

## Third-Order Elastic Constants and the Velocity of Small Amplitude Elastic Waves in Homogeneously Stressed Media

R. N. THURSTON AND K. BRUGGER

*Bell Telephone Laboratories, Murray Hill, New Jersey*

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Third-order elastic constants can be determined from the velocity of small amplitude sound waves in statically stressed media. For this purpose exact expressions are derived for the sound velocity and for a *natural* velocity and their stress derivatives, evaluated at zero stress, in terms of second- and third-order elastic constants. The formulas apply to arbitrary crystal symmetry and to arbitrary stress systems depending on a single scalar variable. Special formulas for hydrostatic pressure and uniaxial stress are listed for the cubic point groups  $O$ ,  $O_h$ ,  $T_d$ , and for isotropic materials. Attention is given to the proper variation of propagation direction with static stress in order to maintain propagation normal to a given crystal face as in ultrasonic experiments, and to the proper separation of isothermal and isentropic coefficients in the results. The simplest and most convenient form of the results employs the *natural* velocity (natural unstressed length at the same temperature divided by the transit time), which is computed directly from experimental data without correcting the path length for the effect of stress.

### 1. INTRODUCTION

**T**HIRD-ORDER elastic constants play an important role in solid-state physics. They allow an evaluation of first-order anharmonic terms of the interatomic potential or of generalized Grüneisen parameters, which enter the theories of all anharmonic phenomena, such as the interaction of acoustic and thermal phonons and the equation of state.

The third-order constants can be determined from velocity measurements on small amplitude sound waves in statically stressed media.<sup>1</sup> Mason<sup>1</sup> and Seeger and Buck<sup>2</sup> calculated the sound velocities in terms of second- and third-order elastic constants for various wave modes in uniaxially and hydrostatically compressed cubic crystals. Using a nonlinear<sup>3</sup> stress-strain relation they derived special equations of motion for the given crystal symmetry and solved them by substituting plane-wave solutions. This procedure is exceedingly laborious, especially for crystals of lower symmetry.

The method presented here, for arbitrary crystal symmetry and arbitrary homogeneous stress systems depending on a single scalar variable, yields general results in a form suitable for algebraic machine reduction<sup>4</sup> to any desired special case. Considerable simplification is obtained by properly maintaining the direction of propagation perpendicular to a chosen crystal face during the deformation, and by introducing instead of the actual wave velocity a *natural* wave velocity which is more readily obtained from experiments. The resulting formulas for the squares of the actual and of this natural velocity and for their stress derivatives, evaluated at zero stress, are exact. The ease of taking these derivatives depends on the thermodynamic

definition of higher order elastic constants given in the following paper.<sup>5</sup>

In Sec. 2, the stress is related to energy functions,<sup>3</sup> and an appropriate general form of the equation of motion is derived.<sup>6</sup> In Sec. 3, the equation of motion is linearized about an arbitrary state of homogeneous strain, and solutions are obtained for small amplitude plane waves superimposed on a homogeneously strained initial state. Section 4 relates the actual propagation direction  $\mathbf{n}$  and velocity  $V$  to the corresponding *natural* direction  $\mathbf{N}$  and *natural* velocity  $W$  used in Sec. 3. For stress systems depending on a single scalar variable, formulas for the stress derivatives of  $\rho_0 W^2$  and  $\rho_0 V^2$ , evaluated at zero stress, are given in Secs. 5 and 6, respectively. Finally, in Sec. 7, we list results for the cubic point groups  $O$ ,  $O_h$ , and  $T_d$  and for isotropic media when the stress is hydrostatic pressure or uniaxial compression.

### 2. EQUATION OF MOTION

From the theory of the mechanics of continua, one has, in the absence of body forces, the equations of motion

$$\rho \ddot{x}_j = (\partial/\partial x_k) \tau_{kj}, \quad (2.1)$$

where the stresses  $\tau_{kj}$  are given by<sup>3,7</sup>

$$\tau_{kj} = - \frac{1}{J} \frac{\partial x_k}{\partial a_p} \frac{\partial x_j}{\partial a_q} t_{pq}. \quad (2.2)$$

The  $a_j$  and  $x_j$  are the coordinates of a material particle in the unstrained and strained states, and the  $\ddot{x}_j$  are the components of its acceleration.  $J$ , the Jacobian of the deformation,

$$J = \left| \frac{\partial x_r}{\partial a_s} \right| = \frac{\rho_0}{\rho} \quad (2.3)$$

<sup>1</sup> T. Bateman, W. P. Mason, and H. J. McSkimin, *J. Appl. Phys.* **32**, 928 (1961).

<sup>2</sup> A. Seeger and O. Buck, *Z. Naturforsch.* **15A**, 1056 (1960).

