Coesite (SiO$_2$) as an extreme case of superheated crystal: An X-ray diffraction study up to 1776 K

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Abstract

The dense SiO$_2$ polymorph coesite has been investigated by X-ray powder diffraction from room temperature up to 1776 K. No phase transition has been detected in this temperature interval. Thermal expansion shows little anisotropy and remains very small since the volume increases by only 1.6% between 300 and 1776 K. As indicated by theoretical simulations, the small dilation results from limited rotations of SiO$_4$ tetrahedra and also from slight expansion of Si–O bonds. In addition, the results demonstrate that coesite can be kept 900° above its metastable congruent temperature of fusion which is about 875 K. Comparisons with measurements made under the same conditions for quartz and cristobalite indicate that, for SiO$_2$ polymorphs with 4-fold coordinated Si, crystal structure exerts a smaller influence than melt viscosity on the extent of superheating.
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1. Introduction

Coesite, which was first observed in the laboratory (Coes, 1953), is the densest SiO$_2$ polymorph in which silicon is tetrahedrally coordinated to oxygen. Its geophysical relevance stems from the fact that it has been identified in materials shocked through meteorite impact (Chao et al., 1960) and in the context of low-temperature, high-pressure metamorphism (Chopin, 1984). Between about 3 and 9 GPa, the stability field of coesite is in fact intermediate between those of quartz and stishovite, the high-pressure SiO$_2$ polymorph stable in which silicon is six-fold coordinated (see Heaney et al., 1994).

Comparison between SiO$_2$ polymorphs are useful to understand how their properties depend on the arrangement of SiO$_4$ tetrahedra. For modeling mineral properties with the polyhedral approach, those of coesite are in particular relevant to dense phases in which silicon remains tetrahedrally coordinated. There are in fact important differences between the properties of coesite and those of the other SiO$_2$ polymorphs with tetrahedrally coordinated Si stable at lower pressure. For instance, coesite has a much smaller thermal expansion coefficient than both quartz and cristobalite. In addition, contrary to these polymorphs, coesite does not undergo α–β transitions at least up to 1300 K, the highest temperature at which it has been hitherto investigated (Skinner, 1962; Galkin et al., 1987).

In this work, our purpose was to investigate the thermal expansion and stability of coesite at higher temperature than made previously. Using the same

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procedure as in our study of quartz and cristobalite (Bourova and Richet, 1998), we have measured the cell parameters from powder X-ray diffraction experiments performed up to about 1800 K. These measurements have also been used as a check for high-temperature lattice dynamics and molecular dynamics simulations of coesite (Bourova et al., 2004). These simulations, in turn, will be used to interpret structurally the present structural data, thus obviating the current lack of high-temperature single-crystal diffraction measurements.

Coesite also deserves interest from a more theoretical standpoint as the highest temperatures at which it could be observed in our X-ray diffraction experiments is much higher than 875 K, its metastable melting temperature determined from thermochemical data (Richet, 1988). In other words, coesite superheats by about 900° and thus represents an extreme case of a phenomenon which is usually assumed to be either impossible or limited to very narrow intervals above the melting point. From available structural data, another goal of this study is thus to account for this unusual feature which throws some light on the melting process and, thus, provides one with an indirect perspective on the liquid state.

2. Experimental methods

Coesite was synthesized at 1293 K and 9 GPa in a MAX80-type multianvil apparatus with a 1000-ton press (Villetaneuse University). Pressures were calibrated from the phase transitions of Bi I–II (2.6 GPa), Bi II–III (5.6 GPa) and Sn (11.4 GPa) as determined from electrical conductivity measurements. The starting material was a small disk of α-quartz, with a height of 1 mm and a diameter of 2 mm. This disk was embedded in a thin Pt foil, surrounded by a cylindrical graphite furnace, and inserted in MgO cube with edge lengths of a 7.2 mm. This assembly was compressed at 9 GPa by 6 cubic tungsten carbide anvils and then heated to 1000 °C for 1 h. The temperature was finally quickly dropped and the pressure slowly released in 12 h. The Raman spectrum of the sample agreed with reported data (Hemley, 1987), but showed a few extra low-intensity peaks that could be attributed to traces of untransformed quartz. Although the same observation was made in the X-ray diffraction patterns, the presence of quartz did not affect the derived unit-cell parameters because of generally limited overlap between the coesite and quartz reflections.

