where C_{ij}, f_r, l, and ρ are, respectively elastic stiffness constant, pulse repetition frequency, length, and density; zero subscripts are, again, for 1 bar values. The parameters were computed at pressure intervals of 0.267 kbar; the volume compressibility, β_V, and the linear compressibilities, $\beta_{||}$ and $\beta_{|}$, were assumed invariant within these pressure intervals.

RESULTS

Single-Crystal Data

Figure 2 shows the plots of C_{ij} versus pressure. The relationships are linear within the experimental error. The values of the pressure derivatives dC_{ij}/dP shown in parentheses were calculated from the least-squares analysis of the data. It should be noted that dC_{44}/dP

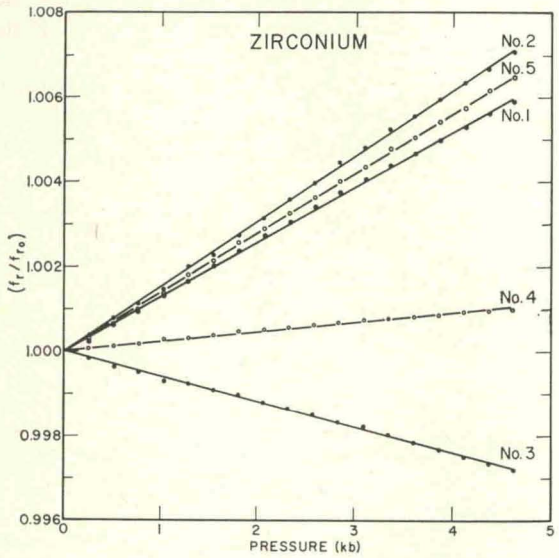

FIG. 1. Frequency ratio versus pressure for the five modes of wave propagation (see Table I for explanation of the modes).

is negative (-0.22) and that dC_{66}/dP is remarkably small (0.26) compared to the pressure derivatives of C_{66} in other hcp metals.

The adiabatic values for $\beta_{||}$, $\beta_{\perp}$, and β_v at various pressures were derived from the C_{ij} values. The isothermal values were obtained from the adiabatic–isothermal relationship. $\beta_T=\beta_s(1+\alpha\gamma T)$, where α, γ, and T, respectively, are the volumetric coefficient of thermal expansion, average Gruneisen parameter, and temperature. The values of $\alpha=1.733\times10^{-5}$/deg and $\gamma=1.01$ were used in these computations.[4]

The isothermal compressibility values versus pressure are shown in Fig. 3. The initial pressure derivatives of the isothermal compressibilities are:

$$d\beta_{||}/dP=-1.9/(\text{Mbar})^2,$$

$$d\beta_{\perp}/dP=-1.3/(\text{Mbar})^2,$$

and

$$d\beta_v/dP=-4.4/(\text{Mbar})^2.$$

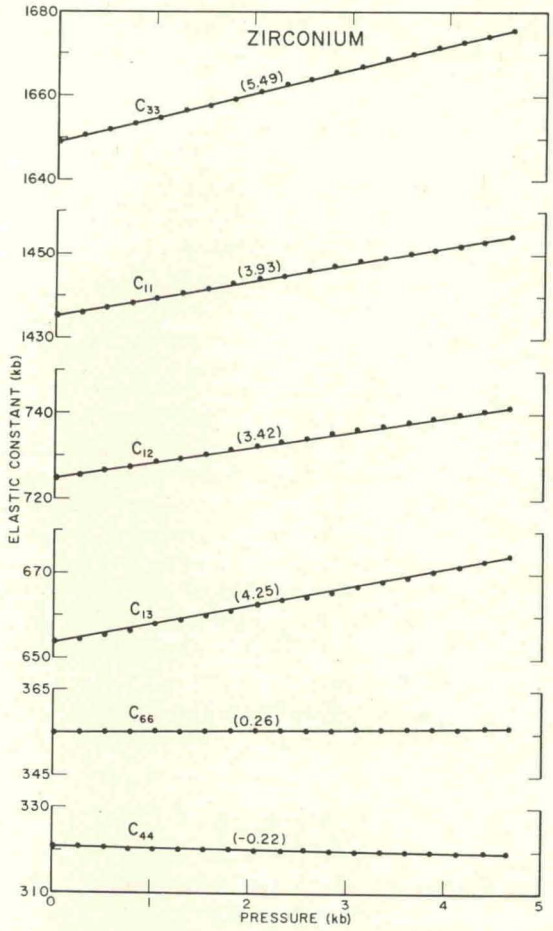

FIG. 2. C_{ij} versus pressure. The dC_{ij}/dP values are shown in parentheses.

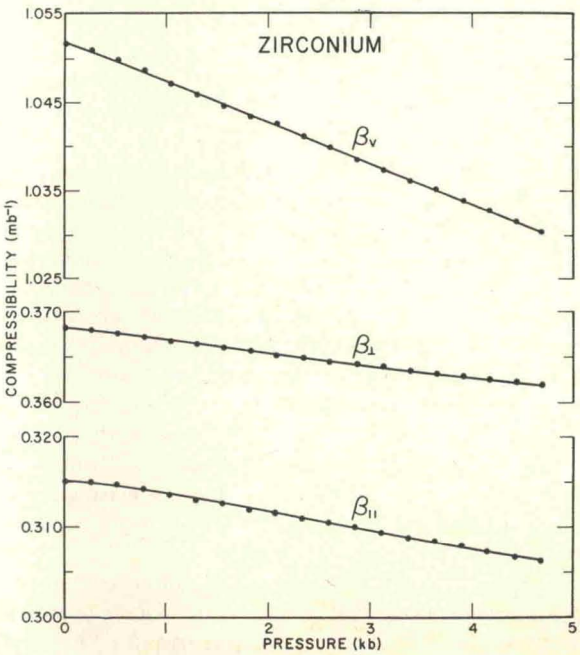

FIG. 3. Isothermal compressibilities versus pressure.

