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THE DENSITIES OF COMPOUNDS AT HIGH PRESSURES AND THE STATE OF THE EARTH'S INTERIOR*

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ABSTRACT

A quantum statistical method, already well developed for pure elements, has been extended to the prediction of the equation of state of compounds at extremely high pressures at absolute zero. Application of a finite-strain condition to possible constituents of the earth, found by Birch to be valid for many materials, leads to satisfactory interpolation between the existing laboratory data and the quantum predictions for these materials. The quantum calculations begin to hold at pressures of the order of 10^{14} dynes/cm², pressures greatly exceeding those obtainable within the earth. The finite-strain interpolative procedure is assumed to predict the pressure-density relationships at pressures corresponding to those prevailing within the earth. From Bullen's pressure-density values for the earth, it is found that, assuming the absence of phase transitions, the base of the mantle has the same density as an olivine possessing 63 per cent Mg_2SiO_4 . By a similar procedure, the earth's outer core cannot be pure iron, but has the same density as a mixture of 90 per cent iron and 10 per cent olivine. For the temperatures prevailing within the earth, the quantum calculations at absolute zero are not significantly altered; a latitude in the interpolative procedure is indicated at these temperatures, leading to a composition of olivine at the base of the mantle ranging between 47 and 63 per cent Mg_2SiO_4 .

I. Introduction

A knowledge of the properties of matter under conditions of extremely high pressures is of considerable importance to the study of the state of the earth's interior. The experimental data of Bridgman (1948a) up to pressures of 10^5 atmospheres correspond to a depth of only 300 km within the earth. At very high pressures, of the order of 10^7 atmospheres or greater, such as occur in the interior of stars, the methods of quantum statistics may be applied to the theoretical determination of the equation of state of the heavy elements.

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Unfortunately, the pressures at which this theoretical method is expected to become applicable are greater than those which obtain within the earth. Elsasser (1951) has compared the earlier results for the elements with the densities and compressibilities found experimentally by Bridgman, and has attempted to interpolate in the gap between 10^5 and 10^7 atmospheres, the interval which is of geophysical interest. Bullen (1952) has criticized Elsasser's extrapolation of the high pressure results to low pressures, and has shown that an earth model based on Elsasser's data becomes internally inconsistent. Bullen concludes that the atomic number to be associated with the material of the outer portion of the earth's core should be at least six units less than the value derived from Elsasser's extrapolation.

The interpolation between the experimental data for silicates and the results of the quantum statistical calculation for compounds should be consistent with Bullen's findings, which required the assigning of a "representative atomic number" to a complex silicate. The interpolation may be performed by means of semi-empirical equations of state, such as those of Grüneisen (1912) and Born (1939), or equations of state based on theories of the deformation of solids. Murnaghan's (1937) theory of finite strain has been applied to the earth's interior by Birch (1952). Birch's formula permits a reasonable fit between Bridgman's experimental data and the results of high pressure computations for compounds based upon the quantum statistical method.

In the work which follows, it is assumed that there are no discontinuities in the pressure-density relations for the materials in the earth's mantle, at the pressures within the earth's mantle. Should it be established that phase changes occur in this region, our results will require revision. If the mantle is to be composed of ultra-basic rocks, the atomic number to be associated with the material near the bottom of the mantle must lie between 10 and 16, with 12.5 as a most probable value. Since Elsasser's curves indicate a value of atomic number approximately equal to 18 for the bottom of the mantle, our results require a shift of approximately six atomic numbers from Elsasser's value in the same direction as required by Bullen from considerations of the core.

II. *Pressure-density relationships for compounds at absolute zero*

Pressure-density relationships at absolute zero (Fig. 1) have been obtained elsewhere (Feynman, Metropolis, and Teller, 1949; Slater and Kruter, 1935; Jensen, 1938) for the pure solid elements under the assumption of a Fermi-Thomas model for the electrons surrounding the nuclei. The several investigators have indicated that the results obtained for the elements may be applied to computations of a similar type for solid compounds of the elements. The Fermi-Thomas model for solid compounds should serve as a basis for the determination of the state of solid matter at great depth within the earth.

The assumptions necessary for the extension of results based upon a quantum model to the state of terrestrial materials at great depth are as follows: (1) that the chemical compounds existing within the earth are composed entirely of atoms whose atomic number, Z , exceeds the value $Z = 6$; (2) that the quantum results obtained at absolute zero are applicable at the elevated temperatures existing

within the earth; and (3) that the pressures within the earth are sufficient to insure the validity of the Fermi-Thomas model.