To avoid orientation effects that could affect the relative intensities of the reflections in the diffraction patterns, we investigated a sample with a very fine grain size of a few microns. After grinding the sample in an agate mortar under ethanol, the very fine suspended fraction was pipetted and then dried. This powder was heated in the 400-μm hole drilled in the 1-mm in diameter Pt–Rh10% heating wire of the high-temperature cell described by Richet et al. (1993). The temperature of the cell was determined from calibrations of the electrical power needed to melt a series of salts and silicates whose congruent melting points are well known. The maximum temperature that could be reached with Pt–Rh wires was about 1900 K.

The X-ray diffraction experiments were made in an energy dispersive configuration on the wiggler line of the DCI storage ring of LURE (Orsay). The X-ray beam was collimated to $200 \times 50\,\mu m$ and the diffracted beam analyzed with a Canberra planar germanium detector at 2θ angles of about 11° for energies between 5 and 50 keV. To optimize the quality of diffraction patterns, the run duration was kept from 23 to 30 min. As a result, the measurements were made in a total time of 252 min between 1480 and 1776 K.

As no attempt was made at determining the diffraction angle, we actually measured relative variations of the cell parameters and volumes. Good resolution was achieved for reflections between 10 and 45 keV, which ensured reliable distance determinations down to 1.5 Å. Up to 24 reflections could be observed. To avoid any bias, however, we used for lattice parameter refinements the 11 most intense reflections that could be followed continuously from 300 K up to the maximum temperature investigated, namely, 130, 111, 040, 220, 022, 131, 150, 112, 260, and 222. The relative uncertainties on the cell parameters determined in this way are about 1‰. The unit-cell volume was then calculated at each temperature from the derived lattice parameters with errors of less than 3‰. Since our experiments were not designed to determine the thermal expansion tensor of coesite (see Paufler and Weber, 1999), we simply determined the volume thermal expansion coefficient from a least-squares fit made to these individual volume data.

3. High-temperature unit-cell parameters and thermal expansion

In agreement with early work (Zoltai and Buerger, 1959; Dachille and Roy, 1959), subsequent studies have shown that coesite has a monoclinic C2/c symmetry (Araki and Zoltai, 1969; Gibbs et al., 1977; Smith et al., 1987; Geisinger et al., 1987). Up to 1776 K, the highest temperature at which cell parameters could be determined, our X-ray diffraction patterns are consistent with this structure. Without evidence for a symmetry change,

the same monoclinic cell thus remained appropriate for assigning all reflections. Except near 1800 K, there was no evidence for partial transformation to either quartz or cristobalite, which are the stable 1-bar polymorphs. Above 1776 K, the recorded diffraction patterns no longer allowed lattice parameters to be calculated likely because of transformation of coesite into cristobalite. Unfortunately, however, the sample could not be kept for further room-temperature examination and we could not determine whether such a transformation was direct or taking place through an intermediate molten state as observed, for platelets, in the case of the transformation of quartz to cristobalite (Mackenzie, 1960).

The derived unit-cell parameters are listed in Table 1. The scatter in these data increases above 1000 K possibly because the reflections of untransformed quartz were less readily separated from those of coesite at higher temperatures. The variations of the unit-cell parameters are compared with previous observations in Fig. 1. To within experimental errors, the data of Galkin et al. (1987) are generally consistent with ours. Exceptions are the c and β parameters for which a change in the slope has been reported by Galkin et al. (1987) near 400 K, indicating a marked anisotropy with an expansion along the a axis twice as great as along the b axis, and 5 times greater than along the c axis. These features are not confirmed by our measurements, which indicate instead an almost isotropic expansion with a mean value of $3.15 \ 10^{-6} \ K^{-1}$ along the three axes up to the highest temperatures investigated.

