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ELASTICITY OF SOLIDS AT HIGH PRESSURE AND THE EARTH'S MANTLE

BY

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ABSTRACT

Elasticity of solids under high pressure is calculated on both theoretical and experimental grounds. It is concluded that the calculated elasticities of dunite and MgO are in good agreement with those obtained from seismic data in the upper mantle and lower mantle respectively. There is some possibility of existence of low-velocity layer or constant-velocity layer just below the so-called Mohorovičić discontinuity and of admixture of metallic iron near the core boundary.

1. Introduction

As the measurement of elasticity of solids has been rapidly advanced, many interesting and valuable data on rock elasticity have been published. In Japan, A. Kubotera (**1**) and D. Shimozuru (**2**) measured velocities of both dilatational and rotational waves in rock samples by the transmission time of ultrasonic impulse. Recently, D. S. Hughes and his co-workers (**3**) have succeeded in measuring elastic wave velocities under variable pressure conditions. Under these circumstances, it is now possible to compare these data with those of the Earth's interior, together with a theoretical treatment. In the present paper, the theoretical extrapolation of high pressure experiments will be made on the basis of the theory of solids.

2. Rock-elasticity

The behaviour of elasticity of rocks under varying pressure is very complex, and the complexity is mainly due to their porosity. But at high pressure, the effect of porosity on elasticity of rocks becomes more and more trivial.

The effect of porosity on elasticity of rocks was studied in my previous paper (**4**), and in the present paper the following points will be emphasized.

A) Both the value of elastic waves and that of compressibility of rocks are exceedingly diverse for each rock-sample of the same kind, but at sufficiently high pressure these values are nearly the same for rocks of the same kind because of the diminution of porosity.

B) Both the velocity of elastic waves and compressibility of rocks are the unique functions of their specific volume at sufficiently high pressure.

With regard to A), Birch (5) and Adams (6) have concluded from their rock-experiments that at high pressure both velocities of elastic waves and compressibility of rocks tend to the values obtained by averaging velocities and compressibilities of the minerals of which the rocks are composed.

With regard to B), the present writer has concluded from D. S. Hughes' experiment used in my previous paper (4) that at high pressure both velocities of elastic waves and compressibilities of rocks become asymptotically functions of their density, free from their temperature.

From the above two points, it is possible to apply the results of rock-experiments to the Earth's mantle, if the data at sufficiently high pressure on rock-experiments are used with suitable care.

It may, therefore, be concluded that in determining the pressure coefficient for both elastic wave velocity and compressibility in the range of high pressure, the use of a bulk modulus-density diagram is more natural and accurate than a direct application of a bulk modulus-pressure diagram with respect to the elimination of the effect of porosity. In Table I some elastic properties of various rocks from D. S. Hughes' experiments are shown, where the pressure coefficients of elasticity are obtained from the bulk modulus-density diagram as in my previous paper (4).

Table I. Elasticity of rocks and MgO at atmospheric pressure and at room temperature.

	Granite	Basalt	Dunite	MgO
V_p (km/sec)	6.0	7.0	8.0	—
k (10^{12} C.G.S.)	0.57	0.86	1.15	1.672
ρ (g/cm^3)	2.7	2.9	3.2	4.0
$\frac{dV_p}{dp}$ (km/sec/10^4 bars)	0.2	0.1	0.1 (0.09~0.14)	—
$\frac{dk}{dp}$ (C.G.S.)	6.6 (6~7)	5.7 (5~6.5)	4.5 (4~5)	4.2 (4~4.5)

References (3) and (20)

3. Elasticity of rocks and minerals at high pressure

In order to compare the elasticity of the Earth's mantle with that of rocks and minerals, the problem of what materials the Earth's mantle consists, has become a very important factor, and investigations were made in my previous paper (7), without reaching a definite conclusion yet. In the present paper, two cases are considered : One case is based upon an assumption that the Earth's mantle consists of dunite, while in the other we assume that the mantle consists of MgO (periclase).