The first of these assumptions is necessary in view of the fact that the Fermi-Thomas model assumes a sufficiently great electron density that Fermi-Dirac

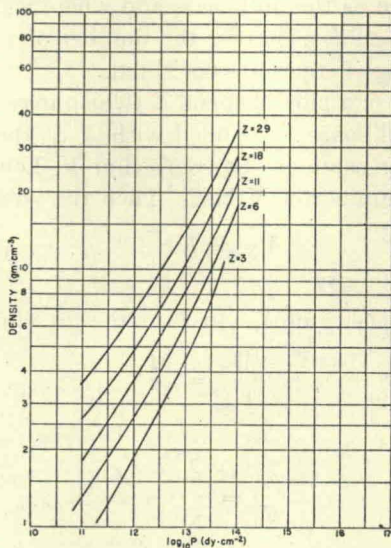


Fig. 1—Pressure-density relationships for the Fermi-Thomas model of the pure solid elements at $T = 0$

statistics may be applied to their distribution in space. The smallest atomic number, $Z = 6$, considered by Feynman, *et al.*, is lower than the atomic numbers of the elements forming the chemical compounds usually assumed to exist in the earth's interior. It is doubtful whether H, He, Li, Be, or B are present in quantity at depth. The element of lowest atomic number assumed to be quantitatively important (Bullen, 1947) is oxygen, necessary to the formation of oxides and silicates. Kuhn and Rittman (1941) have proposed that the earth's interior is composed largely of hydrogen, but this theory has been generally rejected (Birch, 1952, pp. 274-275). The remaining assumptions are investigated in detail in Sections III and IV.

We start by considering a homogeneous material of the chemical composition

$$Y = (A_1)_{n_1}(A_2)_{n_2} \cdots (A_m)_{n_m} \dots \dots \dots (1)$$

where the n_i 's are the numbers of times the elements A_i occur in one molecule of the compound. Each of the elements A_i has a corresponding atomic number Z_i . For each A_i , there is an atomic radius $\mu_i x_{0i}(P)$ computed for the pure element A_i at the pressure P . The unit of length μ_i is (Feynman) $\mu_i = 0.88534a_0 Z_i^{-1/3}$, where a_0 is the Bohr radius for the hydrogen atom.

The volume of the molecule Y at the pressure P may now be computed:

$$V_Y = K \sum_i \frac{n_i x_{0i}^3}{Z_i} \dots \dots \dots (2)$$

where the summation is taken over the elements in the compound and where K is a constant. The mass of the molecule Y is

$$M_Y = 2 \sum_i n_i Z_i \dots \dots \dots (3)$$

where we take the proton as the unit mass and where we assume that the atomic weight of an atom $M_i = 2Z_i$; that is, the number of protons and neutrons are equal and nuclear binding energies are neglected.

Assume the existence of a pure element X (which may have a fractional atomic number), such that if all space were filled with X at the pressure $P(T = 0^\circ\text{K})$, the density would be the same as the compound Y . Let the atomic radius of X be $\bar{\mu}x_0$ and the atomic number of X be \bar{Z} . Then the volume of one atom of X is

$$V_X = K\bar{x}_0^3\bar{Z}^{-1} \dots \dots \dots (4)$$

and the mass of X is $M_X = 2\bar{Z}$.

For the identity of density of X and Y at the pressure P

$$\frac{M_X}{V_X} = \frac{M_Y}{V_Y} \dots \dots \dots (5)$$

Hence it follows that

$$\frac{\bar{Z}^2}{\bar{x}_0^3} = \frac{\sum_i n_i Z_i}{\sum_i \frac{n_i x_{0i}^3}{Z_i}} \dots \dots \dots (6)$$

Thus from the properties of the elementary constituents A_i , at the pressure P , it is possible to find the properties of a pure element X possessing the same pressure-density relationship as the compound Y .

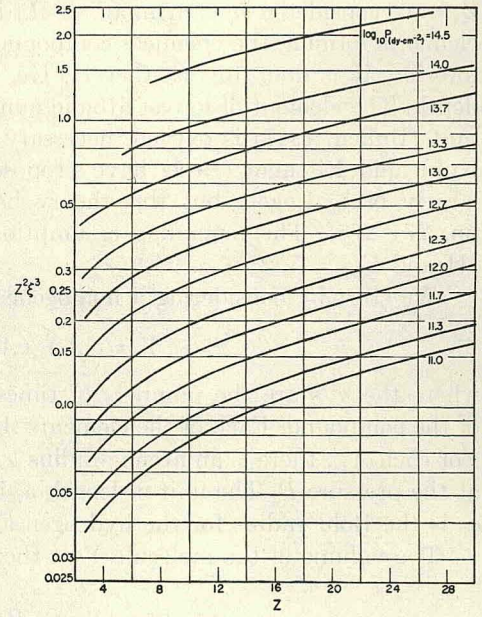
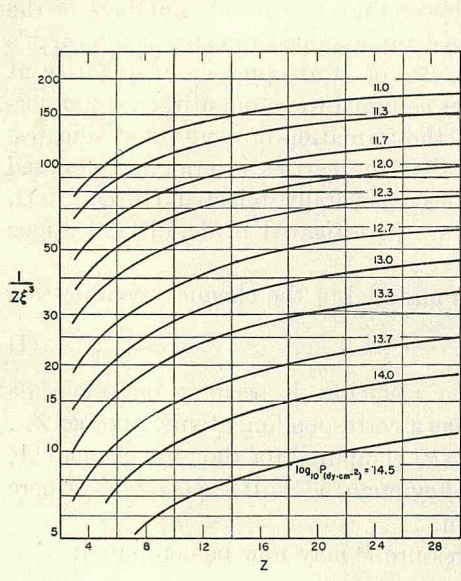