Since Skinner (1962) assumed a pseudo-hexagonal unit cell, comparisons of his unit-cell parameters with those of Table 1 would not be meaningful. We thus compare only volume expansions in Fig. 2, where the
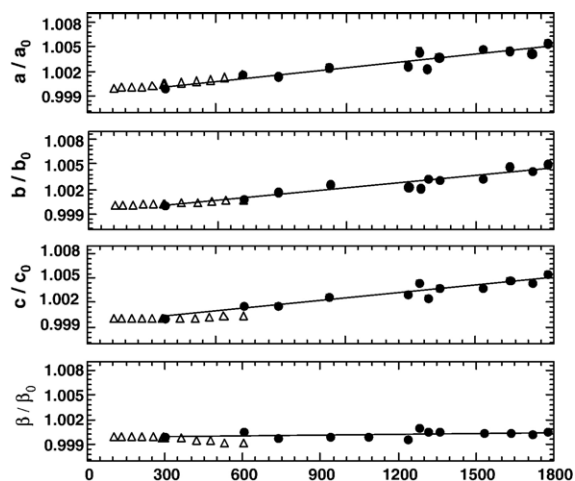

Fig. 1. Relative expansion of the cell parameters of coesite. Data of Galkin et al. (1987, open triangles) and this work (solid circles and solid lines). The size of the symbols corresponds to the experimental errors.

difference between the data of Skinner (1962) and ours reaches only about 3‰ at 1300 K and remains comparable to the combined error margins of the measurements. In view of the near constancy of the angle β of the monoclinic unit cell of coesite, however, this temperature-dependent difference should not be due to the use of a pseudo-hexagonal unit cell by Skinner (1962).

The linear and volume expansion coefficients determined from least-squares fits to our experimental data are listed in Table 2. Constant values are adequate for reproducing all the results. We therefore find no evidence for temperature-dependent values as derived from previous experiments (Skinner, 1962; Galkin et al., 1987) or, consequently, from a more recent assessment of these data (Swamy et al., 1994). The significance of such discrepancies should not be overestimated, however, because the absolute differences between reported volume data are not abnormally high. In fact, the essential feature borne out by all measurements is the

Table 1
High-temperature unit-cell parameters and volume of coesite[a]

T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å³)
300	7.159 (2)	12.329 (4)	7.159 (1)	120.17 (1)	547.82 (35)
602	7.168 (2)	12.374 (5)	7.169 (1)	120.23 (2)	549.44 (47)
737	7.171 (3)	12.374 (7)	7.170 (2)	120.14 (3)	550.40 (69)
936	7.177 (2)	12.392 (5)	7.178 (1)	120.17 (2)	551.92 (48)
1238	7.182 (3)	12.380 (8)	7.181 (2)	120.13 (2)	552.33 (66)
1281	7.187 (2)	12.402 (6)	7.188 (1)	120.22 (2)	553.63 (55)
1315	7.179 (3)	12.391 (8)	7.178 (2)	120.10 (3)	552.37 (75)
1359	7.179 (4)	12.411 (7)	7.184 (2)	120.23 (3)	553.05 (75)
1529	7.185 (3)	12.399 (8)	7.185 (2)	120.17 (3)	553.42 (74)
1632	7.190 (3)	12.432 (8)	7.192 (2)	120.19 (3)	555.58 (72)
1717	7.192 (3)	12.413 (8)	7.192 (2)	120.10 (3)	555.50 (73)
1776	7.195 (3)	12.436 (8)	7.197 (2)	120.19 (3)	556.61 (71)

[a]Determined from the room-temperature parameters $a = 7.135$ Å, $b = 12.372$ Å, $c = 7.174$ Å and $\beta = 120.36°$ as reported by Gibbs et al. (1977).
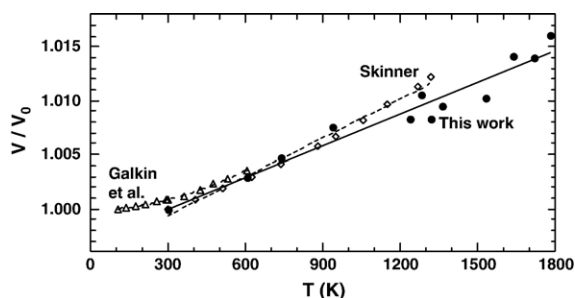

Fig. 2. Volume expansion of coesite against temperature as measured by Skinner (1962), Galkin et al. (1987) and in this work.

