TABLE 5. Comparison of the Results of the Present Study with the Recent Single-Crystal Data of *Kumazawa and Anderson* [1969]

Stiffness	$C_{ij}{}^S$ (kbar)		$(\partial C_{ij}{}^S/\partial P)_T$		$(\partial C_{ij}{}^S/\partial T)_P$ (kbar/°C)	
	a	b	a	b	a	b
$c_{11}{}^S$	3291	3284	8.32	8.47	−0.389	−0.331
$c_{22}{}^S$	2005	1998	5.93	6.56	−0.311	−0.281
$c_{33}{}^S$	2363	2353	6.21	6.37	−0.269	−0.286
$c_{44}{}^S$	672.3	658.9	2.12	2.12	−0.130	−0.128
$c_{55}{}^S$	814.4	812.0	1.65	1.66	−0.144	−0.130
$c_{66}{}^S$	811.4	808.8	2.32	2.37	−0.163	−0.151
$c_{12}{}^S$	663	639	4.30	4.67	−0.117	−0.104
$c_{13}{}^S$	684	688	4.23	4.84	−0.087	−0.082
$c_{23}{}^S$	728	738	3.53	4.11	−0.092	−0.046
K^S	1269	1265	4.80	5.31	−0.178	−0.149
$K_{VRH}{}^S$	1291	1286	4.97	5.37	−0.176	−0.150
$G_{VRH}{}^S$	816	811	1.82	1.80	−0.136	−0.130

Notes.

Columns a, present study.
Columns b, *Kumazawa and Anderson* [1969].

nificantly larger than the standard deviation of the data, and probably reflects error in the expansion coefficients. Based upon this specific example, it seems reasonable to assume that the temperature derivatives listed in Table 4 are accurate to within ±2%.

Comparison of present data with other new single-crystal results. Recently *Kumazawa and Anderson* [1969] have measured the adiabatic second-order elastic constants of another single-crystal specimen of forsterite. Their sample (F) was a synthetic single-crystal in which 1.16% MnO was added to stabilize crystal growth. The density was 3.224 g/cm³. The values obtained by Kumazawa and Anderson are compared with those of the present study in Table 5. In addition, the effective pressure derivatives and the isobaric temperature derivatives were also measured by these investigators. These results are also included in Table 5 for comparison. It should be pointed out, however, that the isobaric temperature derivatives of Kumazawa and Anderson were evaluated at 25°C. Since the temperature derivatives of the present study were evaluated for $T > 200°C$, they are systematically smaller than those of Kumazawa and Anderson, as would be expected. Also included in Table 5 are the single-crystal adiabatic bulk modulus and its isothermal pressure derivative.

The bulk modulus K' and the isotropic value of the rigidity modulus G, and their derivatives with respect to pressure and temperature, have also been calculated from the Voigt-Reuss-Hill (VRH) average scheme [*O. L. Anderson*, 1965] and its extension to the derivatives of the elastic constants for orthorhombic symmetry [*Graham*, 1969]. As suggested by *Barsch* [1968], the pressure derivatives occurring in the equations obtained by differentiating the expressions for the bulk modulus in the approximations of Voigt and Reuss were referred to the thermodynamic rather than the effective elastic constants[3] [*Thurston*, 1967]. The resulting values are also included in Table 5. While the pressure derivatives of the isotropic rigidity modulus agree with those of Kumazawa and Anderson, the pressure derivatives of the bulk modulus differ by 10%. This discrepancy may be primarily attributed to the differences in the pressure derivatives of the off-diagonal constants.

In most cases the data compare favorably, deviations undoubtedly being the result of

[3] Application of the VRH averaging scheme to the pressure derivatives of the elastic constants for cubic, hexagonal, trigonal, and tetragonal symmetry has been made before by *Chung* [1967] and *Soga* [1968], however, by using the pressure derivatives of the effective elastic constants.

minor compositional differences and experimental error.