<sup>3</sup> F. D. Murnaghan, *Finite Deformation of an Elastic Solid* (John Wiley & Sons, Inc., New York, 1951).

<sup>4</sup> W. S. Brown, *Bell System Tech. J.* **42**, 2081 (1963).

<sup>5</sup> K. Brugger, *Phys. Rev.* following paper **133**, A1611 (1964).

<sup>6</sup> C. Truesdell and R. Toupin, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1960), Vol. III/1, p. 226.

<sup>7</sup> R. N. Thurston, in *Physical Acoustics*, edited by W. P. Mason (Academic Press Inc., New York, 1964) **1A**, p. 1.

equals the ratio of unstrained to strained density, and

$$t_{pq} = \rho_0 \left( \frac{\partial U}{\partial \eta_{pq}} \right)_S = \rho_0 \left( \frac{\partial F}{\partial \eta_{pq}} \right)_T, \quad (2.4)$$

with  $U$  and  $F$ , respectively, the internal energy and Helmholtz free energy per unit mass.  $S$  and  $T$  denote entropy and temperature. The Lagrangian strains are given by

$$\eta_{pq} = \frac{1}{2} \left( \frac{\partial x_i}{\partial a_p} \frac{\partial x_i}{\partial a_q} - \delta_{pq} \right). \quad (2.5)$$

Equation (2.4) shows that in the terminology of Truesdell and Toupin,<sup>6</sup> the quantities  $t_{pq}$  are thermodynamic tensions conjugate to the variables  $\eta_{pq}/\rho_0$ , while Eq. (2.2) enables one to identify  $t_{pq}$  as the second Piola-Kirchhoff stress tensor.<sup>6</sup>

Substituting from Eqs. (2.2) and (2.3) into (2.1) and making use of the identity of Euler, Piola, and Jacobi,<sup>6,7</sup>

$$\frac{\partial}{\partial x_k} \left( \frac{1}{J} \frac{\partial x_k}{\partial a_p} \right) = 0, \quad (2.6)$$

the equations of motion become

$$\rho_0 \ddot{x}_j = \partial P_{jp} / \partial a_p \quad (2.7)$$

with

$$P_{jp} = (\partial x_j / \partial a_q) t_{pq}. \quad (2.8)$$

$P_{jp}$  is the first Piola-Kirchhoff stress tensor, or double vector.<sup>6</sup>

### 3. SMALL AMPLITUDE WAVES IN A STRAINED MEDIUM

We now consider the propagation of small amplitude elastic waves in a homogeneously deformed medium. We define, for every initial temperature  $T$ ,  $a_i$  = coordinate in the *natural* or unstressed state,  $X_i(\mathbf{a})$  = coordinate in homogeneously stressed or *initial* state,  $u_i \equiv x_i - X_i$  = component of displacement from initial state due to the wave. We regard  $P_{jp}$  in Eq. (2.7) as a function of the entropy and the deformation gradients  $\partial x_k / \partial a_m$ . To obtain an appropriately linearized equation of motion, we expand  $P_{jp}$  about the initial state of coordinates  $X_i$ , denoting the initial values by  $\sim$  over the symbols, and assuming explicitly that the deviations from  $\mathbf{X}$  to  $\mathbf{x}$  are isentropic:

$$\begin{aligned} P_{jp} - \bar{P}_{jp} &= \frac{\partial P_{jp}}{\partial (\partial x_k / \partial a_m)} \left( \frac{\partial x_k}{\partial a_m} - \frac{\partial X_k}{\partial a_m} \right) + \dots \\ &= \tilde{A}^{sjkpm} \frac{\partial u_k}{\partial a_m} + \dots, \end{aligned} \quad (3.1)$$

where

$$\tilde{A}^{sjkpm} \equiv \left( \frac{\partial P_{jp}}{\partial (\partial x_k / \partial a_m)} \right)_{\mathbf{x}, S}. \quad (3.2)$$

Clearly,

$$\partial \bar{P}_{jp} / \partial a_p = 0. \quad (3.3)$$

Then, substituting from Eq. (3.1) into Eq. (2.7) and retaining only first powers of the displacement gradients  $\partial u_k / \partial a_m$ , we obtain linearized equations of motion for  $u_j$  in the form

$$\rho_0 \ddot{u}_j = \tilde{A}^{sjkpm} \frac{\partial^2 u_k}{\partial a_p \partial a_m}. \quad (3.4)$$

