4. Velocity–density trends

Although the data shown in Figs. 2–4 reveal compositional and crystal structural effects explicitly, they also provide a better test than has been possible hitherto of the applicability of general velocity–density correlations to the effects of phase changes. That is, they test Birch's [1, 2] conjecture that a phase change would move a substance, on average, parallel to his lines of constant mean atomic weight on a velocity–density plot. Liebermann and Ringwood [9] have discussed this question on the basis of their more limited data set, and concluded that the deviations from the trend of the velocity–density correlations can be large for specific transitions, such as the olivine–spinel transition. This conclusion is clearly supported by the present data. Nevertheless, we are concerned here with average trends, in so far as they can be defined by the still limited data set.

In Fig. 3b, for instance, most of the data lie close to a line of slope about 1.3. Thus, a transition between any two of the structures represented would move a material approximately along a line of slope 1.3. In Fig. 2b, the average trend is roughly defined by the olivine–oxides trend, giving a slope of about 1.0. The spinels deviate from this trend, but this is compensated when the olivine–spinel and spinel–oxides trends are averaged. In Fig. 4b, the main trend (excluding α-quartz–coesite) is between about 1.1 (coesite–stishovite) and 1.7 (GeO_2 α-quartz–rutile). Thus the average trend over all of the above cases is probably between slopes of about 1.0 and 1.5, with 1.3 being perhaps the most likely value.

The average trends for v_p and v_s are not so well defined. In Figs. 2a, 3a and 4a, the slopes are about 0.9, 1.1 and 0.7–1.7, respectively, so a representative value would be about 1.1 for v_p. For v_s, a slope between 0.5 and 1.0 might be representative, but there are wide variations. These results are summarized in Table 2.

The slopes in Figs. 2–4 are:

$$C = \frac{\rho^o(v^o - v)}{v^o(\rho^o - \rho)} = \frac{\rho^o \Delta v}{v^o \Delta \rho} \approx \frac{\Delta \ln v}{\Delta \ln \rho} \qquad (3)$$

Thus C is approximately comparable to the parameter λ defined by Shankland and Chung [3, 15, 16] as:

TABLE 2

Slopes $C = \rho^o \Delta v / v^o \Delta \rho$ through selected phase transitions

Transition	C_p	C_b	C_s
Average, all transitions	1.1	1.3	0.5–1.0
Olivine–spinel	1.9	2.0	1.4
Spinel–oxides	0.4	0.1	(0)
Olivine–oxides	0.9	1.0	(0.9)

$$\lambda = \left(\frac{\partial \ln v}{\partial \ln \rho}\right)_A \qquad (4)$$

where A is the mean atomic weight. Shankland and Chung determined λ by fitting the power-law analogue of Birch's [1] originally linear velocity–density correlation to a set of minerals with $A \approx 20$. They found $\lambda_p = 1.25$ and $\lambda_b = 1.25$, approximately [16]. These values are quite comparable to those for C found for phase transitions, above.

Comparisons can also be made with parameters derived from other proposed velocity–density relations. Thus D. Anderson's "seismic equation of state" [17] involved the parameter $n = (\partial \ln \rho / \partial \ln \phi)_A = 1/2\ \lambda_b$. Anderson found $n = 0.323$ [17] and $n = 1/3$ [11], giving $\lambda_b = 1.55$ and 1.5. O. Anderson and Soga [18] suggested that λ_p should have a value of about 1.5. All of these values are slightly higher than the values of C_p and C_b found for phase transitions.

Parameters found from the linear velocity–density correlations [1, 2, 19] can also be compared, with suitable normalization; the quantity found is the derivative $(\partial v / \partial \rho)_A$, and this can be converted to the logarithmic derivative using suitable values of ρ and v. For discussions of the mantle, suitable values are the properties of the oxide mixture (0.9 MgO + 0.1 FeO) + SiO_2 (stishovite): $\rho = 4.0$ g/cm^3, $v_p = 10$ km/sec, $v_s = 7.5$ km/sec. Thus, Birch [1] found, for two selections of rocks and oxides, $(\partial v_p / \partial \rho)_A = 3.05$ and 3.31, giving $\lambda_p = 1.2$ and 1.3, approximately. Wang [19] found $(\partial v_b / \partial \rho)_A = 2.4$ for $A \approx 20$, giving $\lambda_b = 1.3$. These values are all comparable to those for C_p and C_b found for phase changes.