FIG. 2—The quantity $Z^{-1}\xi^{-3}$ plotted as a function of atomic number and pressure

FIG. 3—The quantity $Z^2\xi^3$ plotted as a function of atomic number and pressure

In order to simplify the computation of the right-hand side of equation (6), curves of $Z^{-1}\xi^{-3}$ have been compiled in Figure 2 for values of Z from 3 to 29, a range of values encompassing the elements likely to form significant terrestrial compounds. The variable ξ is defined by the expression

$$\xi = 0.701/x_0 \quad (\text{Feynman}) \dots\dots\dots(7)$$

(We note that for $Z > 28$, the assumption $M = 2Z$ may no longer be used with any assurance for the ordinary isotopes of the elements.)

Similarly, computation of \bar{Z} is simplified by the use of the curves of $Z^2\xi^3$, compiled in Figure 3, for values of Z ranging from 3 to 29, as functions of the pressure. We have used the results obtained by Feynman, Metropolis, and Teller to construct Figures 2 and 3.

If homogeneous mixtures of several compounds Y_i are considered, expression (6) is still valid where it is understood that the n_i represent the occurrences of the atom A_i in a sample of the mixture large enough to be representative.

An example of the method will now be given. Consider a homogeneous earth formed of the material Mg_2SiO_4 . At a pressure of 10^{12} dynes per square centimeter, reading from Figure 2,

$$\bar{Z}^2\bar{\xi}^3 = \frac{2 \times 12 + 1 \times 14 + 4 \times 8}{2 \times 71 + 1 \times 76 + 4 \times 59} = 0.154 \dots\dots\dots(8)$$

and from Figure 3, $\bar{Z} = 10.3$.

For representative compounds, the computed values of \bar{Z} and density are given in Tables 1 and 2 over a pressure range of 10^{11} to $10^{14.5}$ dynes per square centimeter. The densities have been computed according to the expression

$$\rho = \frac{2\bar{Z}M_p}{4/3\pi(\bar{\mu}\bar{x}_0)^3} \dots\dots\dots(9)$$

where M_p is the mass of the proton and where binding energies have again been neglected. Inserting the values of the Bohr radius and the proton mass (Dumond and Cohen, 1952), we obtain

$$\rho = 22.58 \bar{Z}^2\bar{\xi}^3 \text{ gm} \cdot \text{cm}^{-3} \dots\dots\dots(10)$$

where the mean values already computed for the compounds are used. It is noteworthy that the representative atomic number of a compound, under the present definition, has a value in each of the cases considered which is slightly greater than the values obtained by a simple averaging process,

$$\bar{Z} \approx \frac{\sum_i n_i Z_i}{\sum_i n_i} \dots\dots\dots(11)$$

This latter assumption was made by Birch in describing the properties of Mg_2SiO_4 by the representative atomic number, $\bar{Z} = 10$. However, the present results obtained for the representative atomic number suggest a revision of Bullen's (1952, p. 396) statement that "a Z value of 12 would be probably too low to fit in an ultra-basic rock composition." Indeed, the range of values suggested by Bullen for ultra-basic rocks, Z of the order 18 to 23, seems to be too great in view of the present computations.