A. *Case of dunite*

It is well known that the elasticity of dunite is nearly equal to that in the upper part of the upper mantle. Hence, whether the elasticity of dunite at very high pressure is still in good agreement with that of the deeper part of the Earth's mantle, is a very interesting subject. In the following, the elasticity of dunite at very high pressure will be obtained from a theoretical extrapolation.

Rocks and minerals are assumed to belong to ionic crystals, and a theoretical treatment of the elasticity of ionic crystals after Born and Mayer (8) will be applicable.

Taking a unit volume of any mineral, its internal energy E is obtained from summation of a Coulomb interaction and a closed shell interaction, as a function of volume:

$$\left.\begin{aligned} E &= -\frac{A}{v^{1/3}}+Be^{-\alpha v^{1/3}}\,, \\ v_0 &= 1\,, \end{aligned}\right\} \qquad (1)$$

where A, B and α are constants and v is volume, suffix 0 denoting the value at zero pressure. Here a Van der Waals interaction is neglected.

Then from the thermodynamical relation, we obtain

$$p = -\frac{\partial E}{\partial v} = -\frac{1}{3}\left(Av^{-4/3}-B\alpha v^{-2/3}e^{-\alpha v^{1/3}}\right), \qquad (2)$$

$$k = -v\frac{\partial p}{\partial v} = -\frac{1}{9}\left(4Av^{-4/3}-2B\alpha v^{-2/3}e^{-\alpha v^{1/3}}-B\alpha^2 v^{-1/3}e^{-\alpha v^{1/3}}\right), \qquad (3)$$

$$\frac{dk}{dp} = \frac{\frac{16}{3}Av^{-1/3}-\frac{4}{3}B\alpha v^{1/3}e^{-\alpha v^{1/3}}-B\alpha^2 v^{2/3}e^{-\alpha v^{1/3}}-\frac{1}{3}B\alpha^3 ve^{-\alpha v^{1/3}}}{4Av^{-1/3}-2B\alpha v^{1/3}e^{-\alpha v^{1/3}}-B\alpha^2 v^{2/3}e^{-\alpha v^{1/3}}}\,, \qquad (4)$$

where p and k are the pressure and the bulk modulus respectively.

At zero pressure, the following relations hold:

$$p = -\frac{1}{3}\left(A-B\alpha e^{-\alpha}\right) = 0\,, \qquad (2')$$

$$k = -\frac{1}{9}\left(4A-2B\alpha e^{-\alpha}-B\alpha^2 e^{-\alpha}\right) = k_0\,, \qquad (3')$$

$$\frac{dk}{dp} = \frac{\frac{16}{3}A-\frac{4}{3}B\alpha e^{-\alpha}-B\alpha^2 e^{-\alpha}-\frac{1}{3}B\alpha^3 e^{-\alpha}}{4A-2B\alpha e^{-\alpha}-B\alpha^2 e^{-\alpha}} = \left(\frac{dk}{dp}\right)_0. \qquad (4')$$

The values of k_0 and $\left(\frac{dk}{dp}\right)_0$ in the above equations (3′) and (4′) are obtained from rock experiments, so that unknown A, B and α can be determined. In Table II are shown the values of the elasticity of dunite at high pressure which have been calculated from Eqs. (2), (3) and (4) with the help of Eqs. (2′), (3′) and (4′).

