for Ti

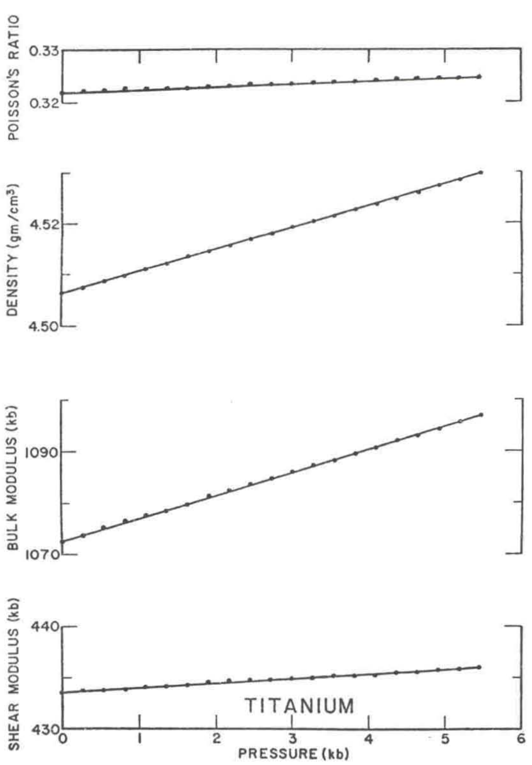

Fig. 4. Shear modulus, Poisson's ratio and bulk modulus vs. pressure as computed from Voigt–Ruess–Hill approximation for polycrystalline Ti with random grain orientation. The density vs. pressure data are obtained from the isothermal volume compressibility data given in Fig. 3.

Anderson[7] has successfully extrapolated the low pressure ultrasonic data to estimate compression of various solids to high pressure. The basic assumptions, given by Murnaghan [8], are that the $(\partial K_T/\partial P)_{P\to 0}$, where K_T is the isothermal bulk modulus, is a constant quantity in this range of extrapolation. The Murnaghan equation of state can be written [4] as

$$V/V_0 = \left[1+\left(\frac{\partial K_T}{\partial P}\right)_T\left(\frac{P}{K_T}\right)\right]^{-1/(\partial K_T/\partial P)_T} \quad (5)$$

where V and V_0 are volumes at pressure P and at zero pressure, respectively. The value of $(\partial K_T/\partial P)$, obtained by using Overton's relationships [9], is calculated to be 4·35. Thus the compression equation becomes

$$V/V_0 = [1+0{\cdot}0040923P]^{-0{\cdot}22978}. \quad (6)$$

In Fig. 5, a comparison between the experimentally determined V/V_0 values and the ultrasonic equation of state is shown. There is a fairly good agreement between the isothermal compressibility data of Bridgman[10] and the ultrasonic equation. There is a poor agreement between the latter and the shock-wave data[11], probably because of the phase change that has been reported for Ti near 90 Kbar[12].

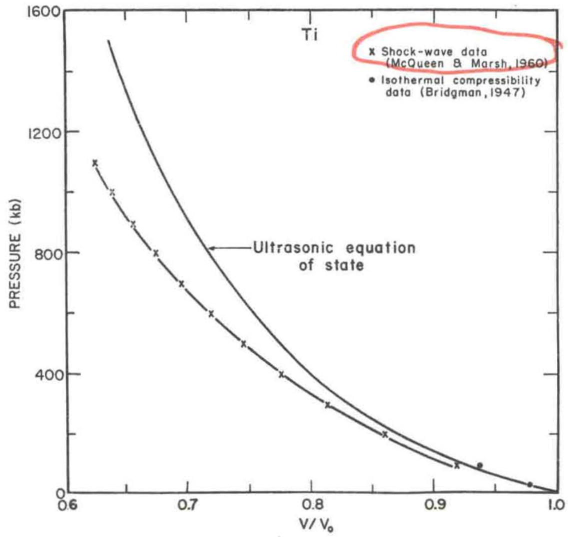

Fig. 5. Comparison of compression data for Ti as obtained from isothermal compressibility measurements of Bridgman[10], from ultrasonic equation of state derived from isothermal dK/dP, where K is the bulk modulus, and from shock wave data given in Ref. [11].

