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THE ELASTIC CONSTANTS OF A CUBIC CRYSTAL SUBJECTED TO MODERATELY HIGH HYDROSTATIC PRESSURE

D. H. CHUNG

Department of Geology and Geophysics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.

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Abstract—This paper presents the results of an analysis of the finite strain theory that goes to the next higher-order term than third-order in the strains for cubic crystals. Theoretical expressions for the effective second-order elastic constants are presented here in terms of the second-, third-, and fourth-order elastic constants and the Lagrangian strain; these have been derived from the rigorous stress-strain relationship set by the Murnaghan theory of finite deformation. Since typical ultrasonic experiments with pressure result in *thermodynamically mixed* elastic constants, the practical ultrasonic expressions of the effective elastic constants are presented for a cubic crystal subjected to moderately high hydrostatic compression. The rigorous relationships between the pressure derivatives of the effective elastic constants and partial contractions of the higher-order elastic constants are presented also, and then the primary experimental quantities that are resulting from the usual ultrasonic-pressure experiments have been identified in terms of the *thermodynamically mixed* second-, third-, and fourth-order elastic constants of the crystal.

1. INTRODUCTION

THE FINITE strain theory for a medium of the cubic symmetry subjected to a finite hydrostatic compression was first developed by Birch[1]. In this work, Birch had defined the free-energy of a crystal in terms of a power series of the energy in the strain components including terms up to the third-order in the strains and then derived expressions for the effective elastic constants of the crystal under hydrostatic pressure. These expressions contained the second- and third-order elastic constants of crystal, and they were shown to describe the effective elastic properties of cubic crystals subjected to relatively 'low' compression.* For a crystal subjected to moderately 'high' compression, however, the higher order terms than the third-order in the strains would play an important role in the description of crystal elasticity under this high pressure.

This paper presents the results of our analysis of the finite strain theory that goes to the next higher order term than the third-order in the strains for cubic crystals. In the following, expressions for the effective elastic constants resulting from the rigorous stress-strain relationship set by the Murnaghan theory of finite deformation[2] will be presented and compared with the earlier work. Since typical ultrasonic experiments with pressure result in *thermodynamically mixed* elastic constants, the derived expressions of the effective elastic constants had to be identified according to their thermodynamic boundary conditions. This is done in Section 3. In Section 4, we present the rigorous relation of pressure derivatives of the effective elastic constants to partial contractions of the higher-order elastic constants. And, in Section 5, the present work is summarized with a brief discussion.

2. THE EFFECTIVE ELASTIC CONSTANTS

Using the usual Cartesian coordinates, we take the principal axes to coincide with the symmetry axes of an unstrained cubic crystal. Let us denote the coordinates of a point p in the crystal before strain by (a_1, a_2, a_3) and

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*The terms 'low' and 'high' compressions as used here are meant to imply the following: For a given solid under hydrostatic pressure, if the change in the second-order elastic constants with pressure is *linear*, this pressure (and up to this pressure) is referred to as relatively 'low' pressure. If the change with pressure is *nonlinear*, the pressures higher than this pressure are referred to as relatively 'high' pressure. Although it is difficult to make a sharp boundary between the 'low' and 'high' pressures, the pressure in the order of 0·05 B^T (where B^T is the isothermal bulk modulus of solid under the study) for most solids can be referred to as the *relatively low* pressure and the pressure in the order of 0·1 B^T may be referred to as the *moderately high* pressure.

those in the crystal after a strain by (x_1, x_2, x_3). These points determine then a displacement vector with components $(x-a_1)$, (x_2-a_2), (x_3-a_3); thus, the components of the displacements are simply

$$u_r = x_r - a_r, \quad (r = 1, 2, 3). \tag{1}$$

For this reason, it is convenient to discuss the strain according to the Lagrangian scheme.

The Lagrangian strain components in Murnaghan's notation are[2]

$$\eta_{rs} = \tfrac{1}{2}\left(\frac{\partial x_p}{\partial a_r}\cdot\frac{\partial x_p}{\partial a_s} - \delta_{rs}\right) \tag{2}$$

where the subscripts ranges are 1, 2, 3 and δ_{rs} are the Kronecker deltas. Using the Jacobian J of the deformation, we can write equation (2) in a compact form as

$$[\eta] = \tfrac{1}{2}(J^*J - I_3) \tag{2a}$$

where J^* is the transpose of J given by

$$J = \frac{\partial(x_1, x_2, x_3)}{\partial(a_1, a_2, a_3)} \tag{3}$$

and I_3 is the unit matrix.