Table II. Elasticity of dunite at high pressure (calculated from Eqs. (2), (3) and (4)).

v/v_0	1.0	0.9	0.8	0.7	0.6
ρ (g/cm^3)	3.2	3.5	4.0	4.5	5.3
p (10^4bars)	0	15	41.4	90	178
$\frac{dk}{dp}$	4.5	4.0	3.7	3.4	3.1
k (10^{12} C.G.S.)	1.15	1.8	2.82	4.5	7.4
$\frac{k}{\rho}$ (10^{11} C.G.S.)	3.6	5.1	7.1	9.8	13.9

B. *Case of MgO (periclase)*

Recently the present author and others have concluded that at very high pressure the decomposition of dunite into MgO and quartz is possible (**9**). The pressure at which the decomposition will occur is suggested as nearly 500,000 bars, and will correspond to that at the depth of nearly 1,000 km in the Earth. Therefore, the elasticity of MgO at high pressure will theoretically be discussed here, in order to compare the observed elasticity of the Earth's mantle with that of MgO.

Internal energy of MgO was determined by Mayer (**10**), and the Coulomb and Van der Waals terms obtained by him are adopted here, but the term of closed shell interaction is assumed to be different from that obtained by Mayer.

Internal energy of MgO per molecule is given by the equation:

$$E = -\left(\frac{A'}{r}+\frac{C'}{r^6}\right) + B_1 e^{-\alpha' r} + B_2 e^{-\sqrt{2}\alpha' r}, \tag{5}$$

where A', C', α', B_1 and B_2 are constants and r is the distance between the nearest neighbours. The first and second terms represent the Coulomb and Van der Waals term respectively, while the third and fourth represent the closed shell interactions between the nearest and second neighbours respectively.

Then from thermodynamic relation we get

$$p = -\left(\frac{A'}{3nr^4}+\frac{2C'}{nr^9}\right)+\frac{B_1}{3nr^2}\alpha' e^{-\alpha' r}+\frac{\sqrt{2}B_2}{3nr^2}\alpha' e^{-\sqrt{2}\alpha' r}, \tag{6}$$

$$k = -\frac{1}{9}\left(\frac{4A'}{nr^4}+\frac{54C'}{nr^9}\right)+\frac{1}{9}\frac{1}{nr^3}(2B_1\alpha' r e^{-\alpha' r}+B_1\alpha'^2 r^2 e^{-\alpha' r}) + \frac{1}{9}\frac{1}{nr^3}(2\sqrt{2}B_2\alpha' r e^{-\sqrt{2}\alpha' r}+2B_2\alpha'^2 r^2 e^{-\sqrt{2}\alpha' r}), \tag{7}$$

$$\frac{dk}{dp} = \left\{\frac{16A'}{3r}+\frac{162C'}{r^6}-\frac{4}{3}B_1\alpha' r e^{-\alpha' r}-B_1\alpha'^2 r^2 e^{-\alpha' r}-\frac{B_1}{3}\alpha'^3 r^3 e^{-\alpha' r} -\frac{4\sqrt{2}}{3}B_2\alpha' r e^{-\sqrt{2}\alpha' r}-2B_2\alpha'^2 r^2 e^{-\sqrt{2}\alpha' r}-\frac{2\sqrt{2}}{3}B_2\alpha'^3 r^3 e^{-\sqrt{2}\alpha' r}\right\} \div\left\{\frac{4A'}{r}+\frac{54C'}{r^6}-2B_1\alpha' r e^{-\alpha' r}-B_1\alpha'^2 r^2 e^{-\alpha' r}-2\sqrt{2}B_2\alpha' r e^{-\sqrt{2}\alpha' r}-2B_2\alpha'^2 r^2 e^{-\sqrt{2}\alpha' r}\right\}, \tag{8}$$

$$v = nr^3,$$

where v is the volume per molecule and n is a constant. At zero pressure, the above equations are written as

$$p = -\left(\frac{A'}{3nr_0^4}+\frac{2C'}{nr_0^9}\right)+\frac{B_1}{3nr_0^2}\alpha' e^{-\alpha' r_0}+\frac{\sqrt{2}B_2}{3nr_0^2}\alpha' e^{-\sqrt{2}\alpha' r_0}=0, \tag{6'}$$

