

correspond to the crystallographic orientation assumed in the theoretical model. The comparison between the stiffnesses at 25°C and zero pressure and the theoretical values is rather good. In the case of the pressure derivatives, the agreement is less satisfactory, but still reasonable. It appears then, that at low temperatures and pressures, the elastic properties of Mg₂SiO₄ are primarily determined by the hep framework of oxygen anions. At high pressures, the effect of the imposed strain on the structure is to increase the crystal field asymmetry and raise the contribution of the Mg²⁺ and Si⁴⁺ cations. That is, the first nearest neighbor cation-anion interactions became increasingly significant, and the central force approximation may also become less valid.

Compression of forsterite at very high pressures. There are several common isothermal equations of state, which are concerned primarily with the effects of compression at high pressures. Two of the most prominent of these equations are the Murnaghan equation of state [Murnaghan, 1944] and the Birch equation of state [Birch, 1952]. These equations are semi-empirical in nature and differ with respect to the initial assumptions made in their derivation. Both the Murnaghan and the Birch equations have been shown to adequately represent the isothermal compression of many metals, oxides, and simple silicates to pressures in the megabar range [O. L. Anderson, 1966] and have recently been examined by Thomsen and Anderson [1969].

The parameters appearing explicitly in the Murnaghan and Birch equations of state can

TABLE 6. Comparison of the Elastic Constants and Their Pressure Derivatives of Mg₂SiO₄ with Theoretical Data for the hep Structure

Index <i>ij</i>	a_{ij}	c_{ij}^s/K^s	$(\partial C_{ij}^s/\partial P)/(\partial K/\partial P)$
11	1.81	1.86	1.59
22	1.81	1.58	1.64
33	2.00	2.59	1.84
44	0.50	0.64	0.72
55	0.50	0.64	0.55
66	0.56	0.53	0.69
12	0.69	0.57	0.58
13	0.50	0.54	0.67
23	0.50	0.52	0.70

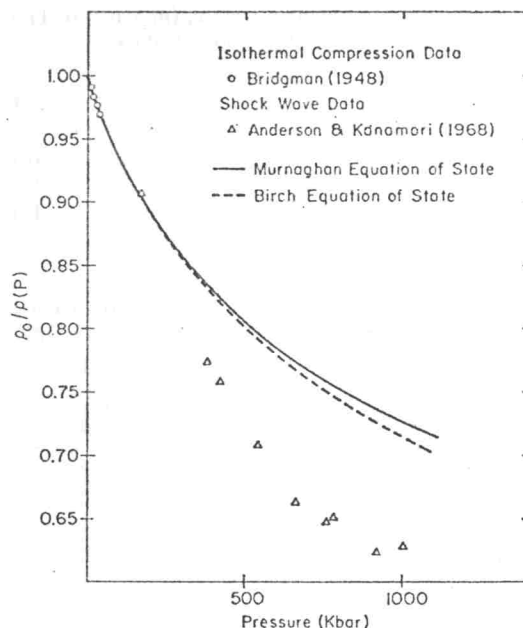


Fig. 3. Compression curves for forsterite at 25°C computed from the single-crystal acoustic data using the Murnaghan and Birch equations of state.

be measured ultrasonically for a given material. The necessary quantities are the isothermal bulk modulus, and the isothermal pressure derivative of the isothermal bulk modulus. The acoustically determined quantities are adiabatic in the case of the elastic moduli, and 'mixed' in the case of the measured derivatives, and must be converted to the pure isothermal quantities by using equations given by Overton [1962]. Using the value of the adiabatic bulk modulus at 25°C in Table 5, determined from the single-crystal acoustic data by means of the VRH average scheme, the isothermal bulk modulus and its isothermal pressure derivative were calculated as $K^T = 1281$ kb and $(\partial K^T/\partial P)_T = 4.99$. These two values were used to predict the compression of an isotropic polycrystal of forsterite to very high pressures at 25°C by using the Murnaghan and Birch equations of state; the results are shown in Figure 3.