The tensor  $A^{sjkpm}$  can be expressed in terms of deformation gradients and derivatives of the internal energy with respect to the classical strain components  $\eta_{ij}$  by making use of the relation

$$\frac{\partial \eta_{ij}}{\partial (\partial x_p / \partial a_q)} = \frac{1}{2} \left( \frac{\partial x_p}{\partial a_j} \delta_{qi} + \frac{\partial x_p}{\partial a_i} \delta_{qj} \right), \quad (3.5)$$

which follows easily from the definition (2.5). By differentiation of Eq. (2.8),

$$\begin{aligned} A^{sjkpm} &= \frac{\partial [(\partial x_j / \partial a_q) t_{pq}]}{\partial (\partial x_k / \partial a_m)} \\ &= \delta_{jk} t_{pm} + \frac{\partial x_j}{\partial a_q} \frac{\partial x_k}{\partial a_i} c^s_{pqmi}, \end{aligned} \quad (3.6)$$

where

$$c^s_{pqmi} \equiv \left( \frac{\partial t_{pq}}{\partial \eta_{mi}} \right)_S = \rho_0 \left( \frac{\partial^2 U}{\partial \eta_{mi} \partial \eta_{pq}} \right)_S. \quad (3.7)$$

The symmetries of  $c^s_{pqmi}$  with respect to permutation of indices have been used in arriving at Eq. (3.6). The quantity  $\tilde{A}^{sjkpm}$  in Eq. (3.4) is then obtained by evaluating Eq. (3.6) at the homogeneously strained initial state:

$$\tilde{A}^{sjkpm} = \delta_{jk} \bar{t}_{pm} + \frac{\partial X_j}{\partial a_q} \frac{\partial X_k}{\partial a_i} \bar{c}^s_{pqmi}. \quad (3.8)$$

We now assume plane sinusoidal waves of the form

$$u_j = A_j \exp[j\omega(t - (\mathbf{N} \cdot \mathbf{a}_i / W))], \quad (3.9)$$

where  $\mathbf{N}$  is a unit vector.

According to this expression, the wave front is a material plane which has unit normal  $\mathbf{N}$  in the natural state; and a wave front moves from the plane  $\mathbf{N} \cdot \mathbf{a} = 0$  to  $\mathbf{N} \cdot \mathbf{a} = L_0$  in the time  $L_0/W$ . Thus  $W$  is the wave speed referred to natural dimensions, and we call it the *natural velocity* for propagation normal to a plane of natural normal  $\mathbf{N}$ .

In a typical ultrasonic experiment, plane waves are reflected between opposite parallel faces of a specimen, the wave fronts being parallel to these faces. One ordinarily measures a repetition frequency  $F$ , which is the inverse of the time required for a round trip between the opposite faces. Hence,

$$W = 2L_0 F. \quad (3.10)$$

The advantages of  $W$  and  $\mathbf{N}$  over the actual velocity  $V$  and actual propagation direction  $\mathbf{n}$  which would

appear in the representation

$$\exp[j\omega(t - (n_i X_i / V))] ]$$

are as follows: (1)  $W$  is proportional to the directly measured frequency  $F$ , whereas  $V$  involves the actual length under stress. (2)  $\mathbf{n}$  may change with static stress, but since the propagation direction remains normal to the same faces of the specimen,  $\mathbf{N}$  is constant.

Substitution of Eq. (3.9) into Eq. (3.4) provides the propagation conditions

$$\rho_0 W^2 u_j = \bar{A}^S_{j k p m} N_p N_m u_k. \quad (3.11)$$

It follows that the possible values of  $\rho_0 W^2$  for plane-wave propagation normal to the material plane of natural normal  $\mathbf{N}$  are eigenvalues of the second rank tensor

$$S_{jk}(\mathbf{N}) = \bar{A}^S_{j k p m} N_p N_m, \quad (3.12)$$

and the possible particle displacement directions are the corresponding eigenvectors. It follows from the symmetry of  $t_{pm}$  and  $c^S_{pqm}$  that  $S_{jk}$  is symmetric, and hence at any state of strain there are three mutually perpendicular particle displacement directions for plane waves corresponding to a given  $\mathbf{N}$ . For three real waves,  $S_{jk}$  must also be positive definite. Criteria for this are discussed in the literature.<sup>8-10</sup> In general,  $S_{jk}$  depends on rotation as well as strain, but the rotational dependence reflects only the obvious fact that the particle displacement directions must rotate with the material. For a given  $\mathbf{N}$ , the eigenvalues  $\rho_0 W^2$  are independent of the rotation.

To obtain a representation completely independent of the rotation, we transform the particle displacement direction  $\mathbf{u}$  back to the natural undeformed direction of the material line along it by the transformation<sup>9</sup>

$$u_j = (\partial X_j / \partial a_q) U_q. \quad (3.13)$$

Then Eq. (3.11) is transformed to

$$\rho_0 W^2 U_j = w_{jk} U_k, \quad (3.14)$$

where

$$w_{jk} = \frac{\partial a_j}{\partial X_r} \frac{\partial X_s}{\partial a_k} S_{rs} \\ = N_r N_s (\delta_{jk} \bar{t}_{rs} + \bar{C}_{qk} \bar{c}^S_{jrqs}) \quad (3.15)$$

and

$$\bar{C}_{qk} = \frac{\partial X_i}{\partial a_q} \frac{\partial X_i}{\partial a_k} = (\delta_{qk} + 2\bar{\eta}_{qk}). \quad (3.16)$$

It is now obvious that all quantities appearing in Eq. (3.15) are independent of the rotation. They depend on the strain and one other thermodynamic variable which may be taken as either the entropy or the temperature. We emphasize the significance of

<sup>8</sup> C. Truesdell, Arch. Ratl. Mech. Anal. 8, 263 (1961).

