## On the compression of stishovite

mantle consists of a mineral assemblage with the density of isochemical mixed oxides, but with a higher iron content than the upper mantle. In order to correlate or compare possible component assemblages of the lower mantle in terms of requisite density and elastic properties, previous investigators have found it convenient to determine  $\rho_0$  and the seismic parameter  $\Phi_0 = K_0/\rho_0$  for the lower mantle by fitting various density distributions with the Birch equation. Considering the present results bearing on the equation of state of stishovite, it is pertinent to examine the procedures and results of compositional models of the lower mantle based on the assumption of a mixture of the isochemical oxides.

Anderson & Jordan (1970) fit pressure-density data for the lower mantle to the Birch equation by a least-squares procedure, thereby determining values for  $\Phi_0$  and  $\rho_0$  representative of lower mantle material. It was assumed that the temperature gradient of the lower mantle approximates the adiabat. However, the results of the shock-wave analysis of stishovite have suggested that the compression of this material is reproduced more accurately by the first-order Murnaghan equation of state than the Birch equation. In the present case, the difference between the bulk modulus calculated by means of the Murnaghan and Birch equations is about 10 per cent. Thus the assumed form of the equation of state has a significant effect on the magnitude of the determined adiabatic constants. Until it is quite clear as to what equation of state is most appropriate for expressing the compression of lower mantle mineral assemblages, the results based on the foregoing assumptions and procedure should be regarded with caution.

In order to assess the iron content of the lower mantle, Anderson & Jordan (1970) used three different methods; these have been reviewed recently by Wang & Simmons (1972). The effect which may be associated with the selection of an inappropriate equation of state may be qualitatively illustrated by considering Anderson & Jordan's (1970) first approach.

Having determined  $\rho_0$  and  $\Phi_0$  for a variety of lower mantle density models as outlined in the preceding section, the mean atomic weight  $\overline{M}$ , which reflects iron content, is derived from the seismic equation of state (Anderson 1967). This equation may be written in the form

$$\frac{\rho}{\overline{M}_i} = A_i \Phi^{n_i} \tag{16}$$

where the constants  $A_1 = 0.048$  and  $n_1 = 0.323$  refer to results obtained from 31 selected rocks and minerals, and  $A_2 = 0.0492$  and  $n_2 = 0.333$  reflect only close-packed oxides relevant to the interpretation of lower mantle data. Estimates of the composition of the upper mantle indicate an average  $\overline{M}$  of about 21.1. By contrast, the estimates of  $\overline{M}_1$  by Anderson & Jordan (1970) for the lower mantle, determined using the first-order Birch equation and seismic equation of state, range from about 22.4-23.4; the corresponding range for  $\overline{M}_2$  is about 21.0-22.0. Thus, as Anderson & Jordan (1970) point out, marginal evidence for an increase in iron content in the lower mantle, relative to the upper mantle, is suggested. However, if the value of  $\Phi_0$  is in error by 10 per cent, this, in itself, results in a 5 per cent uncertainty in the value of  $\overline{M}$ . Recognition of uncertainties of this magnitude associated with the calculated values of  $\overline{M}_1$  and  $\overline{M}_2$  reduce the reliability of conclusions regarding iron enrichment of the lower mantle based on the foregoing procedure.

A second method used by Ringwood (1969) and Anderson & Jordan (1970) involves comparing the density and elasticity of the isochemical oxide mixture MgO-FeO-SiO<sub>2</sub> with lower mantle data. The conclusions resulting from this approach are obviously dependent on the uncertainties associated with the corresponding values of  $\Phi_0$  adopted for the various oxides, especially that of stishovite. Therefore, it is of interest to review the conclusions of Anderson & Jordan (1970)

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## Table 1

Comparison of elastic and crystallographic data for rutile-structure  $SiO_2$ ,  $TiO_2$ , and  $GeO_2$ 

	SiO <sub>2</sub>	GeO <sub>2</sub>	TiO <sub>2</sub>
$\rho_0 \mathrm{g} \mathrm{cm}^{-3}$	4.288	6.279	4.260
$V_{c}^{a}$ (10 <sup>-24</sup> ) cm <sup>3</sup>	46.4	55.3	62.4
K <sup>sb</sup> Kbar	3350	2511	2109
$(\partial K^S / \partial P)_T^b$	5.5	6.48	6.94
$(\partial K^{s}/\partial T)_{P}^{b} K bar/^{\circ} K$	-0.35	-0.38	-0.42

a Unit cell volume.

b single-crystal data is represented by the Reuss average of the  $C_{ij}$  elastic constants.

with respect to the iron content of the lower mantle in view of the value of  $\Phi_0$  for stishovite,  $78 \cdot 1 \pm 4 \cdot 4 \ (\text{km s}^{-1})^2$ , as determined in the present study.

It is assumed that the molar volumes and seismic parameters of lower mantle minerals can be considered to be molar averages of the oxides (Anderson 1969). Thus, both the composition and mineralogy of the lower mantle can be determined by comparing the density and  $\Phi_0$ , inferred from the fit of lower mantle data to the Birch equation, to those predicted for the dense forms of upper mantle minerals. The basic plot of  $\rho_0$  vs  $\Phi_0$  by Anderson & Jordan (1970) is reproduced in Fig. 7 with respect to the olivine and pyroxene systems. In addition, the appropriate values of  $\Phi_0$  and  $\rho_0$ , representing the high-pressure forms of MgSiO<sub>3</sub> and Mg<sub>2</sub> SiO<sub>4</sub> calculated from the stishovite results of the present study, are indicated for comparison. The points Birch II and 200204 represent the preferred solutions of Anderson & Jordan (1970) for the values of  $\Phi_0$  and  $\rho_0$  for the lower mantle. By combining these values inferred for the lower mantle, estimates may be made for mole per cent olivine, pyroxene, SiO<sub>2</sub>, MgO, and FeO. In the present analysis, the following values were used for the component oxides: SiO<sub>2</sub>,  $\rho_0 = 4.288 \text{ g cm}^{-3}$  and  $\Phi_0 = 78.1 \pm 4.4 \text{ (km s}^{-1})^2$ ; MgO,  $\rho_0 = 3.584 \text{ g cm}^{-3}$  and  $\Phi_0 = 45.3 \text{ (km s}^{-1})^2$  (Chang & Barsch 1969); and FeO,  $\rho_0 = 5.948 \text{ g cm}^{-3}$  and  $\Phi_0 = 27.8 \text{ (km s}^{-1})^2$  (Mitzutani *et al.* 1972). Oxide compositions were determined by linear interpolation on an MgO-FeO-SiO<sub>2</sub> triangle superimposed on the  $\rho_0 - \Phi_0$  plot. Results of the present analysis for the Birch II and 200204 models are compared with the conclusions of Anderson & Jordan (1970) in Table 2.

## Table 2

Model Birch II	Anderson & Jordan (1970)	Present analysis
olivine	0.57	0.05-0.68
pyroxene	0.43	0.95 - 0.32
SiO <sub>2</sub>	0.39	$0.47 \pm 0.04$
MgO	0.49	$0.38 \pm 0.03$
FeO	0.12	$0.15\pm0.03$
Model 200204		
olivine	0.20	0-0.32
		*
pyroxene	0.80	>1.00-0.68
SiO <sub>2</sub>	0.46	$0.53 \pm 0.04$
MgO	0.38	$0.26 \pm 0.03$
FeO	0.16	$0.21\pm0.03$

Composition of the lower mantle (mole fraction)

\* Excess silica.