Consider a special strain which is composed of a hydrostatic strain and a subsequent homogeneous strain. By the homogeneous strain, the point p initially at (a_1, a_2, a_3) is brought to the point $(x_1{}^0, x_2{}^0, x_3{}^0)$, given by

$$x_s{}^0 = (1-\alpha)a_s, \quad (s = 1, 2, 3) \tag{4}$$

thus, every line in the crystal is shortened by the factor $(1-\alpha)$, where

$$\alpha \equiv \eta(\tfrac{1}{2}\eta - 1). \tag{5}$$

The additional displacements resulting from the homogeneous strain are then

$$u'_r = \sum_s \beta_{rs} x_s{}^0, \quad (r, s = 1, 2, 3) \tag{6}$$

where $\beta_{rs} = \beta_{sr}$; thus, β_{rs} represent the six homogeneous strain components and they are infinitesimal quantities. The final coordinates are then given by

$$x_r = x_r{}^\circ + u'_r. \tag{7}$$

From these, we find that

$$\frac{\partial x_r}{\partial a_s} = (1-\alpha)(\delta_{rs} + \beta_{rs}). \tag{8}$$

Here, since β_{rs} are infinitesimal quantities as noted above, only the first powers of β_{rs} are retained and all others are neglected. In view of the particular strain defined by equation (7), the Lagrangian strains become

$$\eta_{rs} = \delta_{rs}\eta + \beta_{rs}(1+2\eta). \tag{9}$$

The strain energy density Φ per unit initial volume is usually given by a power series of the Lagrangian strains as

$$\Phi = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \phi_4 + \ldots \tag{10}$$

where ϕ_j contains the jth order terms of η_{ij} and for a body with no initial stresses ϕ_0 and ϕ_1 can be set equal to zero. Thus, ϕ_2, ϕ_3, and ϕ_4 are:

$$\phi_2 = \frac{1}{2!}C_{ijkl}\eta_{ij}\eta_{kl}$$

and

$$\phi_3 = \frac{1}{3!}C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} \tag{11}$$

$$\phi_4 = \frac{1}{4!}C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}$$

where the subscripts ranges are 1, 2, 3 and the Einstein summation convention for repeated subscripts is assumed. The rigorous relation of the stresses T_{rs} to the strains η_{pq} is

$$T_{rs} = \left(\frac{\rho}{\rho_0}\right)\frac{\partial x_r}{\partial a_p}\left[\frac{\partial\Phi}{\partial\eta_{pq}}\right]\frac{\partial x_s}{\partial a_q} \tag{12}$$

or in a compact form

$$[T] = \left(\frac{\rho}{\rho_0}\right)J\left[\frac{\partial\Phi}{\partial\eta}\right]J^*. \tag{12a}$$

Here, ρ_0 and ρ are the crystal densities before and after a strain, respectively, and the compression ratio is

$$\left(\frac{\rho}{\rho_0}\right) = \frac{1}{\det J} \tag{13}$$

and the gradient of Φ with respect to η_{pq} is

$$\frac{\partial\Phi}{\partial\eta_{pq}} = \begin{vmatrix} \dfrac{\partial\Phi}{\partial\eta_{11}} & \dfrac{\partial\Phi}{\partial\eta_{12}} & \dfrac{\partial\Phi}{\partial\eta_{13}} \\ \dfrac{\partial\Phi}{\partial\eta_{21}} & \dfrac{\partial\Phi}{\partial\eta_{22}} & \dfrac{\partial\Phi}{\partial\eta_{23}} \\ \dfrac{\partial\Phi}{\partial\eta_{31}} & \dfrac{\partial\Phi}{\partial\eta_{32}} & \dfrac{\partial\Phi}{\partial\eta_{33}} \end{vmatrix} \tag{14}$$

