

Equations of State and Phase Equilibria of Stishovite and a Coesitelike Phase from Shock-Wave and Other Data¹

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Shock-wave, static-compression (X ray), ultrasonic, thermal expansion, and thermodynamic data are simultaneously inverted to determine the equations of state of stishovite and a coesitelike SiO_2 phase. All the stishovite data except the thermal expansion data are satisfied by a Mie-Grüneisen-type equation of state having a zero pressure bulk modulus K of about 3.50 ± 0.1 Mb, a pressure derivative dK/dP of 3.3 ± 1 , and a Grüneisen parameter, initially 1.25 ± 0.1 , that decreases slowly with compression. The volume coefficient of thermal expansion at ambient conditions is found to be $13 \pm 1 \times 10^{-6}/^\circ\text{K}$, in comparison with 16.4 ± 1.3 measured by Weaver. Some Hugoniot data of Trunin et al. for very porous quartz have densities very close to the density of coesite. However, a calculation of the coesite-stishovite phase line shows that the coesitelike phase persists to about twice the predicted transition pressure at $10,000^\circ\text{K}$. It is suggested that the discrepancy can be explained if this phase is interpreted as a liquid of about coesite density.

Since the discovery of the dense high-pressure silica polymorph stishovite [Stishov and Popova, 1961] and its subsequent identification both in natural silica from a meteor crater [Chao et al., 1962] and as the dense phase obtained in the shock-wave experiments of Wackerle [1962] by McQueen et al. [1963], a variety of experiments have yielded considerable data on stishovite. To date, these data include more shock-wave, static-compression (X ray), thermodynamic, thermal expansion, and, very recently, ultrasonic data. These data, with their sources and other relevant information, are summarized in Table 1. A succession of analyses of these data has accompanied their accumulation [Anderson and Kanamori, 1968; Ahrens et al., 1969, 1970]. This paper is another in that succession.

The Grüneisen parameter γ is an important quantity that characterizes thermal effects in the equation of state. Ahrens et al. [1970], returning to the method used by McQueen et al. [1963], determined the values of γ at large compression from the difference in pressure between Hugoniots corresponding to different initial densities. This method is preferable to

that used by Anderson and Kanamori [1968] and Ahrens et al. [1969], who used the Slater [1939] or Dugdale and MacDonald [1953] formulas for the volume dependence of γ . These formulas have been severely criticized because they fail to take account of the frequently large pressure dependence of the shear modes of vibration [Knopoff and Shapiro, 1969].

Fitting these results with the functional form

$$\gamma = \gamma_0(V/V_0)^A \quad (1)$$

where V is the specific volume, A is a constant, and the subscript 0 denotes zero pressure, Ahrens et al. [1970] adjusted γ_0 until the volume coefficient of thermal expansion α , obtained from the identity

$$\alpha = \gamma\rho C_p/K_s \quad (2)$$

where K_s is determined from the shock-wave analysis, agreed with the measured value. (The value used was the preliminary value of $\alpha = 15 \times 10^{-6}/^\circ\text{K}$, obtained from J. S. Weaver (personal communication, 1969), cf. Table 1.) In (2), K_s is the isentropic bulk modulus, ρ is the density, and C_p is the specific heat at constant pressure.

Since that analysis, several new sets of data have been published. The data of Trunin et al. [1971a] greatly extend the pressure range of the Hugoniot data, and those of Trunin et al. [1971b] extend the range of initial porosities.

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