TABLE 1—Representative atomic numbers for Birch's list of minerals as computed from the Fermi-Thomas model for compounds

Material	Formula	Mean atomic weight	Mean atomic number	Representative atomic number					Assigned representative atomic number
				Log P = 11	Log P = 12	Log P = 13	Log P = 14	Log P = 14.5	
Forsterite	Mg_2SiO_4	20.10	10.0	10.3	10.4	10.4	10.4	10.3	10.4
Fayalite	Fe_2SiO_4	29.11	14.0	15.1	16.0	16.2	16.3	16.4	16.2
Quartz	SiO_2	20.02	10.0	10.4	10.4	10.4	10.4	10.3	10.4
Periclase	MgO	20.16	10.0	10.3	10.4	10.3	10.1	10.2	10.3
Diopside	$CaMgSi_2O_6$	21.65	10.8	11.0	11.3	11.4	11.4	11.6	11.4
Enstatite	$MgSiO_3$	20.08	10.0	10.4	10.4	10.4	10.4	10.3	10.4
Albite	$NaAlSi_3O_8$	20.17	10.0	10.4	10.4	10.4	10.4	10.4	10.4
Rutile	TiO_2	26.63	12.7	13.8	14.1	14.2	14.5	14.4	14.3
Corundum	Al_2O_3	20.39	10.0	10.4	10.4	10.4	10.4	10.4	10.4
Anorthite	$CaAl_2Si_2O_8$	21.40	10.6	10.8	11.0	11.0	11.5	11.4	11.2

In the work which follows, we shall associate a single representative atomic number with each compound. We shall use the mean of the values of atomic number in the pressure interval 10^{12} to $10^{14.5}$ dynes/cm². These values are given in Table 1.

TABLE 2—Densities for Birch's list of minerals as computed from the Fermi-Thomas model for compounds

Material	Formula	Actual density (gm.cm ⁻³) at room temperature, one atmosphere (log P = 6)	Log P	Log P	Log P	Log P	Log P
			= 11	= 12	= 13	= 14	= 14.5
Forsterite	Mg_2SiO_4	3.19	1.72	3.48	8.08	21.6	34.8
Fayalite	Fe_2SiO_4	4.14	2.26	4.42	10.0	26.2	42.2
Quartz	SiO_2	2.654	1.73	3.50	8.08	21.7	35.1
Periclase	MgO	3.56	1.72	3.48	8.04	21.6	34.8
Diopside	$CaMgSi_2O_6$	3.2 -3.38	1.84	3.67	8.47	22.6	36.5
Enstatite	$MgSiO_3$	3.1 -3.43	1.73	3.48	8.08	21.6	35.0
Albite	$NaAlSi_3O_8$	2.57-2.69	1.73	3.48	8.08	21.7	35.0
Rutile	TiO_2	4.2	2.10	4.13	9.42	24.9	40.0
Corundum	Al_2O_3	4.02	1.73	3.48	8.06	21.6	35.0
Anorthite	$CaAl_2Si_2O_8$	2.70-2.76	1.81	3.63	8.40	22.4	36.1

III. The Birch-Murnaghan theory

Since the experimental data on the densities of silicates have been obtained only at relatively low pressures and because the results obtained from the Fermi-Thomas model are valid only at pressures much greater than those of the mantle, it is necessary to interpolate in the gap. Birch has extended and applied Murna-

ghan's theory of finite strain to the earth's mantle. Birch found that, at constant temperature, the pressure P is given by

$$P = \frac{3}{2}K_0[(\rho/\rho_0)^{7/3} - (\rho/\rho_0)^{5/3}]\{1 - \xi[(\rho/\rho_0)^{2/3} - 1] + \dots\} \dots\dots(12)$$

where K_0 is the isothermal incompressibility, ρ_0 is the density at zero pressure, and ξ is a ratio between two coefficients in the power-series expansion of the free energy in terms of the strain. Using experimental data for the alkali metals and for a large number of simple compounds at high compression, Birch found that $|\xi| < \frac{1}{2}$, with the most frequent value $\xi = 0$, in the observed pressure range.

If it be assumed that the value $\xi = 0$ is also valid for the silicates, then we may compute pressure-density relationships (at constant temperature) from the expression

$$P = \frac{3}{2}K_0[(\rho/\rho_0)^{7/3} - (\rho/\rho_0)^{5/3}] \dots\dots\dots(13)$$

The values of K_0 and ρ_0 for silicates at $T = 0^\circ\text{K}$ have not been measured, but the available experimental data (Birch, 1942) suggest that temperature effects are unimportant and that little error will be incurred in adopting the values obtained at room temperature.