From this relation (12), as was done by Birch[1], we can set

$$T_{rs} = -P\delta_{rs} + T'_{rs} \tag{15}$$

where $-P$ is hydrostatic pressure given by

$$-P = \frac{1}{1-\alpha}\left(\frac{\partial\Phi^{(0)}}{\partial\eta_{11}}\right) \tag{16}$$

and T'_{rs} are expressed in terms of the β's and '*a new set*' of elastic constants. This new set of the elastic constants are the effective second-order elastic constants under the hydrostatic pressure and we will denote hereafter to as C_{11}, C_{12} and C_{44}. Since

$$T'_{11} = C_{11}\beta_{11} + C_{12}(\beta_{22} + \beta_{33}) \tag{17}$$

and

$$T'_{12} = 2C_{44}\beta_{12} \tag{18}$$

after having gone through a long algebra, we find the expressions for the effective second-order elastic constants as follows:

$$\begin{aligned} C_{11} = c_{11} &+ \eta(2c_{11}+2c_{12}+c_{111}+2c_{112}) \\ &+ \eta^2(-\tfrac{3}{2}c_{11}-2c_{12}+\tfrac{3}{2}c_{111}+5c_{112}+c_{123} \\ &+ \tfrac{1}{2}c_{1111}+2c_{1112}+c_{1122}+c_{1123}) \end{aligned} \tag{19}$$

$$\begin{aligned} C_{12} = c_{12} &+ \eta(-c_{11}-c_{12}+2c_{112}+c_{123}) \\ &+ \eta^2(c_{11}+\tfrac{3}{2}c_{12}-\tfrac{1}{2}c_{111}-c_{112} \\ &+ c_{1112}+c_{1122}+\tfrac{5}{2}c_{1123}) \end{aligned} \tag{20}$$

$$\begin{aligned} C_{44} = c_{44} &+ \eta(c_{11}+2c_{12}+c_{44}+c_{144}+2c_{166}) \\ &+ \eta^2(-c_{11}-2c_{12}-\tfrac{1}{2}c_{44}+\tfrac{1}{2}c_{111} \\ &+ 3c_{112}+c_{123}+c_{144}+2c_{166} \\ &+ \tfrac{1}{2}c_{1144}+c_{1155}+2c_{1255}+c_{1266}). \end{aligned} \tag{21}$$

Where $c_{\mu\nu}$, $c_{\mu\nu\lambda}$ and $c_{\mu\nu\lambda\xi}$ are the second-, third- and fourth-order elastic constants of crystal in Voigt's notation, respectively, and they are expressed in accordance with the thermodynamic definition[3].

It may be noted that, in equations (19–21), the coefficients of the terms in η with the second- and third-order elastic constants are the conventional expressions for the effective elastic constants[1, 4–6] and they agree with those derived initially by Birch[1] when the third-order elastic constants in Birch's definition are converted into those of more general thermodynamic definition.* However, the coefficients of the terms in η^2 in equations (20) and (21) are at variance with ones given by Ghate[6]. In light of the present analysis, the writer believes that the *minus* signs of the quantities c_{11} and c_{12} found in the η^2 term of Ghate's equation (23) should have been *plus* signs. And, as for the expression for C_{44}, the quantity $(+\tfrac{1}{2}c_{1144})$ should be found in the η^2 term of Ghate's equation (24).

3. THE ULTRASONIC EFFECTIVE ELASTIC CONSTANTS

The expressions of the effective elastic constants as given by equations (19–21) can be either the adiabatic or isothermal expressions, and the proper designation of these is obviously done by adding the proper superscript either 's' or 'T' to all the elastic constants. The acoustic data resulting from the usual acoustic experiments with pressure are neither thermodynamically adiabatic nor thermodynamically isothermal quantities, but they are 'thermodynamically mixed' isothermal-adiabatic quantities[7]. Thus, in this section, we seek for the expressions of the effective elastic constants that may be resulting from the ultrasonic-pressure experiments at high pressures.

