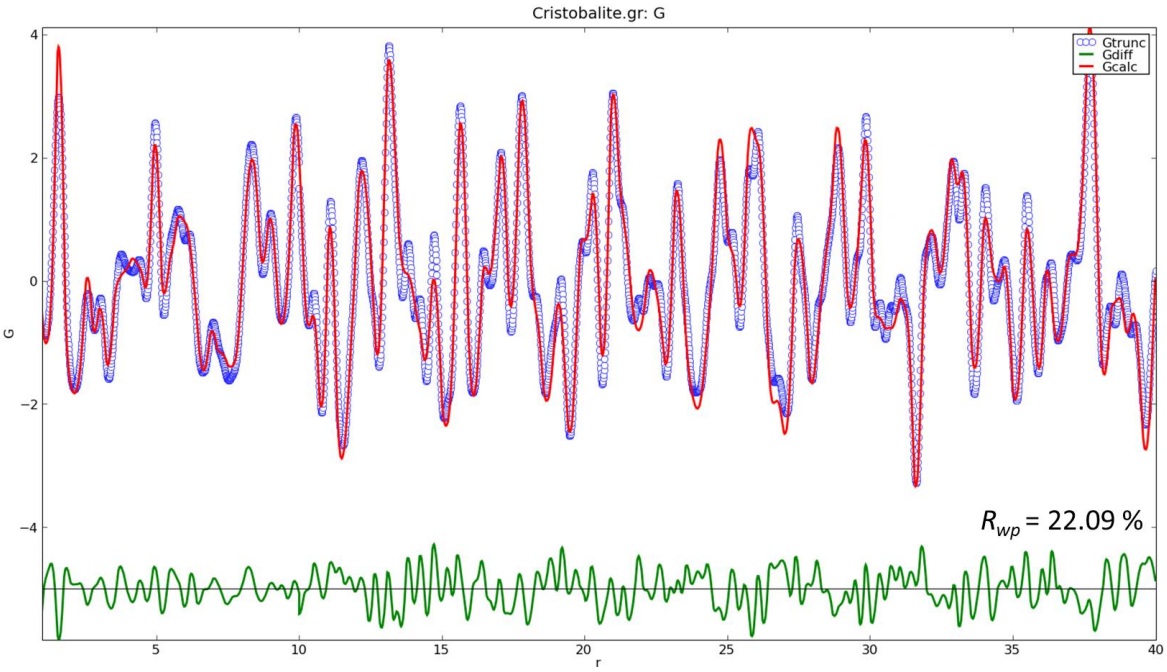

Figure S5 PDF fitting of synthetic cristobalite using structure model with ADPs from Pluth *et al.*, (1985).

Table S1 Atomic coordinates and unit cell parameters of tridymite ($C222_1$) calculated by Rietveld refinement from Figure 3.

Atom	x	y	z	U_{iso}
Si	0.1672(2)	0.5459(2)	0.1877(1)	0.0329(6)
O1	0.3315(5)	0	0.5	0.0455(5)
O2	0	0.5587(7)	0.25	0.0113(3)
O3	0.2522(3)	0.3139(4)	0.2729(3)	0.0134(3)
Lattice parameters: a = 8.7549(5) Å, b = 5.0335(3) Å, c = 8.2118(4) Å				

Table S2 Atomic coordinates and anisotropic thermal displacement parameters of a synthetic tridymite (Kihara *et al*., 1986).

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si	0.1664	0.5467	0.1877	0.037	0.0439	0.0359	-0.0029	0.001	-0.0048
O1	0.3308	0	0.5	0.0971	0.0904	0.0372	0	0	0.0213
O2	0	0.5583	0.25	0.0451	0.0991	0.0128	0	0.0448	0
O3	0.2519	0.3149	0.2733	0.0959	0.0573	0.0923	0.0301	-0.03	0.0094
Lattice parameters: a = 8.756(8) Å, b = 5.024(3) Å, c = 8.213(4) Å									

Table S3 Atomic coordinates and unit cell parameters of tridymite ($C222_1$) calculated by PDF refinement with U_{iso} configuration from Figure 4A.

Atom	x	y	z	U_{iso}
Si	0.1672(2)	0.5459(2)	0.1877(1)	0.029(3)
O1	0.3315(5)	0	0.5	0.039(6)
O2	0	0.5587(7)	0.25	0.027(4)
O3	0.2522(3)	0.3139(4)	0.2729(3)	0.018(3)
Lattice parameters: a = 8.7549(5) Å, b = 5.0335(3) Å, c = 8.2118(4) Å				

Table S4 Atomic coordinates and unit cell parameters of tetragonal cristobalite ($P4_12_12$) calculated by Rietveld refinement from Figure 7.

Atom	x	y	z	U_{iso}
Si	0.3007(3)	0.3007(3)	0	0.0114(3)
O	0.2390(5)	0.1041(2)	0.1787(2)	0.0178(3)
Lattice parameters: a = 4.9727(6) Å and c = 6.9257(5) Å				

Table S5 Atomic coordinates and unit cell parameters of tetragonal cristobalite ($P4_12_12$) calculated by PDF refinement U_{iso} configuration from Figure 8A.

Atom	x	y	z	U_{iso}
Si	0.3007(3)	0.3007(3)	0	0.009(2)
O	0.2390(5)	0.1041(2)	0.1787(2)	0.019(3)
Lattice parameters: a = 4.9727(6) Å and c = 6.9257(5) Å				

Table S6 Atomic coordinates and unit cell parameters of tetragonal cristobalite (Downs & Palmer, 1994).

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si	0.3003(1)	0.3003(1)	0	0.0096(1)	0.0096(1)	0.0097(1)	-0.0003(2)	0.0014(1)	-0.0014(1)
O	0.2392(2)	0.1044(2)	0.1787(1)	0.0306(7)	0.0108(5)	0.0151(2)	-0.0016(4)	0.0047(3)	0.0008(3)
Lattice parameters: a = 4.9717(4) Å and c = 6.9223(3) Å									

Table S7 Atomic coordinates and unit cell parameters of tetragonal cristobalite (Pluth *et al*., 1985).

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si	0.3005(3)	0.3005(3)	0	0.0130(6)	0.0130(6)	0.0136(4)	0.024(5)	0.004(3)	-0.004(3)
O	0.2392(3)	0.1037(2)	0.1786(2)	0.0399(8)	0.0086(6)	0.0218(4)	-0.004(5)	0.003(3)	0.006(2)
Lattice parameters: a = 4.9709(1) Å and c = 6.9278(2) Å									