In Figure 4 are shown the experimental pressure-density relations, a graph

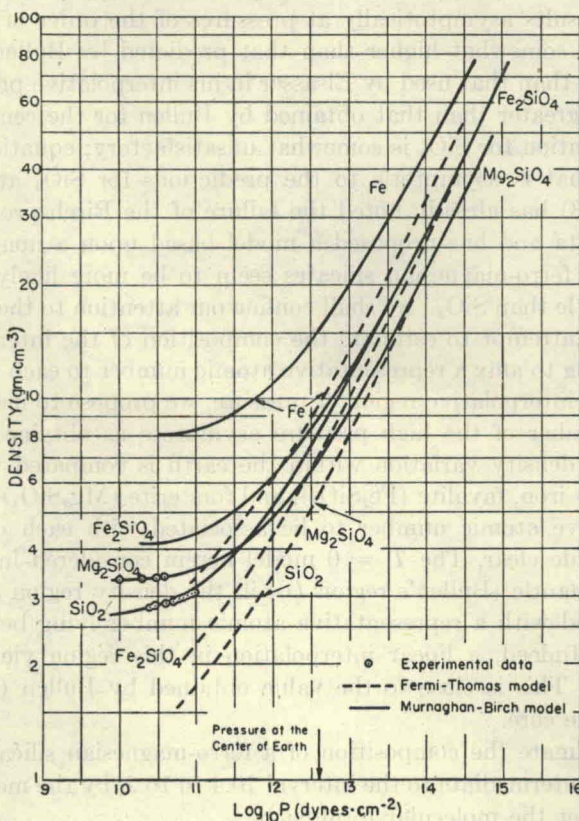


FIG. 4—The experimental data, the Birch-Murnaghan computation, and the Fermi-Thomas computations for four materials

using equation (13), and the present theoretical quantum statistical predictions for very high pressures for SiO_2 , Mg_2SiO_4 , Fe_2SiO_4 , and Fe. The initial constants used in constructing the curves of Figure 4 based upon the Birch model are given in Table 3 (obtained from Birch, 1952, p. 264). It is seen that Birch's procedure

TABLE 3—Densities and bulk moduli for several materials at one atmosphere and room temperature

Material	Formula	ρ_0	K_0
		<i>gm · cm⁻³</i>	<i>dynes · cm⁻²</i>
Forsterite	Mg_2SiO_4	3.29	1.19×10^{12}
Quartz	SiO_2	2.65	0.37
Fayalite	Fe_2SiO_4	4.07	1.04
Iron	Fe	7.87	1.684
Nickel	Ni	8.9	1.87

provides a reasonable fit with Bridgman's (1948*b*) experimental data for olivine (reduced to the density 3.29 at one atmosphere) and approaches the theoretical high pressure results asymptotically at pressures of the order of 10^{14} dynes/cm². This pressure is somewhat higher than that predicted by Bullen and Feynman, *et al.*, and larger than that used by Elsasser in his interpolative procedure. Indeed, this pressure is greater than that obtained by Bullen for the center of the earth.

The interpolation for SiO_2 is somewhat unsatisfactory; equation (13) does not yield a curve that is asymptotic to the predictions for SiO_2 at high pressures. Verhoogen (1953) has already noted the failure of the Birch procedure to fit the experimental data and has proposed a model based upon a non-zero value of ξ . However, since ferro-magnesian silicates seem to be more likely constituents of the earth's mantle than SiO_2 , we shall confine our attention to the olivine minerals and iron in our attempt to estimate the composition of the interior of the earth.

In attempting to affix a representative atomic number to each of the significant materials in the interpolative region of pressure, we propose to use the representative atomic number of the high pressure asymptote as obtained in Table 1. If Bullen's (1947) density variation within the earth is compared with that of the three materials—iron, fayalite (Fe_2SiO_4), and forsterite (Mg_2SiO_4)—as in Figure 5, the representative atomic number to be associated with each of the regions is immediately made clear. The $T = 0$ model herein considered indicates that the bottom of the mantle (Bullen's region *D*), in the density region 5.5 of the earth, can be associated with a representative atomic number lying between the limits 10.4 and 16.2. Indeed, a linear interpolation in this region yields the absolute zero value 12.5. This is close to the value obtained by Bullen (1952) from considerations of the core.

We may estimate the composition of a ferro-magnesian silicate possessing an atomic number intermediate to the interval 10.4 to 16.2, by the methods developed in Section II. Let the molecular formula be

