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

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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

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

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 $K = \rho(dP/d\rho)$,

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

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 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 $P \simeq 0.5K_0$.

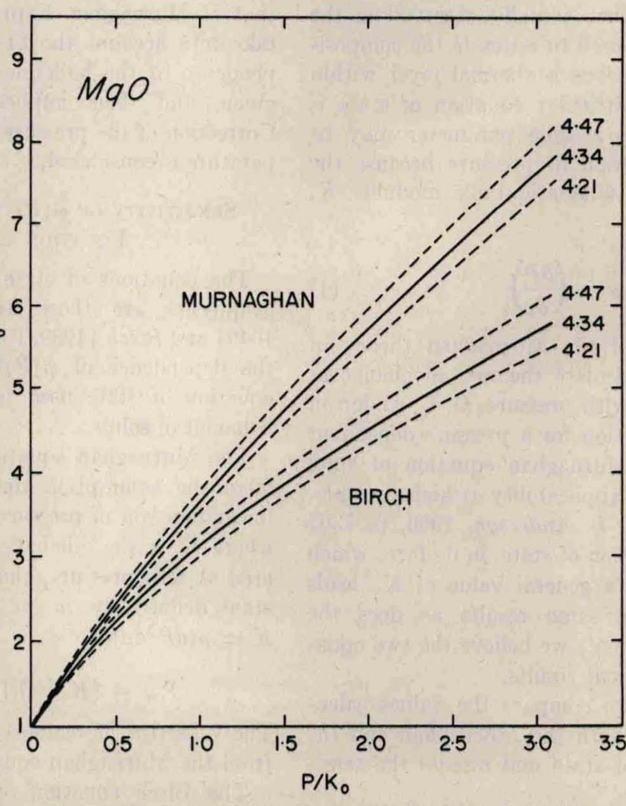

Fig. 1. Comparison of the seismic ϕ calculated from the Birch and the Murnaghan equations for periclase (at 298°K).