Direct compression data of forsterite are available from Bridgman [1948] who measured the isothermal compression of a natural peridot sample up to pressures of 40 kb. Although this sample contained about 12% fayalite (Fe₂SiO₄),

TABLE 7. The Zero Pressure Lattice Parameters a_i^0 and the Exponents m_i, n_i (in Mb^{-1}) of Thurston's Equation of State

	i	$a_i^0, \text{\AA}$	m_i	n_i
a_0	1	4.758	-0.05596	+0.0317
b_0	2	10.214	-0.08877	-0.0068
c_0	3	5.984	-0.06368	-0.0249

which corresponds to a density of 3.364 g/cm^3 , its bulk elastic properties are probably sufficiently close to forsterite such that the results are included in Figure 3 for comparison. Shock compression data for pure forsterite polycrystals have been measured up to 1 Mb [D. L. Anderson and Kanamori, 1968]. Although the polycrystals exhibited a porosity of 2-3%, it is assumed that such effects are minimized under conditions of shock compression, and the data has been reduced in Figure 3 using the theoretical density of pure forsterite. The shock-wave data are also plotted in Figure 3 for comparison with the acoustic equation of state curves. Only one shock-wave data point compares well with the calculated equations of state. Since this point occurs at a pressure of somewhat less than 200 kb, it appears that

this measurement was made within the olivine structure stability range. Above 380 kb however, the shock compression data begin to systematically differ from the calculated curves. It is apparent, therefore, that somewhere within the pressure range 180-380 kb a solid-solid phase transition occurs.

Pressure dependence of lattice parameters. In addition to the calculation of the isothermal equation of state the ultrasonic data of the elastic constants and their pressure derivatives may also be used for calculating the pressure dependence of the crystallographic lattice parameters from Thurston's generalization of Murnaghan's equation of state [Thurston, 1967]

$$\lambda_i = \frac{a_i(P)}{a_i^0} = [1 + (\partial \ln K^T / \partial P)_T^0 P]^{m_i} e^{n_i P} \quad (6)$$

Here λ_i denotes the principal stretches, a_i the orthorhombic lattice constants ($i = 1, 2, 3$), and the index 0 refers to zero pressure. The parameters m_i and n_i depend on the isothermal elastic constants and their isothermal pressure derivatives according to equations (I, 88), (I, 90), (II, 9) and (II, 15) of Thurston [1967]. The numerical values calculated from the isothermal

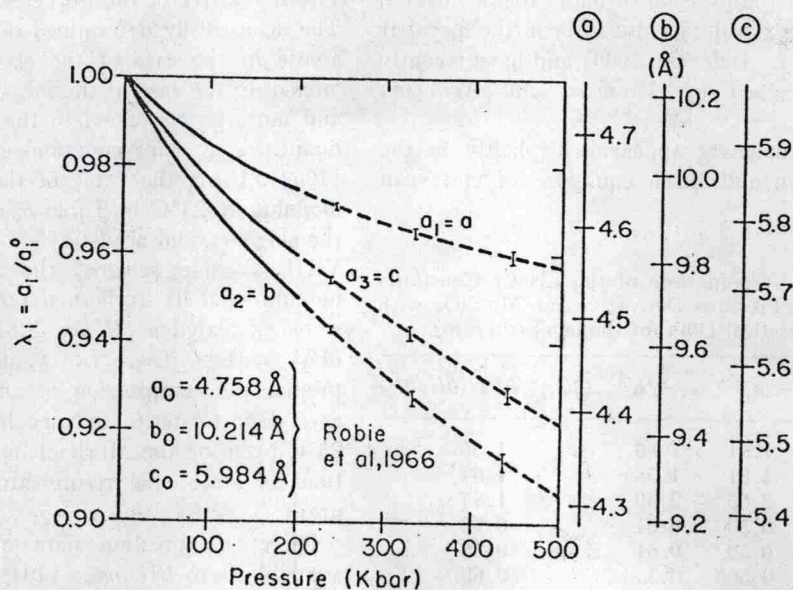


Fig. 4. Principal stretches λ_i and lattice parameters a_i of forsterite versus hydrostatic pressure calculated from ultrasonic elastic data according to Thurston's equation of state.