$$[a \text{ Mg} + (1 - a) \text{ Fe}]_2 \text{SiO}_4 \dots \dots \dots (14)$$

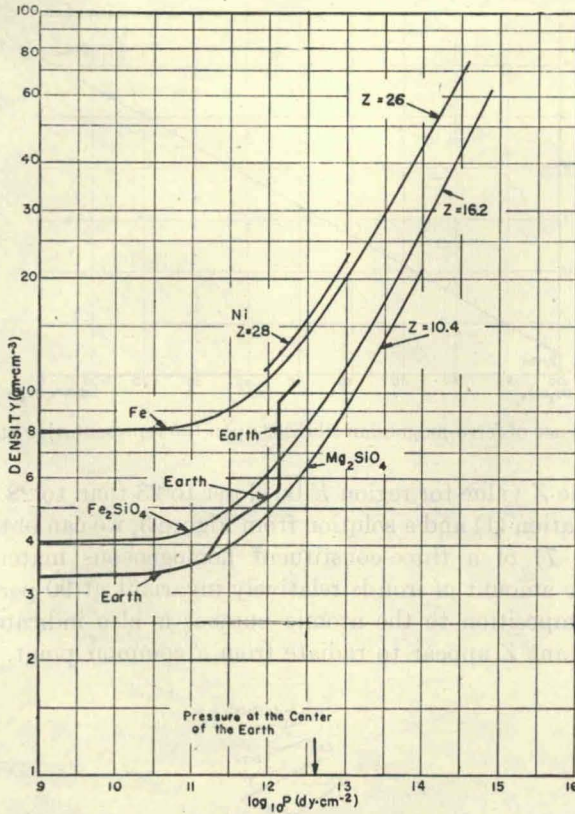


FIG. 5—The pressure-density relation for the earth in relation to the interpolated curves for fayalite (Fe_2SiO_4), forsterite (Mg_2SiO_4), iron, and nickel at $T = 0^\circ K$

where $a \leq 1$. Then for a given atomic number at the pressure 10^{12} dynes/cm², by equation (6),

$$\bar{Z}^2 \xi^3 = \frac{24a + 52(1 - a) + 14 + 32}{2a(70.5) + 2(1 - a)94 + 76 + 4(59.5)} = \frac{98 - 28a}{502 - 47a} \dots (15)$$

Solutions for this expression, obtained with the aid of Figure 3, are indicated in Figure 6. Corresponding to the representative atomic number 12.5, the composition of the silicate is

$$(0.635 Mg + 0.365 Fe)_2SiO_4 \dots \dots \dots (16)$$

The curve of Figure 6 indicates that use of a linear interpolation between the magnesium and iron silicates is satisfactory.

Insofar as the outer core (Bullen's region *E*) is concerned, the present method of interpolation yields information regarding the purity of the material within this region. The density required for region *E* is greater than that of the most dense of the olivine minerals and is in turn less than that of the iron-nickel group of pure elements. An interpolation in the region corresponding to the surface of the core yields as an atomic number 22. This value is in close agreement with Bullen's

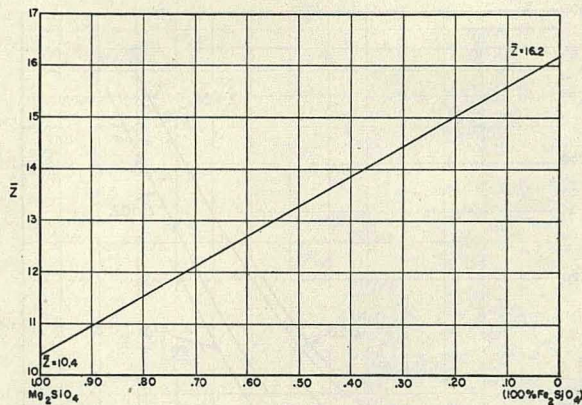


FIG. 6—Dependence of ferro-magnesian silicates upon the representative atomic number Z

suggestion that the Z value for region E be closer to 23 than to 28. Again from an application of equation (1) and a solution from Figure 3, we can obtain the possible percentages (Fig. 7) of a three-constituent homogeneous material having the value $Z = 22$; the amount of iron is relatively invariant at 90 per cent. The sensitivity of the composition to the atomic number is also indicated in Figure 7. The lines of constant Z appear to radiate from a common point.

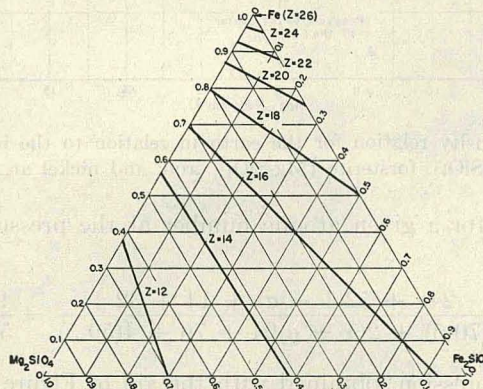


FIG. 7—Iso- Z lines in the three-component system $\text{Fe} - \text{Fe}_2\text{SiO}_4 - \text{Mg}_2\text{SiO}_4$ at a pressure of 1.3 megabars

It is of interest to note that the high densities suggested by Bullen (1950) for the inner core fall in the region of density above the values required for pure iron. The density given by Bullen for his model B at the center of the earth is a figure somewhere between 17 and 18 $\text{gm} \cdot \text{cm}^{-3}$. At this pressure (3.9×10^{12} dynes $\cdot \text{cm}^{-2}$), this density is greater than the interpolated value of density for iron, but is not inconsistent with the interpolated densities for cobalt or nickel. A density of 18 at the center of the earth is, however, the upper limit of density allowable for any material consistent with either a silicate or iron-nickel structure.

