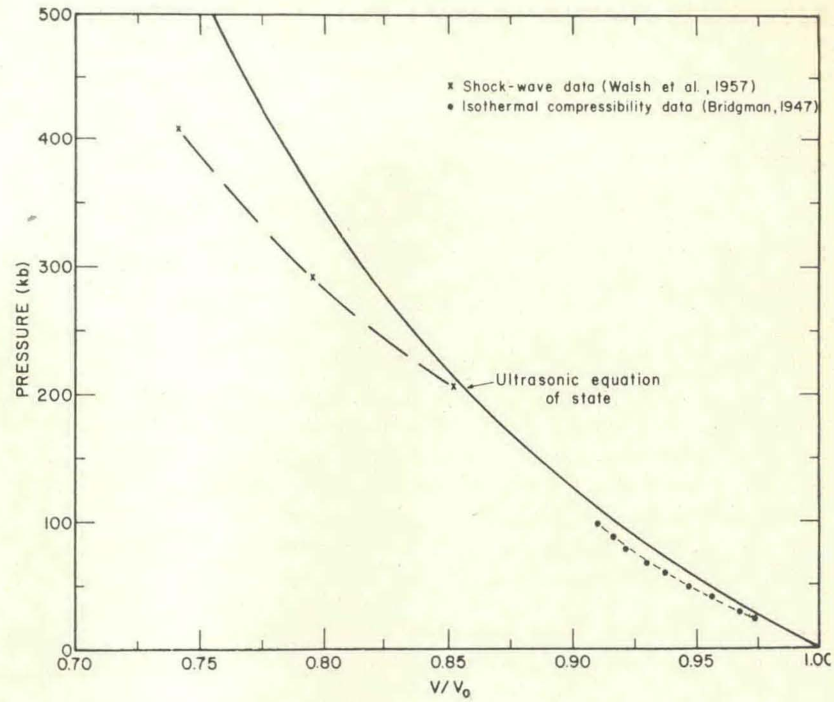

FIG. 5. Comparison of compression data for Zr as obtained from measurements of isothermal compressibility, ultrasonic-wave velocities and shock-wave velocities.

Thus, the interaction between the ultrasonic waves and other lattice waves must come into existence at higher temperatures and perhaps increases in degree as the transformation from hcp to bcc is approached. Measurements of the pressure coefficients of the elastic moduli at high temperatures are needed to look further into this question.

One can also calculate $\bar{\gamma}_H$ and $\bar{\gamma}_L$ values from the isotropic elastic moduli and pressure derivatives. The equations are given in Ref. 7. These relations give $\bar{\gamma}_H$

$$\bar{\gamma}_H(ISO)=0.59,\ \bar{\gamma}_L(ISO)=0.34.$$

Here, again, $\bar{\gamma}_H$ is considerably below $\bar{\gamma}_H(\alpha_V)$ from polycrystalline thermal expansion because of the negative pressure coefficient for the shear modulus μ_H calculated from the single-crystal data.

TABLE VII. Values of the parameters in Eqs. (15) and (16) used for computing $(\partial K_T/\partial P)_T$ at 298°K.

Parameter	Value	Unit
K_s	953.1	kbar
K_T	948.44	kbar
$(\partial K_s/\partial P)_T$	4.08	
α_V	17.35×10^{-6}	deg^{-1}
$(\partial\alpha_v/\partial T)$	1.0×10^{-8}	deg^{-2}
C_p	2.82×10^{6}	erg/g/deg
γ	0.95	
$(1+\alpha_v\partial T)$	1.005	
$(\partial K_s/\partial T)_P$	-9.35×10^{-2}	kbar/deg
$(\partial K_T/\partial T)_P$	-11.1×10^{-2}	kbar/jeg
T	298°K	deg
$(\partial K_T/\partial P)_T$	4.11	

Estimation of Compression of Zr to Higher Pressures

Anderson[25] has shown that the low-pressure ultrasonic data can be used to estimate compression of solid at high pressures below the phase-transition pressure by means of Murnaghan's equation of state

$$V/V_0=[1+(\partial K_T/\partial P)_T(P/K_T)]^{-1/(\partial K_T/\partial P)_T},\quad(14)$$

where V and V_0 are volumes at a given pressure and at zero pressure, respectively, and K_T is the isothermal bulk modulus. For zirconium, K_T was calculated from the relationship $K_T=K_S(1+\alpha\gamma T)^{-1}$ to be 950.1 kbar. To calculate $(\partial K_T/\partial P)_T$ from $(\partial K_s/\partial P)_T$, Overton's[26] relationships were used:

$$\left(\frac{\partial K_T}{\partial P}\right)_T=\left(\frac{\partial K_s}{\partial P}\right)_T+T\alpha_v\gamma\left(\frac{C_v}{C_p}\right)\left[\frac{-2}{\alpha_vK_T}\left(\frac{\partial K_T}{\partial T}\right)_P-2\left(\frac{\partial K_s}{\partial T}\right)_P\right]+\left[T\alpha_v\gamma\left(\frac{C_v}{C_p}\right)\right]^2\left[\left(\frac{\partial K_s}{\partial P}\right)_T-\frac{1}{\alpha_v^2}\left(\frac{\partial\alpha}{\partial T}\right)_P-1\right],\quad(15)$$

and

$$\left(\frac{\partial K_T}{\partial T}\right)_P=\left(\frac{\partial K_s}{\partial T}\right)_P(1+T\alpha_v\gamma)^{-1}-\frac{K_s\gamma}{(1+T\alpha_v\gamma)^2}\left[\alpha_v+T\left(\frac{\partial\alpha}{\partial T}\right)\right]_P.\quad(16)$$

Table VII shows the values of various parameters in Eqs. (15) and (16) used for deriving the values of $(\partial K_T/\partial P)$ which is 4.11. Thus the compression equation for zirconium is

$$V/V_0=[1+0.00433P]^{-0.243}. \quad (17)$$

In Fig. 5, a comparison of the ultrasonic equation of state (17) is made with the shock-wave data,[27] and Bridgman's isothermal compressibility data.[28] There is a poor agreement between Bridgman's data to 98 kbar and our results. This is partially explained by the phase transformation in Zr.[9] At higher pressures (760 kbar) the ultrasonic equation of state certainly cannot be used to estimate compression.

SUMMARY OF CONCLUSIONS

Attempts to correlate volume thermal expansion in Zr with the temperature and hydrostatic pressure derivatives of the elastic moduli lead to the conclusion that the elastic shear moduli and the transverse phonon modes are more dependent on the c/a ratio in this hcp structure than on the volume changes. In Zr, where the anisotropy in linear compressibility is the inverse of the anisotropy in linear thermal expansion, the strong coupling of the shear mode frequencies to the c/a ratio leads to a wide deviation between the high-temperature Gruneisen $\bar{\gamma}_H$ determined from the hydrostatic pressure derivatives of the elastic moduli and the Gruneisen parameter calculated from thermal-expansion data. Measurements of the elastic modulus changes under uniaxial stresses are needed to answer the questions raised in this study. Measurements of the high-temperature hydrostatic pressure derivatives should be helpful in deciding whether volume changes, rather than relative axial expansion, produced the effects on the lattice vibrations that lead to the hcp to bcc transformation. The pressure-induced phase change in Zr[9] at 60 kbar may be a result of the negative pressure derivative of the C_{44} shear modulus in Zr.

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