Recalling the usual behaviors of ultrasonic wave velocities in the medium of a cubic crystal[8, 9], we note that a longitudinal stiffness c_{11} and shear stiffness c_{44} result directly from measurements of the longitudinal and transverse wave velocities in the [001] direction of the crystal, respectively. If one measures a transverse wave velocity in [110] polarized in the $[1\bar{1}0]$ direction, the resulting stiffness constant is $(c_{11}-c_{12})/2$. Thus, from this, one finds immediately the elastic constant c_{12} as a typical procedure. Following exactly the same procedure as the above but subjected to hydrostatic pressure, we find the *ultrasonic* effective elastic constants of cubic crystals as:

$$\begin{aligned} C_{11(\text{ultrasonic})} = c^s_{11} &+ \eta(c^s_{11}+C_a{}^m+3B^T) \\ &+ \eta^2(-\tfrac{1}{2}c^s_{11}+C_a{}^m+\tfrac{1}{2}C_d{}^m \\ &+ C_e{}^m+\tfrac{1}{2}C_a{}^T+C_b{}^T-3B^T) \end{aligned} \tag{22}$$

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*The relations between the $c_{\mu\nu\lambda}$ defined by Brügger ($c^{Br}_{\mu\nu\lambda}$) and those by Birch ($c^{Bi}_{\mu\nu\lambda}$) are: $c^{Br}_{111} = 6c^{Bi}_{111}$, $c^{Br}_{112} = 2c^{Bi}_{112}$, $c^{Br}_{123} = c^{Bi}_{123}$, $c^{Br}_{456} = \tfrac{1}{8}c^{Bi}_{456}$, $c^{Br}_{144} = \tfrac{1}{2}c^{Bi}_{144}$, and $c^{Br}_{166} = \tfrac{1}{2}c^{Bi}_{166}$. It is noted that the relation between Birch's c_{456} and Brügger's c_{456} should be as given in this paper, provided c_{456} term in the expression of the strain energy is $[\tfrac{1}{2}c_{456}(\eta_{12}\eta_{23}\eta_{31}+\eta_{21}\eta_{32}\eta_{13})]$. However, if the term in the expression of the strain energy is $[c_{456}(\eta_{12}\eta_{23}\eta_{31}+\eta_{21}\eta_{32}\eta_{13})]$ as in Birch's original paper (e.g. equation 12 of[1]), the relation should be $c^{Br}_{456} = \tfrac{1}{4}c^{Bi}_{456}$.

$$C_{12(\text{ultrasonic})} = c_{12}^{s} + \eta(c_{12}^{s} + C_b{}^m - 3B^T) + \eta^2(-\tfrac{1}{2}c_{12}^{s} + C_b{}^m + C_e{}^m + \tfrac{3}{2}c_{1123}^{m} - \tfrac{1}{2}C_a{}^T - C_b{}^T + 3B^T) \qquad (23)$$

$$C_{44(\text{ultrasonic})} = c_{44} + \eta(c_{44} + C_c{}^m + 3B^T) + \eta^2(-\tfrac{1}{2}c_{44} + C_c{}^m + \tfrac{1}{2}C_f{}^m + C_g{}^m + \tfrac{1}{2}C_a{}^T + C_b{}^T - 3B^T). \qquad (24)$$

Where $B^T = (c_{11}^T + 2c_{12}^T)/3$ and the C_j are

$$C_a = c_{111} + 2c_{112} \qquad (25)$$
$$C_b = 2c_{112} + c_{123} \qquad (26)$$
$$C_c = c_{144} + 2c_{166} \qquad (27)$$
$$C_d = c_{1111} + 2c_{1112} \qquad (28)$$
$$C_e = c_{1112} + c_{1122} + c_{1123} \qquad (29)$$
$$C_f = c_{1144} + 2c_{1155} \qquad (30)$$
$$C_g = 2c_{1255} + c_{1266}. \qquad (31)$$

The superscripts '*s*', '*T*' and '*m*' designate *thermodynamically adiabatic*, *thermodynamically isothermal*, and *thermodynamically mixed* elastic constants, respectively. Since the C_j are related to the pressure derivatives of the linear elastic constants $c_{\mu\nu}$, these relationships are to be found.