Table 2

Volume thermal expansion coefficient, $1/V\,(\partial V/\partial T)_P = \alpha_0 + \alpha_1 T + \alpha_2/T$, and expansivity of cell parameters (X), $dX/dT = \alpha_0 + \alpha_1 T + \alpha_2/T$

	T	T_0	Variable	V_0 (cm³/mol)	α_0, 10^{-5}	α_1, 10^{-9}	α_2
Skinner (1962)	297–1045	297	V	20.647	0.5430	8.320	−0.0061
Galkin et al. (1987)	103–602	103	a	7.1357	0.53788	48.254	
			b	12.3678	0.25679	44.266	
			c	7.1726	−0.34116	24.122	
			V	20.563	0.0651	18.704	
Swamy et al. (1994)	300–4000	298	V	20.641	0.5430	7.600	
This study	300–1800	300	a	7.159	2.359		
			b	12.329	1.621	20.188	
			c	7.159	2.2885		
			V	20.619	1.0167	−0.4534	

very small thermal expansion of coesite. Even over the 1500° interval of our experiments, the volume increase is only 1.6%.

4. Discussion

4.1. Thermal expansion

Coesite is the only silica polymorph made up of two different kinds of SiO_4 tetrahedra with five different oxygen sites and eight non-equivalent Si–O bonds (Grandinetti et al., 1995). These so-called Si1 and Si2 tetrahedra define two kinds of four-membered rings which are mutually linked to form a double crankshaft chain similar to that observed in feldspars: one is parallel to the <101> axis whereas the other is approximately parallel to the <110> axis (Geisinger et al., 1987). Both kinds of chains run parallel to [101] and are cross-linked by oxygen atoms to form a three-dimensional framework. This close packing of SiO_4 tetrahedra involves short distances between second-neighbor oxygens along with a wide distribution of the intertetrahedral angle Si–O–Si, which ranges from 138° to 180°.

Expansion is much smaller for coesite than for quartz and cristobalite (Fig. 3). This small expansion is a direct consequence of the high pressure of formation of coesite because the compact packing of SiO_4 tetrahedra prevents Si–O–Si angles from varying much with increasing temperatures. According to lattice dynamics calculations (Bourova et al., 2004), these variations are the smallest, but of the opposite sign, for the intrachain angles Si–O_3–Si and Si–O_4–Si with values lower than 0.2% between 300 and 1600 K. With an increase of only 0.6% from 300 to 1600 K, the variations are the greatest for the Si–O_2–Si angle between oxygen atoms cross-linking the chains running parallel to <101> and <110>. But the actual dilation mechanisms are more complicated for coesite than for other SiO_2 polymorphs. The reason is that the usually negligible expansion of Si–O bonds also contributes to thermal expansion because of the small variations of the coesite intertetrahedral angles.

For quartz and cristobalite, the high dilation of the α phase is a premonitory effect of the α–β transition. At this transition, the distances between second-neighbor oxygens increase abruptly and dynamical disorder sets in through precession of the oxygen atoms around Si–O–Si bonds (see Bourova et al., 2000, 2004). For the β phases of both polymorphs, the thermal expansion coefficient then becomes negative (Bourova and Richet, 1998, and references therein). Although extrapolation of the data indicates that coesite and quartz would have the same volume near 2000 K (Fig. 3), this feature is purely coincidental as the distribution functions calculated for cristobalite and coesite differ markedly at this temperature, in particular for the distances between second-neighbor oxygen atoms (Bourova et al., 2000, 2004).