$$\begin{aligned} k &= -\frac{1}{9}\left(\frac{4A'}{nr_0^4}+\frac{54C'}{nr_0^9}\right)+\frac{1}{9}\frac{1}{nr_0^3}(2B_1\alpha' r_0 e^{-\alpha' r_0}+B_1\alpha'^2 r_0^2 e^{-\alpha' r_0}) \\ &\qquad +\frac{1}{9}\frac{1}{nr_0^3}(2\sqrt{2}B_2\alpha' r_0 e^{-\sqrt{2}\alpha' r_0}+2B_2\alpha'^2 r_0^2 e^{-\alpha'\sqrt{2}r_0}) \\ &= k_0, \end{aligned} \tag{7'}$$

$$\begin{aligned} \frac{dk}{dp} &= \left\{\frac{16A'}{3r_0}+\frac{162C'}{r_0^6}-\frac{4}{3}B_1\alpha' r_0 e^{-\alpha' r_0}-B_1\alpha'^2 r_0^2 e^{-\alpha' r_0}-\frac{B_1}{3}\alpha'^3 r_0^3 e^{-\alpha' r_0}\right. \\ &\qquad \left. -\frac{4\sqrt{2}}{3}B_2\alpha' r_0 e^{-\sqrt{2}\alpha' r_0}-2B_2\alpha'^2 r_0^2 e^{-\sqrt{2}\alpha' r_0}-\frac{2\sqrt{2}}{3}B_2\alpha'^3 r_0^3 e^{-\sqrt{2}\alpha' r_0}\right\} \\ &\quad \div\left\{\frac{4A'}{r_0}+\frac{54C'}{r_0^6}-2B_1\alpha' r_0 e^{-\alpha' r_0}-B_1\alpha'^2 r_0^2 e^{-\alpha r_0}-2\sqrt{2}\frac{B_2}{3}\alpha' r_0 e^{-\sqrt{2}\alpha' r_0}-2B_2\alpha'^2 r_0^2 e^{-\sqrt{2}\alpha' r_0}\right\} \\ &= \left(\frac{dk}{dp}\right)_0, \end{aligned} \tag{8'}$$

$$v = nr^3 = 2r_0^3,$$

where r_0 is the distance between the nearest neighbours at zero pressure.

The right-hand sides of the above equations are all determined from high pressure experiments, so that the unknown α', B_1 and B_2 are obtained from the above simultaneous equations.

Table III. Elasticity of MgO at high pressure (calculated from Eqs. (6),(7) and (8)).

v/v_0	1.0	0.9	0.8	0.7	0.6
ρ (g/cm^3)	3.6	4.0	4.5	5.1	6.0
p (10^4bars)	0	22	60	127	247
$\frac{dk}{dp}$	4.2	3.8	3.5	3.2	3.0
k (10^{12} C.G.S.)	1.67	2.54	3.91	6.14	9.8
$\frac{k}{\rho}$ (10^{11} C.G.S.)	4.7	6.3	8.7	11.9	16.4

The elasticity of MgO at high pressure thus calculated is given in Table III. It should be noticed that in the above theoretical calculation dunite and MgO are assumed to be ionic crystals. Strictly speaking, this is not the case, and dunite and MgO contain some electron pair bonds. The nature of such electron pair bonds is still unknown and in the present paper the assumption is regarded to be correct in a first approximation.

4. Comparison of the calculated elasticity of dunite and MgO with those observed in the Earth's mantle.

Velocities of seismic waves in the Earth's mantle obtained by Jeffreys (**11**) and Gutenberg (**12**) are in good agreement except in low-velocity layer. The elasticity of the Earth's mantle is known exact enough to compare it with that of rocks at high pressure evaluated in § 4. In the following a discussion will be given, for convenience, in two parts, i.e., in the upper and lower mantle respectively.

1. *Upper mantle*

Both k/ρ obtained from seismic wave velocity in the Earth's mantle, where ρ denotes density, and that calculated in § 3, are shown in Fig. 1, where the data of pressure in the Earth's mantle are taken from Bullen's (**13**).