TABLE III. Isotropic elastic parameters of zirconium and their pressure derivatives.

Elastic parameter, X	Value	(dX/dP)
Adiabatic bulk modulus, K_s	953.1 kbar	4.08
Shear modulus, μ_H	361.3 kbar	0.02
Compressional-wave velocity, v_p	4.697 km/sec	4.23×10^{-3} km/sec/kbar
Shear-wave velocity, v_s	2.357 km/sec	-1.27×10^{-4} km/sec/kbar
Poisson's ratio, σ_s	0.3317	6.2×10^{-4}/kbar
Density, ρ	6.505 g/cm³	6.8×10^{-3} g/cm³/kbar

Pressure Dependence of Isotropic Elastic Parameters

The isotropic elastic moduli for zirconium were computed from the Voight–Reuss–Hill[14] approximation. The values of the various isotropic elastic parameters at ambient conditions and their initial pressure derivatives are given in Table III. The pressure dependence of the bulk modulus K, shear modulus μ, Poisson's ration σ, and density ρ are shown in Fig. 4. The change with pressure of the shear modulus is irregular. The value of $d\mu/dP$ is small but, in general, positive (0.06) to about 3 kbar and it becomes negative at higher pressures. It should be noted that this unusual phenomenon may be related to the pressure-induced phase change at ~60 kbar.[9]

DISCUSSION

Calculation of Intrinsic Temperature Coefficients of the C_{ij}

The pressure coefficients of the C_{ij} are related to the temperature derivatives through the following variation of Eq. (1)

$$C_{ij}^{-1}(dC_{ij}/dT)=C_{ij}^{-1}(\partial C_{ij}/\partial T)_V - (\alpha_V/\beta_V C_{ij})(\partial C_{ij}/\partial P)_T, \quad (3)$$

where the first term on the right side of the equation represents the intrinsic temperature dependence of the elastic modulus, and the second term is the temperature dependence caused by volume change (thermal expansion). For a quasiharmonic solid the lattice frequencies are not an intrinsic function of temperature and dC_{ij}/dT is dependent only on volume. In real solids the vibrational energy will vary with applied stress and the change with temperature of this effect contributes to the intrinsic term, along with possible intrinsic effects of electron excitation. In those fcc metals where $(\partial C_{ij}/\partial P)_T$ has been measured the volume change effect generally accounts for at least $\frac{1}{3}$ of the total temperature coefficient.[15]

The two unusual features in the observed temperature dependence of the elastic moduli of Zr are mentioned in the introduction to this paper. The total temperature coefficients for Zr, at 298°K, the calculated volume dependent terms, and the intrinsic terms that remain are listed in Table IV. It is clear that dC_{66}/dT and dC_{44}/dT at 298°K are derived almost completely from the intrinsic contribution and only about $\frac{1}{7}$ of dC_{11}/dT is due to the volume change during thermal expansion. In contrast, about 86% of dK_s/dT is derived from the volume change.

The very evident changes[2] in the total temperature derivatives of the elastic moduli at temperatures above 400°K could, however, be a consequence of the in-

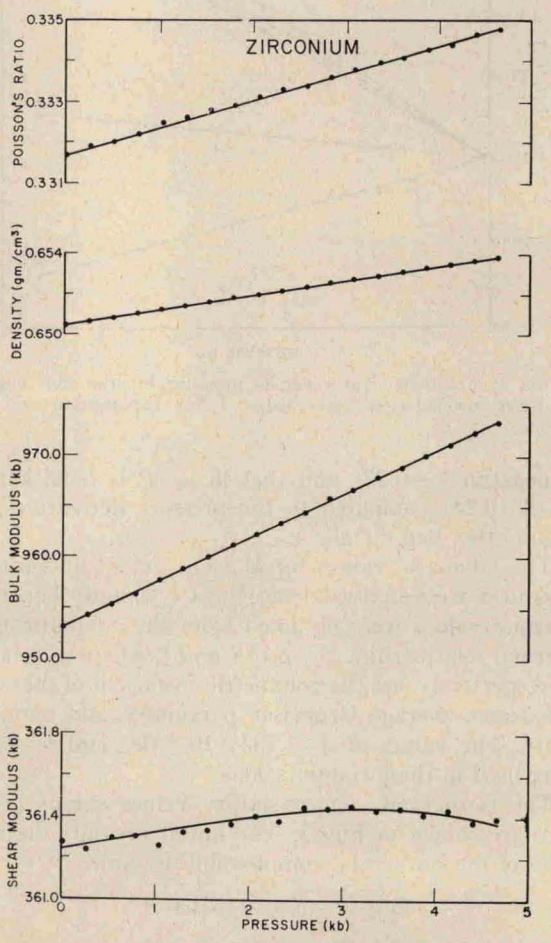

FIG. 4. Isotropic bulk and shear moduli, Poisson's ratio and density versus pressure.