For β-cristobalite and β-quartz, molecular dynamics calculations indicate that dynamical disorder is related to the existence of three and two distinct crystal structures, respectively, which are characterized by slightly different potential energies (Bourova et al., 2000, 2004). In contrast, similar simulations yield a
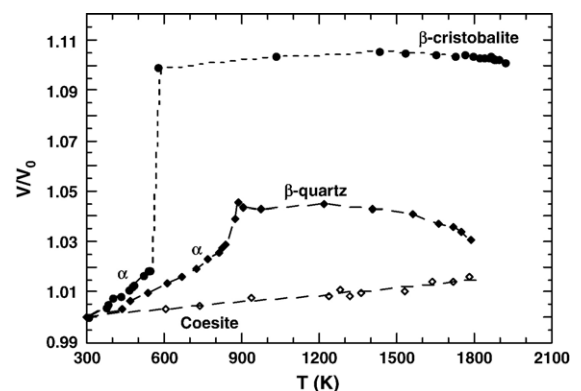

Fig. 3. Comparison between the volumes of quartz, cristobalite and coesite. Data from Bourova and Richet (1998) and this work.

single crystal structure for coesite at all temperatures, which thus accounts for the lack of an $\alpha-\beta$ transition for this polymorph. This feature is related to the high pressure of formation of coesite, since the steeper slopes of potential energy wells associated with the high density of this polymorph leave little room for the existence of two or more energetically comparable minima. Molecular dynamics simulations have nonetheless shown that dynamical disorder exists in coesite. As revealed by a considerable broadening of the distributions of Si–O–Si angles and of O–O second-neighbor distances (Bourova et al., 2004), it does not set abruptly, but progressively above 1000 K, i.e., at temperatures higher than the 520 and 850 K of the $\alpha-\beta$ transitions of cristobalite and quartz, respectively (Richet et al., 1982).

4.2. Superheating

The metastable melting point of coesite is given by the temperature at which the Gibbs free energy of formation of the crystal is equal to that of amorphous SiO_2. From thermochemical data for coesite and SiO_2 glass and liquid, this temperature was found to be 875 ± 200 K (Richet, 1988). This result has been confirmed by the new thermodynamic functions derived from a redetermination of the low- and high-temperature heat capacity of coesite (Hemingway et al., 1998), which yield a melting temperature of about 800 K.

Previously, coesite has been observed up to about 1300 K by X-ray diffraction (Skinner, 1962) and Raman spectroscopy (Gillet et al., 1990). Although this temperature is much higher than the metastable melting point of coesite, it is lower than 1480 K, the standard glass transition temperature (T_g) of pure SiO_2 (Richet et al., 1982). At such temperatures, coesite does not melt but partially decomposes to an amorphous solid. This solid state amorphization has been studied by Brazhkin et al. (1991) and especially by Gong et al. (1996) who observed that it is a rather slow heterogeneous nucleation-and-growth process. Progressing from the sample surface, the amorphous layer had for instance a thickness of only 60 nm after 3.5 h at 1200 K. Under these circumstances, amorphization is similar to that described at lower temperatures for stishovite (see review by Richet and Gillet, 1997), which is thermodynamically unstable at all temperatures with respect to SiO_2 glass. At room pressure, this metastability of stishovite could also considered as a form of superheating (Richet, 1988) where the relevant amorphous phase is a solid that of course lacks the dynamical nature of the melt. Then, the common point between coesite

and stishovite is that low thermal energy induces progressive decomposition to an amorphous phase, which is devoid of long-range order, and not reconstructive transition to the stable low-pressure polymorph.

Compared to these observations, a noteworthy difference of our experiments is that they extend to 1776 K, i.e., a temperature much higher than the glass transition range of SiO_2. Superheating is especially significant as the total time spent above 1480 K was of the order of 1 h in the experiments. We cannot exclude the possibility that partial amorphization, below T_g, or melting, above T_g, took place before reaching the highest temperature investigated, although significant partial transformation to quartz or cristobalite is ruled out under these conditions. Given the small grain size of the sample, however, it seems unlikely that good diffraction patterns could have been obtained with a significant volume fraction of melt. In any case, the occurrence of such transformations would not affect the actual extent of superheating because X-ray diffraction yields unambiguous sample characterization. Compared to other silicates for which superheating is restricted to a few tens of degrees (see the summary given by Greenwood and Hess, 1998), coesite brought to 1776 K therefore represents an extreme case of superheated crystal. In fact, superheating should be even more extensive for large single crystals in which heterogeneous nucleation would be slower than with the very fine grain size of our material. As an example, quartz platelets have been kept for short periods of time up to 2000 K (Ainslie et al., 1961), whereas the maximum temperature reached in our X-ray study of a fine quartz powder was only 1785 K (Bourova and Richet, 1998).