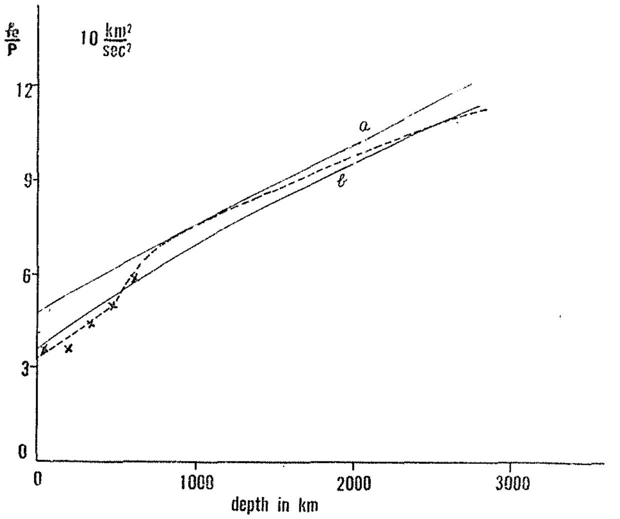

Fig. 1. Calculated elasticity of dunite and MgO
(a) : k/ρ of MgO, (b) : k/ρ of dunite
broken line : k/ρ of the Earth's mantle from seismic observation by Jeffreys (**11**)
×× : k/ρ by Gutenberg (**12**), abscissa being the depth in the Earth's mantle.

As seen in Fig. 1, the elasticity of dunite at high pressure is in good agreement with that from seismic data in the upper mantle. Especially increasing rate of the elasticity of dunite under high pressure is in very good agreement with that in the upper mantle, except in low-velocity layer.

From these relations, the effect of temperature and inhomogeneity in the upper mantle are considered small and the velocity increase in the upper mantle is regarded to be due mainly to compression with the overlying materials, except in low-velocity layer.

With regard to the region just below the so-called Mohorovičić discontinuity, temperature effects should not be neglected, because in this region temperature gradient is considered to be large. In order to make the temperature correction in this region, it is necessary to know the distribution of temperature in the upper mantle, but it is not yet accurately determined up to the present. Consequently a very simple correction due to temperature-effect will be given in the following. It is assumed in a first approximation that the velocity of elastic wave in solids is a function of density alone, the relation being valid excepting the case when the temperature is near the melting point of the solids. If the relation is satisfied in the upper mantle, i. e., the temperature in the upper mantle is below the melting point of rocks, then a correction due to temperature-effect will be obtained simply.

The variations of elastic wave velocity (V_p) and the bulk modulus with increasing depth are given by the equations:

$$\frac{dV_p}{dh}=\frac{dV_p}{d\rho}\frac{d\rho}{dh}=\frac{dV_p}{d\rho}\frac{\rho_{h+\Delta h}-\rho_h}{\Delta h}, \qquad (9)$$

$$\frac{dk}{dh}=\frac{dk}{d\rho}\frac{d\rho}{dh}=\frac{dk}{d\rho}\frac{\rho_{h+\Delta h}-\rho_h}{\Delta h}, \qquad (10)$$

where ρ_h and $\rho_{h+\Delta h}$ are the densities at the depths of h and $h+\Delta h$ in the upper mantle respectively.

Then these equations are written in the forms:

$$\frac{dV_p}{dh}=\frac{dV_p}{d\rho}\left(\frac{\rho}{k}\Delta p-\beta\rho\Delta T\right)\Big/\Delta h, \qquad (11)$$

$$\frac{dk}{dh}=\frac{dk}{d\rho}\left(\frac{\rho}{k}\Delta p-\beta\rho\Delta T\right)\Big/\Delta h, \qquad (12)$$

where p, T and β are pressure, temperature and thermal expansion coefficient, at the depth of h, and Δp and ΔT are the pressure- and the temperature-differences between the depths of h and $h+\Delta h$.

