

assign  $Z = 3$  to all three rare earth metals and thus estimate the proximity of the Er results to the pure electrostatic case assuming  $dZ/dV = 0$ . The results of calculating the weighted  $\pi_{ij}^e$  contributions to  $\pi_{44}$ ,  $\pi_{66}$ , and  $\pi_{CH}$  are given in Tables 7, 8 and 9, respectively. We note that the values of  $c_{44}^e$ , as calculated from  $Z = 3$  and the  $M_{44}$  values computed by Cousins, are in fair agreement with the observed values of  $c_{44}$  in Gd, Dy and Er. The ratio  $R_{44}^e = c_{44}^e/c_{44}$  is a useful gauge of the

relative electrostatic and observed values and is carried through to Tables 8 and 9 for the  $c_{66}^e$  and  $C_H^e$  contributions.

The near electrostatic character of the shear moduli of Er is reflected consistently in the weighted contributions to the  $\pi_{ij}$  values, where the difference

$$\pi - \pi^e R^e = \pi^b R^b \quad (7)$$

becomes a useful parameter for estimating the band structure contributions to the observed

Table 7. Evaluation of weighted electrostatic and band structure components to  $\pi_{44}$ , from equation (6)

	Z	$c_{44}^e$	$R_{44}^e = c_{44}^e/c_{44}$	$\pi_{44}^e R_{44}^e$	$\pi_{44}^b R_{44}^b$	$\pi_{44}^b$	$d\pi_{44}^b/dP$
Gd	3	283	1.29	-1.79	+1.45	-5.00	-0.84
Dy	3	323	1.25	-1.63	+0.89	-3.56	-0.56
Er	3	339	1.14	-1.83	+0.29	-2.07	-0.19
Mg	2.168	210	1.14	-1.72	-1.60	+11.48	+0.66
Be	2.137	1021	0.62	-0.68	-1.02	-2.84	+1.5
Zr	4	796	2.19	-2.07	+2.73	-2.29	-1.05
Ti	4	1179	2.32	-3.46	+2.27	-1.72	-1.08

Table 8. Evaluation of weighted electrostatic and band structure components to  $\pi_{66}$

	$c_{66}^e$	$R_{66}^e$	$\pi_{66}^e R_{66}^e$	$\pi_{66}^b R_{66}^b$	$\pi_{66}^b$	$d\pi_{66}^b/dP$
Gd	405	1.72	-2.30	+1.61	-2.24	-1.02
Dy	429	1.59	-2.12	+1.43	-2.42	-0.98
Er	445	1.47	-2.00	+0.61	-1.30	-0.49
Mg	352	1.87	-2.51	-0.28	+0.32	+0.15
Be	1333	0.98	-1.29	-0.47	-2.35	+0.54
Zr	1153	2.61	-3.39	+2.69	-1.67	-1.25
Ti	1664	3.73	-5.00	+3.65	-1.34	-1.52

Table 9. Evaluation of electrostatic and band structure components to  $\pi_{CH}$

	$C_H^e$	$R_H^e$	$\pi_H^e R_H^e$	$\pi_H^b R_H^b$	$\pi_H^b$	$d\pi_H^b/dP$
Gd	559	2.24	-3.00	+2.35	-1.89	-1.37
Dy	581	2.01	-2.67	+2.00	-1.98	-1.40
Er	600	1.74	-2.40	+0.12	-0.16	-0.09
Mg	502	2.22	-2.99	-0.88	+0.72	+0.58
Be	1799	1.116	-1.45	-0.14	+1.20	+0.20
Zr	1597	3.10	-3.97	+3.53	-1.68	-1.92
Ti	2290	3.71	-5.00	+3.19	-1.18	-1.84

$\pi$ . For Er the  $\pi^b R^b$  difference does not exceed 1/3 of  $\pi_{ij}^e R_{ij}^e$  for any one of the three moduli, whereas a relatively large  $\pi_{ij}^b R_{ij}^b$  is necessary to account for at least one of the values observed for each of the other metals listed. Important examples of the latter are the  $\pi_{44}$  values for Mg and Be, where  $\pi_{44}^b R_{44}^b \geq \pi_{44}^e R_{44}^e$ .

Other interpretations of the data may be equally plausible at the present state of the theory of the rare earth metals. It is, for example, possible that  $dZ/dV \neq 0$ , thus contributing to  $\pi_{ij}^e$  in a positive way, i.e. making  $\pi_{ij}^e$  more negative by an increase in effective electron charge density in the spaces between the ions. The results for Er are, however, remarkably consistent with a simple Coulomb model with  $dZ/dV = 0$ . Since the highest magnetic ordering temperatures in Gd and Dy are higher than in Er, i.e. closer to the temperature of the present measurements, one might suspect that interactions between the conduction band and the 4f electrons are reflected in the Gd and Dy results. A direct effect of short range magnetic ordering on the shear modulus results seems improbable, however, since we see in Table 5 that the observed  $\pi_{44}$  and  $\pi_{66}$  of Gd at  $T < T_c$  are not greatly different than in the paramagnetic phase.

#### (b) Analysis of $\pi_{11}$ and $\pi_{33}$

It can be seen in Table 4 that the  $\pi$  values for the longitudinal stiffnesses,  $c_{11}$  and  $c_{33}$ , are considerably larger than those for the shear moduli. This is the usual case for solids and is qualitatively understood as a result of the fact that volume changes are produced by compressional waves but not shear waves. There will thus be a large contribution from the free electrons in the metal even when the core repulsion is relatively small. In the present case, it appears proper to consider the coupled plasma model of Bohm and Staver in which the electron-lattice interaction is derived from the screening by the free electrons of the charge produced by ionic motion [12, 21]. In this model the ion-core interaction

is pure Coulombic and the phonon frequencies become wave number dependent because of the electron response. The result is that the sound velocity for a longitudinal wave is given as

$$V_l^2 = \left[ \frac{m}{3M} Z \right] V_f^2. \quad (8)$$

Here  $M$  and  $Z$  are the ionic mass and charge and  $m$  and  $V_f$  are the electron mass and velocity, respectively. Since  $V_f^2 = 2E_f/m$ , where  $E_f$  is the Fermi energy, the sound velocity that is given by the Bohm-Staver equation will depend on the assumed valence as well as the Fermi energy,  $E_f$ . The general history of this equation [21] shows that it does indeed give reasonably good agreement, i.e. within 10 per cent, in the case of the alkali metals, where  $Z = 1$  and  $E_f$  is computed from the free electron gas model. In other metals, including Mg, the deviation from observed values of longitudinal velocities exceeds 20 per cent. It is, therefore, significant that the values of  $V_l$  calculated from equation (10) for Gd, Dy, and Er, with  $Z = 3$  and  $E_f$  values calculated for the free electron gas, are remarkably close to the observed longitudinal sound velocities in either the [0001] directions or in perpendicular directions, as shown in Table 10. In all cases the free electron calculated  $V_l$  are within 3 per cent of the observed values. The second values of  $E_f$  noted in the

Table 10. Comparison of Bohm-Staver longitudinal sound velocity with measured values for Gd, Dy and Er at 300°K

Metal	$E_f$ (Rydbergs)	$V_l$ calculated (cm/sec) $\times 10^{-5}$		
		$V_{11}$	$V_{33}$	
Gd	0.540*	3.002	2.91	3.02
	0.425 (Ref. [23])	2.66		
Dy	0.558*	3.002	2.95	3.03
	0.450 (Ref. [23])	2.696		
Er	0.568*	2.987	3.09	3.07
	0.452 (Ref. [23])	2.664		

\*Free electron gas model.