

## EQUATIONS OF STATE AND PHASE EQUILIBRIA

TABLE 1a. Shock-Wave and Static-Compression Data for Stishovite

Code	Source	No. of Points	Initial Density, g/cm <sup>3</sup>	Pressure Range, Mb
S1	Wackerle [1962]	12	2.65	0.4 to 0.7
S2	Altshuler et al. [1965]	3	2.65	0.6 to 2.0
S3	Trumh et al. [1971a]	12	2.65	0.4 to 6.5
S4	Wackerle [1962]	3	2.20	0.5 to 0.6
S5	H. Shipman (private communication, 1969)	5	2.20	0.6 to 1.6
S6	McQueen [1968]	34	2.20	0.4 to 0.8
S7	Trumh et al. [1971b]	2	2.20	0.5 to 1.6
S8	Jones et al. [1968]	6	1.98	0.4 to 1.4
S9	Trumh et al. [1971b]	6	1.77	0.2 to 2.3
S10	Trumh et al. [1971b]	3*	1.55	0.3 to 0.6

Code	Source	No. of Points	Initial Density, g/cm <sup>3</sup>	Pressure Range, Mb
X1	Liu et al. [1972]	9	0 to 2.23†	0 to 2.23†
X2	Bassett and Barnett [1970]	14	0 to 85†	0 to 85†

\*May be interpreted as coesite-stishovite mixture (see text).  
†Value in kilobars.

The resultant wide spread of the Hugoniot provides stronger constraints on  $\gamma$ . Also, Mizutani et al. [1972] have measured ultrasonically the compressional- and shear-wave velocities of stishovite, and thus another constraint on  $K_s$  is provided. In addition to benefiting from the newly available data and using a different form of the equation of state (discussed below), the present analysis determines simultaneously the compressional and thermal parts of the equation of state by adjusting simultaneously all free parameters to give a least-squares fit to all the data. This procedure accomplishes implicitly the two sequential stages of the analysis of Ahrens et al. [1970].

Although coesite is stable at room temperature in the approximate pressure range 30–70 kb between the stability fields of quartz and stishovite, coesite has not previously been observed in shock-wave experiments, the transformation usually being directly from quartz to stishovite. There are enough other coesite data (Table 2) that, when they are combined with these Hugoniot data and when it is assumed that they do

TABLE 1b. Other Data for Stishovite

Quantity	Source	Value
Compressional-wave velocity	Mizutani et al. [1972]	$V_p = 11.0$ km/sec
Shear-wave velocity		$V_s = 5.50$ km/sec
Isentropic bulk modulus		$K_s = 3.46 \pm 0.24$ Mb
Volume coefficient of thermal expansion (300°K)	Weaver [1971]	$\alpha = 16.4 \pm 1.3/\text{°K}$
Specific heat at constant pressure (300°K)	Holm et al. [1967]	$C_p = 7.15 \times 10^6$ ergs/g °K
High temperature limit of Debye temperature	Kieffer and Kamb [1972]	$\theta_D = 1120^\circ\text{K}$
Density, zero pressure, 298°K	Hobie et al. [1966]	$\rho_0 = 4.287$ g/cm <sup>3</sup>

TABLE 2a. Shock-Wave and Static-Compression Data for Coesite

Code	Source	No. of Points	Initial Density, g/cm <sup>3</sup>	Pressure Range, kb
<i>Shock-Wave Data</i>				
S11	<i>Trunin et al.</i> [1971b]	3	1.35	119 to 322
S12	<i>Trunin et al.</i> [1971b]	2	1.35	454 to 552
S13	<i>Trunin et al.</i> [1971b]	5	1.15	65 to 477
<i>Static-Compression Data</i>				
X3	<i>Bassett and Barnett</i> [1970]	11		0 to 80

indeed represent coesite, the equation of state can be approximately determined. The success of this procedure seems to support the coesite identification, but other calculations suggest otherwise, as will be seen.

*Trunin et al.* [1971b] also calculated approximate Hugoniot temperatures and suggested that the boundary separating the coesite and stishovite fields in a pressure-temperature plot represented the coesite-stishovite phase transition line. Hugoniot temperatures have been recalculated here, and, in addition, the coesite-stishovite phase line has been independently calculated from the equations of state of the two phases, the coesite identification again being assumed. There is a large discrepancy between the two approaches. It is suggested that the new phase may in fact be a liquid of approximately the density of coesite rather than coesite itself. Because some of the

properties of this liquid are unknown, it is necessary to proceed as if the phase were solid coesite and to examine the plausibility of the results.

#### ANALYSIS

A complete equation of state must account for both compressional and thermal effects. Previous studies have accounted for these effects by invoking the Mie-Grüneisen equation, incorporating a finite strain description of compressional effects with various expressions for the Grüneisen parameter to describe thermal effects, as was discussed in the introduction. The problem is to find an expression for  $\gamma$  that does not involve overrestrictive assumptions and that has some theoretical foundation.

*Thomsen* [1970] has considered the question of incorporating the results of the theory of anharmonic lattice dynamics into finite strain

TABLE 2b. Other Data for Coesite

Source	Quantity	Value
<i>Skinner</i> [1966]	Volume coefficient of thermal expansion (293°K)	$\alpha = 8.0 \times 10^{-6}/^{\circ}\text{K}$
<i>Holm et al.</i> [1967]	Specific heat at constant pressure (300°K)	$C_p = 7.46 \times 10^6 \text{ ergs}/^{\circ}\text{K}$
<i>Kieffer and Kamb</i> [1972]	High temperature limit of Debye temperature	$\theta_D = 1170^{\circ}\text{K}$
<i>Robie et al.</i> [1966]	Density, zero pressure, 298°K	$\rho_0 = 2.91 \text{ g}/\text{cm}^3$
<i>Mizutani et al.</i> [1972]	Compressional-wave velocity Shear-wave velocity Isentropic bulk modulus	$V_p = 7.53 \text{ km}/\text{sec}$ $V_s = 4.19 \text{ km}/\text{sec}$ $K_g = 0.97 \text{ Mb}$