The foregoing conclusions are all predicated upon the assumption of the absence of phase transitions in the several minerals in the range of pressures obtained within

the earth. In the event a phase transition occurs, the appropriate curves drawn in Figure 5 would be modified. It is important to note that the presence of phase transitions would modify the present estimates in the direction of lower iron content in the outer core, with corresponding increase in the silicate content.

IV. Temperature effects

It may well be questioned whether computations based upon the assumption of a temperature of absolute zero are valid when the interior regions of the earth may have temperatures of the order of several thousand degrees. An extension of the quantum model for the pure elements to the case of non-zero temperatures was given by Feynman, Metropolis, and Teller. By a perturbation method, they obtained for the pressure

$$P = \frac{8\pi}{3h^3} (2m)^{3/2} (kT)^{5/2} I_{3/2}(\eta) \dots \dots \dots (17)$$

where

$$\eta = \frac{\pi\Phi(x_0)}{2Tx_0(2\zeta)^{1/2}} \dots \dots \dots (18)$$

$$\zeta = \frac{\pi^2 k^2 \mu^2}{8Z^2 e^4} \dots \dots \dots (19)$$

and m is the electronic mass, h is Planck's constant, e is the electronic charge, k is Boltzmann's constant, T the absolute temperature, and x_0 and μ have been defined in Part II. The function Φ is the electrostatic potential. The Fermi-Dirac function $I_{3/2}(\eta)$ is given by the integral

$$I_{3/2}(\eta) = \int_0^\infty \frac{x^{3/2} dx}{e^{x-\eta} + 1} \dots \dots \dots (20)$$

It can be shown (Sommerfeld, 1928; Gilham, 1936; Stoner, 1936; McDougall and Stoner, 1936) that, for large values of the argument,

$$I_{3/2}(\eta) \approx \frac{2}{5} \eta^{5/2} \left(1 + \frac{5\pi^2}{8\eta} \right) \quad (\eta \gg 1) \dots \dots \dots (21)$$

This expression is important in the consideration of small temperature perturbations. For a given density, the fractional error in computing the pressure is given by

$$\frac{5\pi^2}{8\eta} \dots \dots \dots (22)$$

Instead of computing the temperature perturbed electrostatic potential, we approximate the ratio $\Phi(x_0)/x_0$ by the corresponding quantity evaluated at $T = 0$ and computed without the inclusion of exchange effects. Under the latter condition,

$$P \approx \frac{Ze^2}{10\pi\mu^4} \left(\frac{\Phi(x_0)}{x_0} \right)^{5/2} \dots \dots \dots (23)$$

Thus

$$\frac{5\pi^2}{8\eta} = \frac{5}{8} \frac{\pi^2 kT}{(10\pi PZ)^{2/5}} \cdot (0.88534a_0e)^{-3/5} \dots \dots \dots (24)$$

Inserting the values of the atomic constants, k , a_0 , and e into equation (24), we obtain

$$\frac{5\pi^2}{8\eta} = 3.244TP^{-2/5}Z^{-2/5} \dots\dots\dots (25)$$

where P is in dynes·cm⁻² and T is in degrees absolute. For the values $P = 10^{13}$ dynes/cm², $Z = 10$, and $T = 10^4$ degrees Kelvin,

$$\frac{5\pi^2}{8\eta} = 0.0815 \dots\dots\dots (26)$$

Since the values of pressure and atomic number used above are below the values corresponding to the asymptotic behavior considered in this analysis, and since the value of T used is well above the limit placed by the melting-point gradient (Uffen), we conclude that very small errors (less than 8 per cent) are introduced by using the quantum calculations at absolute zero insofar as the earth is concerned.

There remains the determination of the influence of temperature upon the computations based upon the theory of finite strain. Slater (1939) has indicated that the pressure at a non-zero temperature may be written as

$$P = P_0 + P_t \dots\dots\dots (27)$$

where P_0 is the pressure of the ensemble of molecules at zero temperature and P_t is the thermal pressure due to the vibrating ensemble. Debye (1913)—see Roberts (1940)—deduced the thermal pressure to be

$$P_t = \frac{9\gamma kTN}{y_0^3 V} \int_0^{y_0} \frac{x^3 dx}{e^x - 1} \dots\dots\dots (28)$$

for a sample of volume V , where N is Avogadro's number, γ is Grüneisen's ratio (assumed independent of temperature), and $y_0 = \Theta_D/T$, where Θ_D is the Debye characteristic temperature.