If we assume $\frac{k}{\rho}=35\,\mathrm{km^2/sec^2}$, $\beta=4\cdot10^{-5}$ and $\frac{dV_p}{d\rho}=6\,\mathrm{km/sec/g/cm^3}$ in this region, the variation of the velocity of dilatational wave with depth in the upper mantle is obtained, when the temperature distribution in the upper mantle is given.

In Table IV and Fig. 2 the the velocity of dilatational wave at various depths in the upper mantle is shown, where the temperature distribution is adopted from Gutenberg (**14**), Daly (**15**), and Jeffreys (**16**).

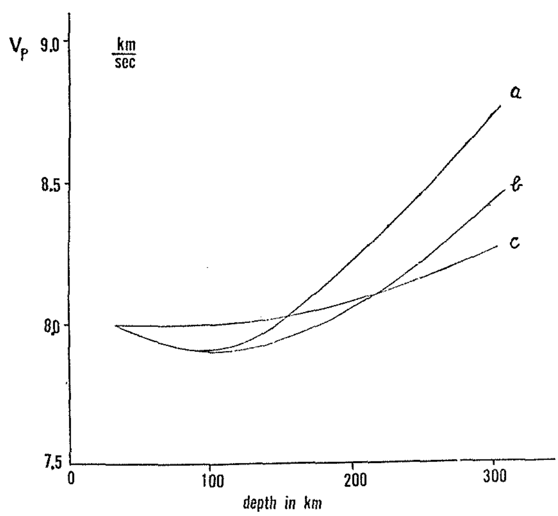

Fig. 2. Dilatational wave-velocity of dunite *versus* depth in the Earth's mantle.
Temperature distributions are after (a) Gutenberg, (b) Daly, and (c) Jeffreys respectively.

Table IV. Seismic wave velocity in the upper mantle.

	Dilatational wave velocity (km/sec)		
Depth (km)	A	B	C
30∼50	8.0	8.0	8.0
100	<7.9	<7.9	8.0
200	8.1	8.3	8.15
300	8.5	8.8	8.3

Temperature distributions for models A, B and C are after Daly, Gutenberg and Jeffreys respectively.

The velocity at the depth of 30 km is assumed to be 8.0 km/sec as is seen in Fig. 2. At depths between 50 and 100 km, a low-velocity layer is obtained from Gutenberg's and Daly's temperature distribution and a constant-velocity layer from Jeffreys'. It will safely be concluded that the existence of a low-velocity layer or a constant-velocity layer is theoretically and observationally possible.

Needless to say, the present discussion is correct only in a rough approximation, and it contains ambiguity in the point of simplification. According to Born and others (**8**) the bulk modulus of solids is given in the form, $k=f(v)+g(v, T)$ where f and g are functions of volume alone, and of volume and temperature respectively. In the above procedure, the second term is neglected because of the assumption that the temperature in the upper mantle is below the melting point of rock. Near the melting point, elasticity of solids becomes very rapidly small. Recent experiments on the elasticity of solids below and above the melting point of solid show that temperature effect becomes suddenly large at the temperature very near the melting point. According to Birch (**17**) and Shimozuru (**18**), when $T/T_m \approx 0.95$, the effect of temperature becomes predominant, where T_m is the melting point of the solid. If the melting point of dunite is assumed to be 1,500°C, the effect of temperature will become very large above 1,400°C. But there is no evidence that temperature in the upper mantle is within 100°C lower than the melting point of rocks at the prevailing pressure in this region. Therefore the assumption in the above procedure is not far from the actual condition in the upper mantle. Moreover, if the second term is taken into account, temperature effect will be larger than that in the above discussion, and the existence of a low-velocity layer becomes more probable.

2. *Lower mantle*

As seen in Fig. 1, the elasticity of MgO is in good agreement with that in the Earth's lower mantle. The elasticity of dunite at high pressure is in good agreement with that in the Earth's upper mantle, but not in the lower mantle.