Melting is generally considered to be either a homogeneous mechanical instability of the crystal or a phase transition governed by heterogeneous nucleation and growth. As reviewed by Greenwood and Hess (1998), to whom we refer for a detailed discussion, the former theories are not adequate to our purpose since one of their aims is to account for the usually assumed lack of superheating. Hence, interest is paid to the latter theories for which experimental evidence exists below T_g, such as the observations of Gong et al. (1996) for coesite. These theories are also used to describe crystal nucleation and growth, with shortcomings that are now well known at high degrees of supercooling (e.g., Weinberg and Zanotto, 1989). These shortcomings stem in part from the actually incongruent nature of the phase transition and from the fact that melt viscosity is not the right scaling parameter to account for transport of all

elements to the crystal–melt interface (Roskosz et al., 2005). Both of these problems are irrelevant to crystallization and melting of SiO_2 polymorphs, however, in view of their congruent nature and also because the diffusivities of Si and O in the melt are not too different.

When viewing melting as a heterogeneous nucleation-and-growth process, variations in the extent of superheating for a given crystal reflects primarily differences in sample grain size because only the second step of growth is really probed. But the availability of data obtained under the same conditions for different SiO_2 polymorphs (having similar SiO_4 tetrahedral units) provides a unique opportunity to evaluate the respective roles of crystal structure and melt properties on superheating and thus, at least indirectly, on melt nucleation and growth. As expected, the extent of superheating is a regular function of the crystal stability of SiO_2 polymorphs. Superheating is negligible for fine cristobalite powders because no diffraction patterns could be recorded in analogous experiments above the melting point of 1999 K (Bourova and Richet, 1998). For quartz, the lattice parameters could be determined up to 1785 K, i.e., above the metastable melting temperature of 1700 K (Bourova and Richet, 1998). As a matter of fact, this temperature is nearly the same as that reached for coesite. Despite the large density difference observed between quartz (2.568 g/cm^3) and coesite (2.865 g/cm^3) at this temperature, the kinetics of decomposition and eventual transformation of both minerals into cristobalite (2.187 g/cm^3) appear to be similar. This similarity thus suggests that differences in density, crystal structure or dynamical disorder between coesite and quartz are not crucial as long as superheating is concerned.

Empirically, it has long been known that superheating takes place when the melt is very viscous, in which case growth of the liquid phase is made difficult by slow element diffusivity. That melt viscosity could be the limiting factor for the initial stages of melting is indeed suggested by the fact that both coesite and quartz could be superheated to nearly the same temperature of 1780 K. If so, then, as noted by Greenwood and Hess (1998), superheating is favored by low configurational entropy of the melt through the quantitative relationship between viscosity and configurational entropy (Richet, 1984). From this standpoint, some numbers can be put on timescales relevant to the melting process. At 1780 K, the viscosity (η) of molten SiO_2 is $10^{7.9}$ Pa s (Urbain et al., 1982) and the shear modulus at infinite frequency G_∞ is 3.5 10^{10} Pa as calculated from the Brillouin scattering data of Polian et al. (2002). From the Maxwell's

relationship $\tau = \eta / G_\infty$, then one derives a structural relaxation time of 2.3 10^{-3} s for SiO_2 liquid, which represents an upper bound to the configurational changes connected with melt nucleation and growth. In accordance with the Eyring relationship, which relates melt viscosity to silicon diffusivity (see Mysen and Richet, 2005), silicon mobility is negligible at such timescales with a self-diffusivity of 10^{-19} m^2/s. This indicates that the melting front advances through disordering of successive atomic layers, without significant diffusion in the amorphous phase, even at temperature much higher than the glass transition range. In other words, the melting mechanisms are likely similar near the liquidus and as described below T_g (Gong et al., 1996).

Acknowledgments

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