The Debye temperature has been estimated from seismic data by Uffen and Birch (1952) for the core-mantle boundary to be 1280°K for forsterite. We shall investigate the integral for P_t for small values of the variable y_0 corresponding to the much larger values of temperature in the mantle.

$$P \approx \frac{3\gamma k\rho}{m} (T - \frac{3}{8} \Theta_D) \quad \frac{T}{\Theta} \gg 1 \dots\dots\dots (29)$$

where m is the mass of an oscillator in the ensemble. This expression is accurate within 10 per cent for temperatures greater than $0.7\Theta_D$.

If \bar{M} is the "mean atomic weight," we can write

$$P_t \approx \frac{3\gamma k\rho N}{\bar{M}} (T - \frac{3}{8} \Theta_D) \dots\dots\dots (30)$$

At the base of the mantle P is 1.37×10^{12} dynes/cm². Let us assume the mantle to be composed of a more basic member of the olivine series than one whose representative atomic number is 12.5. For example, choose the extreme case Fe₂SiO₄. The zero-temperature value of pressure obtained from Figure 5 is 0.69×10^{12} dynes/cm² at a density corresponding to the bottom of the mantle. Thus,

$$P_t = 0.68 \times 10^{12} \text{ dynes} \cdot \text{cm}^{-2} \text{ for } \text{Fe}_2\text{SiO}_4$$

Inserting the values $\gamma = 0.79$ (Birch), $\bar{M} = 29.1$, $\rho = 5.69 \text{ gm} \cdot \text{cm}^{-3}$ (for fayalite), we obtain for the temperature to which Fe_2SiO_4 must be raised to correspond to the pressure and density of the bottom of the mantle

$$T = 17,200^\circ\text{K}$$

By means of a linear interpolation for the zero-point pressure of intermediate silicates, we find the temperature distribution shown in Figure 8 as a function of

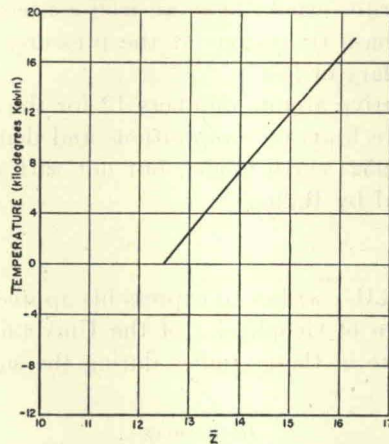


FIG. 8—The numerical solution of equation (30) as a function of the representative atomic number of the homogeneous constituent

the representative atomic number of the silicates. Uffen finds from seismic data the value of the melting point at the core boundary to be $5,300^\circ\text{K}$. Thus, we find that the atomic number corresponding to the bottom of the mantle must fall in the interval 12.5 to 13.5, for temperatures in the range 0°K to $5,300^\circ\text{K}$. The corresponding range of composition of olivine is 47 to 63 per cent Mg_2SiO_4 (Fig. 6).

V. Summary.

The method of Feynman, Metropolis, and Teller for computing the densities of elements at very high pressures has been extended to compounds. It is found that a "representative atomic number" can be assigned to compounds; that is, the atomic number of a hypothetical pure element which would have the same pressure-density relationship as the compound. For a number of compounds of geophysical interest, this representative atomic number is close to the "mean atomic number"; hence, if the earth's mantle is composed of ultra-basic rocks, the representative atomic number must be near 12.

Interpolation in the pressure interval between Bridgman's laboratory data and the quantum statistical high-pressure computations has been made with the aid of Birch's finite-strain method, with the important result that the pressure-density curves for all probable constituents of the deep earth become asymptotic at pressures of the order of 10^{14} dynes/cm². It has been shown that if the actual temperature at the core boundary is less than 10^4 degrees absolute, the errors in

the quantum statistical computations will be less than 8 per cent. If the temperature lies between zero and 5,300° absolute, the atomic number corresponding to the base of the mantle will be between 12.5 and 13.5, and the corresponding range of composition for an olivine mantle would be between 47 and 63 per cent Mg_2SiO_4 .

The representative atomic number corresponding to the outer part of the core was found to be 22, which is intermediate between that of iron and the silicates. The density required by Bullen, for the outer part of the core, is greater than the most dense of the olivine minerals but less than that of iron. Corresponding to an atomic number of 22, it was found that a core composed of the three constituents—iron, fayalite, and forsterite—would have an iron content of nearly 90 per cent, provided there are no phase transitions at the pressures corresponding to those at the core-mantle boundary or less.

The use of representative atomic numbers 12 for the base of the mantle and 22 for the top of the core leads to compositions and densities which are in conformity with Bullen's (1952) earth model, but not with earlier models proposed by Elsasser and criticized by Bullen.

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