4. RELATION OF PRESSURE DERIVATIVES OF THE EFFECTIVE ELASTIC CONSTANTS TO PARTIAL CONTRACTIONS OF THE HIGHER-ORDER ELASTIC CONSTANTS

The pressure-dependent second-order elastic constants are[7, 10]

$$C_{ijkl}^{s}(P) = \frac{\lambda}{V^\circ}\left[\frac{\partial^2 U(V^\circ, S, \tilde{\boldsymbol{\eta}})}{\partial\eta_{ij}\partial\eta_{kl}}\right]_{\substack{V^\circ \\ S=\text{const.} \\ \tilde{\eta}=\epsilon 1}} + PD_{ijkl} \qquad (32)$$

where $D_{ijkl} = \delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl}$. V denotes the volume of crystal at reference state characterized by the hydrostatic pressure P, and $\tilde{\boldsymbol{\eta}}$ is the strain tensor corresponding to an arbitrarily deformed state characterized by that pressure P. V° is defined by the relation $(V/V^\circ) = \lambda^3$, where λ is a factor given by the coordinates of a material point in two reference states a_i and a_i° according to $(a_i/a_i^\circ) = \lambda$. The Lagrangian strain tensors corresponding to these two reference states are η_{ij} and η_{ij}°, and they are related by

$$\eta_{ij}^\circ = \lambda^2\eta_{ij} + \epsilon\delta_{ij}$$

where $\epsilon = \frac{1}{2}(\lambda^2 - 1)$. Since from thermodynamics $(\partial/\partial P)_T = -(V/B_T)(\partial/\partial V)_T$ and $(\partial\lambda/\partial V)_0 = \frac{1}{3}V^\circ$, we find by differentiating equation (32) that

$$\left(\frac{\partial C_{ijkl}^{s}}{\partial P}\right)_T = -\frac{1}{3B^T}\left[\frac{1}{V^\circ}\left\{\frac{\partial^2 U(V^\circ, S, \tilde{\boldsymbol{\eta}})}{\partial\eta_{ij}\partial\eta_{kl}}\right\}_{\substack{V^\circ \\ S=\text{const.} \\ \tilde{\eta}=0}} + \frac{1}{V^\circ}\left\{\frac{\partial}{\partial\eta_{mm}}\left(\frac{\partial^2 U(V^\circ, S, \tilde{\boldsymbol{\eta}})}{\partial\eta_{ij}\partial\eta_{kl}}\right)_{\substack{V^\circ \\ S=\text{const.}}}\right\}_{\substack{V^\circ \\ S=\text{const.} \\ \tilde{\eta}=0}}\right] + D_{ijkl}. \qquad (33)$$

Note that the first term in equation (33) is by definition the zero-pressure second-order elastic constants. The second term is, however, thermodynamically mixed third-order elastic constants at zero pressure. Thus, from equation (33), it follows that[7]

$$\left(\frac{\partial C_{ijkl}^{s}}{\partial P}\right)_T = -\frac{1}{3B^T}\left[C_{ijkl}^{s} + C_{ijklmm}^{m}\right] + D_{ijkl} \qquad (34)$$

where

$$C_{ijklmm}^{m} = \frac{1}{A}\left[C_{ijklmm}^{s} + T\gamma_G\left\{-\beta C_{ijkl}^{s} + 3\left(\frac{\partial C_{ijkl}^{s}}{\partial T}\right)\right\}\right]. \qquad (35)$$

γ_G is the Grüneisen constant, β is the coefficient of volume expansion, and A is the ratio of the adiabatic bulk modulus to the isothermal bulk modulus and it is given by $A = 1 + T\beta\gamma_G$. The quantities given by equation (35) are the primary experimental quantities which result from the usual ultrasonic-pressure experiments at low pressures. For cubic crystals, equation (35) reduces to:

$$C^{m}_{1111ii} = c^{m}_{111} + 2c^{m}_{112} = -\left[3B^{T}\left(\frac{\partial c^{s}_{11}}{\partial P}\right)_{T} + 3B^{T} + c^{s}_{11}\right] = C_{a}{}^{m} \tag{36}$$

$$C^{m}_{1122ii} = 2c^{m}_{112} + c^{m}_{123} = -\left[3B^{T}\left(\frac{\partial c^{s}_{12}}{\partial P}\right)_{T} - 3B^{T} + c^{s}_{12}\right] = C_{b}{}^{m} \tag{37}$$

$$C^{m}_{1212ii} = c^{m}_{144} + 2c^{m}_{166} = -\left[3B^{T}\left(\frac{\partial c_{44}}{\partial P}\right)_{T} + 3B^{T} + c_{44}\right] = C_{c}{}^{m}. \tag{38}$$

