# Equations of State and Phase Equilibria of Stishovite and a Coesitelike Phase from Shock-Wave and Other Data[1]

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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 $3.50 \pm 0.1$ Mb, a pressure derivative $dK/dP$ of $3.3 \pm 1$, and a Grüneisen parameter, initially $1.25 \pm 0.1$, that decreases slowly with compression. The volume coefficient of thermal expansion at ambient conditions is found to be $13 \pm 1 \times 10^{-6}/°K$, in comparison with $16.4 \pm 1.3$ 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 $10,000°K$. 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 $\gamma$ 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 $\gamma$ 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 $\gamma$. 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

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

where $V$ is the specific volume, $A$ is a constant, and the subscript 0 denotes zero pressure, *Ahrens et al.* [1970] adjusted $\gamma_0$ until the volume coefficient of thermal expansion $\alpha$, obtained from the identity

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

where $K_s$ is determined from the shock-wave analysis, agreed with the measured value. (The value used was the preliminary value of $\alpha = 15 \times 10^{-6}/°K$, obtained from J. S. Weaver (personal communication, 1969), cf. Table 1.) In (2), $K_s$ is the isentropic bulk modulus, $\rho$ 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.