4. DISCUSSION OF RESULTS

In Table 2 the pressure derivatives of the stiffness moduli for Ti are compared with those of other h.c.p. metals[13–15]. The purpose of this comparison is to show that there is a general decrease with the c/a ratio of the pressure derivatives of the C_{ij}, where $i=j$, and that the pressure derivatives of the C_{44} and C_{66} shear moduli are very significantly reduced at $c/a < 1{\cdot}62$. The following discussion is based on the presumption that the

Table 2. Pressure derivatives at 25°C of the adiabatic stiffness moduli for Ti compared to those for Zr, Gd, Mg, *and* Cd

	Ti	Zr*	Gd†	Mg‡	Cd§
c/a ratio	1·587	1·593	1·590	1·62	1·88
dC_{11}/dP	5·01	3·93	3·12	6·11	9·29
dC_{33}/dP	4·88	5·49	6·02	7·22	7·26
dC_{44}/dP	0·52	−0·22	0·07	1·58	2·38
dC_{66}/dP	0·45	0·26	0·36	1·36	2·59
dC_{12}/dP	4·11	3·42	2·39	3·39	4·10
dC_{13}/dP	4·05	4·25	3·55	2·55	5·66
dK_s/dP	4·31	4·08	3·22	4·05	7·02

*Ref. [1]
†Ref. [13]
‡Ref. [14]
§Ref. [15].

effect of changing the c/a ratio during application of hydrostatic pressure assumes a more significant role in changing the C_{ij} and the phonon frequencies when the initial $c/a < 1{\cdot}62$. We first present a simple formal approach to show that the wide difference in dC_{44}/dP between Ti and Zr, and other differences between the elastic properties of the two metals, can be explained by the difference between the respective $\beta_\perp$ values. We then show that the differences between the average mode Grüneisen $\gamma^p(q)$, $\bar{\gamma}_H$, as calculated from the dC_{ij}/dP ($i =$ or $\neq j$) for Ti and Zr and as calculated from the volume thermal expansion can probably be explained by the differences in $d(c/a)dV$ between the two experimental conditions.

(a) *Separation of* ΔV *and* $\Delta(c/a)$ *effects on the* C_{ij}

The following equations are developed to show the parameters that relate the volume change and the c/a change, separately, to the total measured dC_{ij}/dP:

$$dC_{ij}/dP = (\partial C_{ij}/\partial P)_{c/a} + (\partial C_{ij}/\partial(c/a))_V \frac{d(c/a)}{dP} \quad (7)$$

$$= -\beta_V V(\partial C_{ij}/\partial V)_{c/a} - (\partial C_{ij}/\partial(c/a))_V \left(\frac{\partial(c/a)}{\partial V}\right)_T \frac{dV}{dP} \quad (8)$$

$$= -\beta_V C_{ij}(\partial \ln C_{ij}/\partial \ln V)_{c/a} + (c/a)(\beta_\perp - \beta_\parallel)(\partial C_{ij}/\partial(c/a))_V. \quad (9)$$

For cubic metal crystals[16] the measured dC_{ij}/dV values in all cases are negative ($dC_{ij}/dP > 0$), as expected for normal solids with positive values of the Grüneisen γ, so we can reasonably expect $(\partial C_{ij}/\partial V)_{c/a}$ to be negative. Thus the occurrence of a negative value for dC_{ij}/dP will depend on the difference $(\beta_\perp - \beta_\parallel)$ and the value of $(\partial C_{ij}/\partial(c/a))_V$. Since $(\beta_\perp - \beta_\parallel)$ is positive for Zr and negative for Ti, the wide difference in dC_{44}/dP for the two metals can be simply related to a relatively large and negative value for $(\partial C_{44}/\partial(c/a))_V$. If we go further and assume that the values for the two partial derivatives for each C_{ij} are the same for Ti as in Zr, an assumption which is perhaps reasonable in view of the many other similar properties, we arrive at the quantitative values given in Table 3. The first two columns list the values for the two unknowns that are obtained by simultaneously solving equation (9) with the known coefficients and measured dC_{ij}/dP for Ti and Zr. The components of dC_{ij}/dP due to ΔV and to $\Delta(c/a)$ for each metal are listed in columns 3 and 4, respectively. For Ti the change in modulus due to the c/a change is less than 4 per cent of the total pressure derivative for C_{11}, C_{33}, C_{12}, and C_{13}, whereas, the contributions to dC_{44}/dP and dC_{66}/dP are about 24 and 11 per cent, respectively. For Zr the $\Delta(c/a)$ contributions are considerably larger, because of the relatively large anisotropy in $\beta_\perp$ and $\beta_\parallel$, and the negative contribution to dC_{44}/dP overwhelms the positive effect of the volume decrease.

(b) ΔV *and* $\Delta(c/a)$ *effects on the normal mode frequencies of lattice vibrations*

In the quasi-harmonic approximation the