Alternately, the expressions for $C_{a}{}^{m}$, $C_{b}{}^{m}$ and $C_{c}{}^{m}$ can be obtained directly from the effective elastic constants given earlier by taking the pressure derivatives and evaluating them at zero-pressure. Thus, we find

$$C_{a}{}^{m} = -3B^{T}\left[1 + \left\{\frac{\partial C^{s}_{11}}{\partial P}\right\}_{P=0}\right] - c^{s}_{11} \tag{36a}$$

$$C_{b}{}^{m} = -3B^{T}\left[-1 + \left\{\frac{\partial C^{s}_{12}}{\partial P}\right\}_{P=0}\right] - c^{s}_{12} \tag{37a}$$

$$C_{c}{}^{m} = -3B^{T}\left[1 + \left\{\frac{\partial C_{44}}{\partial P}\right\}_{P=0}\right] - c_{44}. \tag{38a}$$

To obtain the relation of the second pressure derivatives of the elastic constants to partial contractions of the higher-order elastic constants, we start from equation (34). By taking the pressure derivatives of $(\partial C^{s}_{ijkl}/\partial P)_{T}$ and arranging the result,

$$\left(\frac{\partial^{2} C^{s}_{ijkl}}{\partial P^{2}}\right)_{T} = \frac{1}{(3B^{T})^{2}}\left[C^{s}_{ijkl}\left\{1 + 3\left(\frac{\partial B^{T}}{\partial P}\right)_{T}\right\} + \left\{4 + 3\left(\frac{\partial B^{T}}{\partial P}\right)_{T}\right\}C^{m}_{ijklmm} + C^{m}_{ijklmmnn}\right] \tag{39}$$

where $C^{m}_{ijklmmnn}$ are certain linear combinations of the fourth-order elastic constants and

$$\left(\frac{\partial B^{T}}{\partial P}\right)_{T} = -\frac{1}{9B^{T}}\left[C_{a}{}^{T} + 2C_{b}{}^{T}\right]. \tag{40}$$

Therefore, solving equation (39) for $C^{m}_{ijklmmnn}$, we find explicitly the followings:

$$C_{d}{}^{m} + 2C_{e}{}^{m} = (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T})\left[1 + \left(\frac{\partial c^{s}_{11}}{\partial P}\right)_{T}\right] + c^{s}_{11} - 2C_{a}{}^{m} + (3B^{T})^{2}\left(\frac{\partial^{2} c^{s}_{11}}{\partial P^{2}}\right)_{T} = C_{A}{}^{m} \tag{41}$$

$$2C_{e}{}^{m} + 3C^{m}_{1123} = (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T})\left[-1 + \left(\frac{\partial c^{s}_{12}}{\partial P}\right)_{T}\right] + c^{s}_{12} - 2C_{b}{}^{m} + (3B^{T})^{2}\left(\frac{\partial^{2} c^{s}_{12}}{\partial P^{2}}\right)_{T} = C_{B}{}^{m} \tag{42}$$

$$C_{f}{}^{m} + 2C_{g}{}^{m} = (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T})\left[1 + \left(\frac{\partial c_{44}}{\partial P}\right)_{T}\right] + c_{44} - 2C_{c}{}^{m} + (3B^{T})^{2}\left(\frac{\partial^{2} c_{44}}{\partial P^{2}}\right)_{T} = C_{C}{}^{m}. \tag{43}$$