DISCUSSION

Comparison with the theoretical data for a hcp structure. The members of the olivine solid solution series are orthorhombic in crystal symmetry and belong to the space group Pbnm. The structure was originally determined by *Bragg and Brown* [1926] and refined by *Gibbs et al.* [1964]. Essentially, the structure of forsterite consists of a framework of approximately hexagonally close-packed (hcp) oxygen anions with the Mg^{++} cations occupying $\frac{1}{2}$ of the available octahedral sites, and the Si^{4+} cations occupying $\frac{1}{8}$ of the available tetrahedral sites. The deviation from hexagonal symmetry is rather small, and simple electrostatic rules combined with packing considerations permit a qualitative explanation of the structural distortions [*Gibbs et al.*, 1964].

The suggestion has been made [*O. L. Anderson*, 1965] that the elastic properties of oxide compounds and simple silicates are predominantly determined by the oxgyen anion framework, especially for hexagonally close-packed and cubic close-packed structures, and are relatively independent of the nature of the cations occurring within the anion interstices. *D. L. Anderson* [1969] has shown that, in general, the elastic parameter $\psi_0 = (\rho_0/\bar{M})\Phi^{-1/3}$ (where ρ_0 is the zero pressure density, $\bar{M}$ is the mean atomic weight, and Φ is the ratio of the zero pressure bulk modulus to the density) decreases with increasing cell volume per oxygen anion. The experimental values of the elastic constants of Al_2O_3 and their first pressure derivatives agree approximately with theoretical values calculated for an hcp model of oxygen anions [*Gieske and Barsch*, 1968]; it was therefore concluded that the elastic properties of Al_2O_3 are primarily determined by the slightly distorted hcp framework, and that the aluminum cations occupying 2/3 of the octahedral interstices have only minor effects. In view of these observations and the hcp structure of forsterite, it was of interest to investigate the extent to which the elastic properties of this material are dominated by the oxygen anion framework.

Theoretical elastic constant values have been calculated by *Leibfried* [1955] for the hcp structure from a central force model in which only nearest neighbor interaction is considered. The stiffness coefficients may be represented in terms of the bulk modulus K by the following relation:

$$c_{ij} = a_{ij}K \qquad (i, j = 1, \cdots, 6) \qquad (4)$$

The coefficients a_{ij} are numbers that depend on the crystal symmetry only and, for the hcp structure, are given by *Leibfried* [1955]:

$$a_{ij} = \frac{1}{48} \begin{bmatrix} 87 & 33 & 24 & 0 & 0 & 0 \\ 33 & 87 & 24 & 0 & 0 & 0 \\ 24 & 24 & 96 & 0 & 0 & 0 \\ 0 & 0 & 0 & 24 & 0 & 0 \\ 0 & 0 & 0 & 0 & 24 & 0 \\ 0 & 0 & 0 & 0 & 0 & 27 \end{bmatrix} \qquad (5)$$

For the theoretical model of Leibfried, the bulk modulus is $K = [4f/3(2)^{1/2}d]$, where f denotes the force constant, and d the nearest neighbor distance. The above theoretical model refers to a static lattice; however, the effect of thermal motion may be expected to be small at room temperature.

If the force constant f is assumed to be a function of interatomic distance only, (4) is valid at arbitrary pressure and may be differentiated with respect to pressure with the a_{ij} coefficients treated as constants. Therefore, the pressure derivatives of the elastic coefficients are proportional to the pressure derivative of the bulk modulus with the same a_{ij} coefficients as in (4) serving as the constants of proportionality. It should be pointed out, however, that the pressure derivatives occurring in such relations are those of the 'thermodynamic' elastic constants. The conversion of the pressure derivatives of the 'effective' elastic coefficients c_{ij}, measured by ultrasonic wave velocities, to those of the 'thermodynamic' coefficients c_{ij}^*, is given by *Thurston* [1965].

The comparison of the hcp theoretical model with the experimental values of Mg_2SiO_4 is made in Table 6. The elastic coefficients and the pressure derivatives of the thermodynamic constants, are listed in Table 6 in units of the bulk modulus and the pressure derivative of the bulk modulus, respectively, together with the theoretical values a_{ij}. The crystallographic axes a and c of forsterite have been interchanged to