In summary, the various velocity–density correlations for mean atomic weights near 20 have yielded slopes which are comparable to, and in some cases slightly greater than, the trends found here for phase

changes. However, trends through specific phase transitions can deviate widely from these average values.

5. Geophysical implications

Liebermann and Ringwood [9] have pointed out that the wide range of velocity–density trends through phase transitions which they observed may require that some previous interpretations of the mantle transition zone be revised. The present results indicate that the velocity–density relations which have been used are probably reasonable representations of the average effects of phase changes, but not of specific phase changes which may be important in the mantle. The point made by Liebermann and Ringwood is thus reinforced.

In particular, the spinel–oxides transition involves only a small increase in v_p, and possibly also of v_s (Fig. 2). Bassett and Ming [20] have reported evidence from static compression X-ray experiments that fayalite (Fe_2SiO_4) breaks down to the oxides FeO and SiO_2 above about 200 kilobars pressure. This suggests that the post-spinel phase of magnesium-rich olivines, $(Mg, Fe)_2SiO_4$ might be the mixture 2(Mg,Fe)O (rocksalt) + SiO_2 (rutile). If the major component of the mantle is olivine, the present results suggest that in the sequence of transformations olivine–β-phase–spinel–oxides most of the total increase of velocities would be accounted for by the olivine–spinel part of the sequence, and hence that this behavior should be reflected in the seismic velocity profiles of the mantle. In this connection, it is interesting to note that some recent v_p models of Helmberger and Wiggins [21, 22] show this tendency – the sharp velocity increase near 650 km depth is only about 4% in their models, whereas in some other models [23, 24] the increase is about 8–11%.

If the mantle is composed mainly of olivine, then the mean trend from olivine to oxides is the relevant quantity with which to compare velocity–density relations which have been used to interpret the transition zone as a whole. Thus the effect of the intermediate β- and spinel phases, which lie above the average trends defined by the other structures in Figs. 2–4, can be neglected in this comparison. For olivine–oxides, C_p is about 0.9 and C_b is about 1.0 (Table 2). Birch [2, 25] and D. Anderson [26], for instance, used values of $(\partial v_p/\partial\rho)_A$ of 3.31 and 3.05, corresponding to values of λ_p of about 1.3 and 1.2, respectively. Thus Birch's [25] solution I for the mantle density may have underestimated the density increase through the transition zone, while Anderson [26] may have overestimated the velocity increase to be expected for a pure olivine model – it thus may not be necessary to invoke an increasing iron content through the transition zone to match the observed compressional velocity below the transition zone. In Birch's [25] solution II, $(\partial v_p/\partial\rho)_A$ was determined to be 2.64 km/sec, corresponding to a λ_p of about 1.05. This may be more consistent with an olivine model of the mantle. D. Anderson and Jordan [27] and D. Anderson et al. [28] used $\lambda_b = 1.5$ and 1.55, in effect, in the seismic equation of state to determine the mean atomic weight of the lower mantle from extrapolated zero-pressure values of the velocities and density. These high values may have caused the mean atomic weight to be overestimated.

In some recent earth models [29, 30] both the density and velocities have been determined entirely from seismic data. The velocity–density trends through the transition zones of these models may therefore be compared directly with the present results. Liebermann [31] examined some characteristics of the "400-km" discontinuity in these models, and concluded that none of them were compatible with experimentally observed characteristics of the olivine–spinel or olivine–β-phase transitions. The seismic (free oscillation) data did not give very good resolution of the details of the transition zone for any of these models. Since Model B1 of Jordan and Anderson [30] seems to employ the most reasonable assumptions about the transition zone, it will be examined further here. The parameters C_p, C_b and C_s for the discontinuities at 420 km and 670 km depth in Model B1 are listed in Table 3. The corresponding parameters for the olivine–spinel, spinel–

TABLE 3

Values of $C = \rho^0\Delta v/v^0\Delta\rho$ through the transition zone of Model B1 [30]

Depth (km)	C_p	C_b	C_s
420	1.2	0.6	1.8
670	1.0	0.3	1.8
(420–670)	1.1	0.9	1.3