Or, from the effective elastic constants given by equations (22–24), we find that

$$C_{A}{}^{m} = c^{s}_{11} - 2C_{a}{}^{m} + (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T}) \times \left[1 + \left\{\frac{\partial C^{s}_{11}}{\partial P}\right\}_{P=0}\right] + (3B^{T})^{2}\left\{\frac{\partial^{2} C^{s}_{11}}{\partial P^{2}}\right\}_{P=0} \tag{41a}$$

$$C_{B}{}^{m} = c^{s}_{12} - 2C_{b}{}^{m} + (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T}) \times \left[-1 + \left\{\frac{\partial C^{s}_{12}}{\partial P}\right\}_{P=0}\right] + (3B^{T})^{2}\left\{\frac{\partial^{2} C^{s}_{12}}{\partial P^{2}}\right\}_{P=0} \tag{42a}$$

$$C_{C}{}^{m} = c_{44} - 2C_{c}{}^{m} + (6B^{T} - C_{a}{}^{T} - 2C_{b}{}^{T}) \times \left[1 + \left\{\frac{\partial C_{44}}{\partial P}\right\}_{P=0}\right] + (3B^{T})^{2}\left\{\frac{\partial^{2} C_{44}}{\partial P^{2}}\right\}_{P=0}. \tag{43a}$$

Thus, from equations (28–31) and equations (41–43), we have

$$C_{A}{}^{m} = c^{m}_{1111} + 4c^{m}_{1112} + 2c^{m}_{1122} + 2c^{m}_{1123} \tag{44}$$

$$C_B{}^m = 2c^m_{1112} + 2c^m_{1122} + 5c^m_{1123} \quad (45)$$

$$C_C{}^m = c^m_{1144} + 2c^m_{1155} + 4c^m_{1255} + 2c^m_{1266}. \quad (46)$$

These are the primary experimental quantities that are resulting from the ultrasonic-pressure experiments at high pressures.

5. SUMMARY AND CONCLUDING NOTES

Summarizing the foregone sections, the followings may be stated:

(i). Expressions for the effective elastic constants of a cubic crystal subjected to moderately high hydrostatic pressure are derived from the consideration of the rigorous stress-strain relation set by Murnaghan's theory of finite deformations, and these have been compared with the earlier work. Discrepancies were found in the expressions of the effective second-order elastic constants C_{12} and C_{44}. The expressions as ones presented here may be derived from the strain-energy density considerations, and this method may be used to distinguish the observed discrepancies.

(ii). Expressions for the effective second-order elastic constants are

$$C_{\mu\nu} = c_{\mu\nu} + C_I\eta + C_{II}\eta^2$$

where C_I and C_{II} are certain linear combinations of the second- and the higher-order elastic constants of crystal and η is the Lagrangian strain which depends upon pressure. The present expressions are distinguished from the expressions of Birch[1], Seeger and Buck[4], and Thurston[5] and others mainly by the appearance of the $C_{II}\eta^2$ terms in the expressions of the effective elastic constants of cubic crystals.

(iii). Ultrasonic effective second-order elastic constants at high hydrostatic pressures were derived and presented in terms of *thermodynamically mixed* higher-order elastic constants. The rigorous relationships between the pressure derivatives of the elastic constants and partial contractions of the higher-order elastic constants were presented also. And, then, the primary experimental quantities that may be resulting from the ultrasonic-pressure experiments have been identified in a useful form in terms of the *thermodynamically mixed* second-, third-, and fourth-order elastic constants of the crystal under the study.

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REFERENCES

1. BIRCH F., *Phys. Rev.* **71**, 809 (1947).
2. MURNAGHAN F. D., *Am. J. Math.* **59**, 235 (1937); and also, *Finite Deformation of an Elastic Solid* Wiley, New York (1951).
3. BRÜGGER K., *Phys. Rev.* **133**, A1611 (1964).
4. SEEGER A. and BUCK O., *Z. Naturf.* **15A**, 1056 (1960).
5. THURSTON R. N., *J. acoust. Soc. Am.* **37**, 348 (1965).
6. GHATE P. B., *Phys. Status Solidi* **14**, 325 (1966).
7. BARSCH G. R., *Phys. Status Solidi* **19**, 129 (1967): see also the references cited by Barsch.
8. See, for example, HUNTINGTON H. B., *Solid State Physics* (Edited by Seitz F. and Turnbull D.), Vol. 7. Academic Press, New York (1958).
9. THURSTON R. N., *Physical Acoustics* (Edited by Mason W. P.), Vol. IA. Academic Press, New York (1964).
10. LEIBFRIED G. and LUDWIG W., *Solid State Physics* (Edited by Seitz F. and Turnbull D.), Vol. 12. Academic Press, New York (1961).