Recently, the present author and others pointed out that olivine will decompose into MgO and SiO_2 at very high pressure, and the coincidence of elasticity of MgO with that in the lower mantle supports this possibility. The elasticity of MgO at depths from 1,000 km to 3,000 km is especially in good agreement with that in the lower mantle. It was concluded in our previous paper (**9**) that the pressure at which the decomposition of olivine will occur corresponds to a depth of about 1,000 km. This previous estimation was ascertained also from the point of view of elastic property. Therefore, in this region of the lower mantle (at depths from 1,000 to 2,000 km), MgO is to be regarded as a main constituent mineral.

Below the depth of 2,000 km in the lower mantle, the elasticity of MgO is larger than that obtained from a seismic observation, as seen in Fig. 1. This fact will be explained as due to admixture of low velocity materials—metallic iron. If we assume that the constituent of the Earth's core is metallic iron and if the elasticity of a mixture is given by a weighted mean of elasticities of constituents, the difference between the elasticity of the core boundary observed from seismic waves and that of MgO at pressure corresponding to that depth, will be explained as due to an admixture of 10 per cent metallic iron in weight. But the propriety of theoretical extrapolation of elasticity of MgO to this depth in the lower mantle is considered questionable, and a definite conclusion must be postponed. A rapid development in experimental research in this field is earnestly desired.

5. Concluding remarks

1) The elasticity of dunite as calculated from the theory of solids is in good agreement with that observed in the Earth's upper mantle excepting the region just below the so-called Mohorovičić discontinuity.

2) Taking into account the effect of temperature, an existence of low-velocity layer or constant-velocity layer just below the crust is presumed to be probable.

3) The calculated elasticity of MgO is in good agreement with that in the region of depths from 1,000 to 2,000 km, and from this the existence of MgO in the lower mantle is considered to be probable.

4) Below the depth of 2,000 km in the lower mantle, an admixture of metallic iron is suggested as probable.

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REFERENCES

1. A. Kubotera, J. Physics Earth, **2** (1954), 33.
2. D. Shimozuru, Bull. Earthq. Res. Inst., **30** (1952), 63.
3. D. S. Hughes *et al.*, Geophysics, **16** (1951), 577; **21** (1956), 277; **22** (1957), 23.
4. T. Nishitake, Mem. Coll. Sci., Kyoto Univ. A, **28** (1957), 73.
5. F. Birch, Bull. Geol. Soc. America, **54** (1943), 263.
6. L. H. Adams and E. D. Williamson, J. Franklin Inst., **195** (1923).
7. T. Nishitake, Mem. Coll. Sci., Kyoto Univ., **29** (1958), 37.
8. M. Born and J. E. Mayer, ZS f. Phys., **75** (1932), 1.
9. T. Nishitake *et al.*, Report of I.U.G.G. in Toronto (1957).
10. J. E. Mayer and M. McC Maltibie, ZS f. Phys., **75** (1932), 748.
11. H. Jeffreys, *The Earth*, (Camb. Univ. Press, 1952).
12. B. Gutenberg, Bull. Seis. Soc. America, **43** (1953) 223.
13. K. E. Bullen, *An Introduction to Theory of Seismology*, (Camb. Univ. Press, 1952).
14. B. Gutenberg, *Internal Constitution of the Earth*, (Dover Publication, 1951).
15. R. A. Daly, Bull. Geol. Soc. America, **54** (1943), 401.
16. H. Jeffreys, loc. cit.
17. F. Birch, J. Chem. Phys., 8 (1940), 641.
18. D. Shimozuru, Bull. Earthq. Res. Inst., **34** (1956), 88.
19. J. E. Mayer and M. L. Huggins, J. Chem. Phys., **1** (1933), 643.
20. F. Birch *et al.*, *Handbook of Physical Constants*, Geol. Soc. America, Special Paper No. 36 (1954).