JOURNAL OF GEOPHYSICAL RESEARCH VOL. 75, NO. 26, SEPTEMBER 10, 1970

On the Calculation of the Seismic Parameter ϕ at High Pressure and High Temperatures

D. H. CHUNG, HERBERT WANG, AND GENE SIMMONS

Department of Earth and Planetary Sciences
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Comparison of the Murnaghan equation of state with the Birch equation shows that, for a given value of pressure, the values of (ρ/ρ_0) calculated from the two equations differ by less than 1% to a pressure equal to 0.5 K_0 (where K_0 is the zero-pressure isothermal bulk modulus), but the corresponding values of the seismic parameter ϕ differ by 10%. The value of ϕ is extremely sensitive to the choice of the equation of state because ϕ is the derivative of pressure with respect to density. The good agreement between the two equations of state for pressure as a function of density observed for some materials does not imply the same agreement in the relationship between ϕ and pressure. Expressions for $\phi(P)$ that take into account the first order nonlinear dependence of the bulk modulus on pressure are presented, and their applications are discussed. Temperature correction of the pressure-dependent ϕ is also considered.

Comparison of the seismic parameter ϕ_{LAB}, determined in the laboratory for various materials, with the values actually observed in the field, ϕ_{FLD}, can be used to estimate the composition of a homogeneous isothermal layer within the earth. If a particular equation of state is assumed, then the seismic parameter may be written as a function of pressure because the definition of the adiabatic bulk modulus K_s implies that

$$\phi = \left(\frac{\partial P}{\partial \rho}\right)_s \qquad (1)$$

Birch [1939] used the Murnaghan theory of finite strain to calculate the rate of change of seismic velocities with pressure. O. L. Anderson presented an equation for a pressure-dependent ϕ based on the Murnaghan equation of state and illustrated its applicability at high pressure. He concluded [*O. L. Anderson*, 1966, p. 730] that 'Birch's equation of state, in its form which is appropriate to a general value of K_0, leads to essentially the same results as does the Murnaghan equation'; we believe the two equations lead to different results.

In this paper we compare the values calculated for ϕ from both the Murnaghan and the Birch equations of state and discuss the sensitivity of $\phi(P)$ to the choice of the equation of state; we believe the Birch form superior to that of Murnaghan. Expressions for $\phi(P)$ that take into account the first-order nonlinear dependence of the bulk modulus on pressure are given, and their implications are discussed. Correction of the pressure-dependent ϕ for temperature is considered.

SENSITIVITY OF $\phi(P)$ TO THE CHOICE OF EQUATION OF STATE

The equations of state most widely used in geophysics are those of *Murnaghan* [1944, 1949] and *Birch* [1939, 1947, 1952]. We examine the dependence of $\phi(P)$ on the form of the equation of state used to describe the elastic behavior of solids.

The Murnaghan equation of state is derived from the assumption that bulk modulus is a linear function of pressure: $K(P) = K_0 + mP$, where K_0 is the adiabatic bulk modulus evaluated at zero pressure, and m is a material constant defined by $m = \{(\partial K/\partial P)_s\}_{P=0}$. Since $K = \rho(dP/d\rho)$,

$$P_M = (K_0/m)[(\rho/\rho_0)^m - 1] \qquad (2)$$

The subscript M denotes parameters calculated from the Murnaghan equation of state.

The Birch equation of state, derived from Murnaghan's theory of finite strain [*Murnag-*

han, 1951] with cubic and quadratic terms retained in the Helmholtz free energy of strain retained in the Helmholtz free energy [*Birch*, 1947, 1952], leads to

$$P_B = (3K_0/2)[(\rho/\rho_0)^{7/3} - (\rho/\rho_0)^{5/3}] \cdot \{1 + (\tfrac{3}{4})(m - 4)[(\rho/\rho_0)^{2/3} - 1]\} \quad (3)$$

The subscript B refers to the parameters calculated from the Birch equation of state.

From equation 2, we find the derivative

$$dP_M/d\rho = \phi_0(\rho/\rho_0)^{m-1} \quad (4)$$

where $\phi_0 = (K_0/\rho_0)$. To express ϕ as a function of pressure, we substitute equation 2 in the form

$$\rho/\rho_0 = [1 + m(P_M/K_0)]^{1/m} \quad (5)$$

and obtain

$$= dP_M/d\rho$$

$$= (K_0/\rho_0)[1 + m(P_M/K_0)]^{(m-1)/m} \quad (6)$$

Equation 6 corresponds to equation 8 of *O. L. Anderson*'s [1966] paper, and it is noted that he derived this expression in a different way.

Similarly, from the Birch equation of state, we have

$$P_B = (3K_0/2)y^5\{(y^2 - 1) + b_1(y^2 - 1)^2\} \quad (7)$$

and

$$\phi_B = dP_B/d\rho = (\phi_0/3)\{3y^4[1 + 2b_1(y^2 - 1)] + (5/y^3)(P_B/K_0)\} \quad (8)$$

where $y = (\rho/\rho_0)^{1/3}$ and $b_1 = (3/4)(m - 4)$. To obtain ϕ_B as a function of pressure, the Birch equation of state must be solved numerically for (ρ/ρ_0) as a function of pressure.

It has previously been recognized that the Murnaghan equation 2 will be limited to values of $P < 0.5K_0$ in estimating (V/V_0) [e.g., *O. L. Anderson*, 1968, p. 170]. We show below that its validity for ϕ does not extend as high as $P \simeq 0.5K_0$.

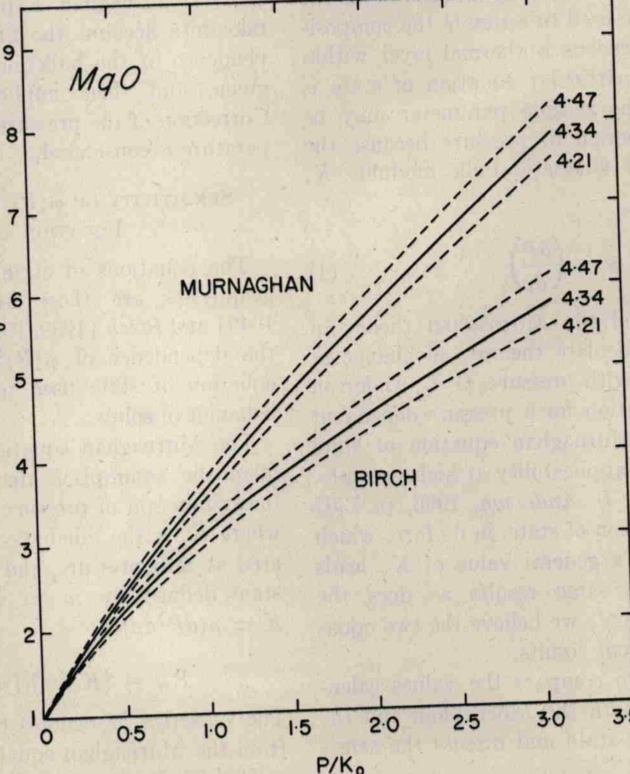

Fig. 1. Comparison of the seismic ϕ calculated from the Birch and the Murnaghan equations for periclase (at 298°K).