<sup>9</sup> R. A. Toupin and B. Bernstein, J. Acoust. Soc. Am. 33, 216 (1961).

<sup>10</sup> C. Truesdell and R. Toupin, Arch. Ratl. Mech. Anal. 12, 1 (1963).

Eq. (3.14): The possible values of  $\rho_0 W^2$  for propagation normal to a material surface of natural undeformed normal  $\mathbf{N}$  are the eigenvalues of  $w_{jk}$ , and the material lines along the corresponding eigenvectors  $\mathbf{U}$  are rotated by the deformation [i.e., transformed by Eq. (3.13)] into the actual particle displacement directions  $\mathbf{u}$ . The three eigenvectors  $\mathbf{U}$  corresponding to a given  $\mathbf{N}$  are not in general orthogonal.

#### 4. PROPAGATION DIRECTION AND VELOCITY

In the definitive paper of Truesdell<sup>8</sup> and in other published work,<sup>7,9</sup> results have been expressed in terms of actual propagation direction and velocity. To permit ready comparison, we shall relate  $\mathbf{N}$  and  $W$  in Eq. (3.9) to the actual propagation direction  $\mathbf{n}$  and velocity  $V$ .

In the homogeneous deformation, the material point at  $\mathbf{a}$  in the natural state moves to  $\mathbf{X}$ , where

$$a_i = (\partial a_i / \partial X_j) X_j. \quad (4.1)$$

It follows that the actual plane wave front in the homogeneously deformed body has coordinates  $X_j$  satisfying

$$\mathbf{N} \cdot \mathbf{a} = N_i (\partial a_i / \partial X_j) X_j = \text{const.}$$

Thus, the propagation direction has the direction numbers  $N_i \partial a_i / \partial X_j$  and the direction cosines

$$n_j = (f_N)^{-1} N_i (\partial a_i / \partial X_j), \quad (4.2)$$

where the normalization factor  $f_N$  satisfies

$$f_N^2 = N_i N_k \frac{\partial a_i}{\partial X_j} \frac{\partial a_k}{\partial X_j} = \bar{C}_{ik}^{-1} N_i N_k. \quad (4.3)$$

[It is readily verified that  $(\partial a_i / \partial X_j) (\partial a_k / \partial X_j)$  is the  $ik$  element in the inverse of the tensor  $\bar{C}_{pq}$ .]

To obtain the actual path length and propagation velocity, we note that a material line segment of unit length along  $\mathbf{N}$  in the unstrained state is rotated and stretched by the homogeneous deformation into a new line segment having the components  $(\partial X_i / \partial a_j) N_j$ . Letting  $\mathbf{m}$  denote a unit vector along its new direction, and  $\lambda_N$  the stretched length, we have

$$\lambda_N \mathbf{m}_j = \frac{\partial X_j}{\partial a_k} N_k. \quad (4.4)$$

By projecting the slant distance  $\lambda_N$  back onto the new normal  $\mathbf{n}$ , we find the ratio of deformed to undeformed perpendicular distance between material planes of natural, undeformed normal  $\mathbf{N}$ :

$$\frac{L}{L_0} = \lambda_N \mathbf{m} \cdot \mathbf{n} = \frac{1}{f_N} \frac{\partial a_i}{\partial X_j} \frac{\partial X_j}{\partial a_k} N_i N_k = \frac{1}{f_N}. \quad (4.5)$$

Hence, the actual propagation velocity  $V$ , given by  $LW/L_0$ , is

$$V = W / f_N. \quad (4.6)$$

The geometric relationships involved here are pictured in Fig. 1. They may be summarized as follows:  $\mathbf{N}$  denotes the original unit normal to a pair of parallel material planes. The originally normal material line segment  $L_0\mathbf{N}$  connecting the planes is deformed into  $\lambda_N L_0\mathbf{m}$  while the material planes acquire the new unit normal  $\mathbf{n}$ . The separation of the planes changes from  $L_0$  to  $L = \lambda_N L_0 \mathbf{m} \cdot \mathbf{n} = L_0 / f_N$ .

From Eq. (4.2),

$$N_k = f_N n_j (\partial X_j / \partial a_k). \tag{4.7}$$

In view of Eq. (4.6), the possible values of  $\rho_0 V^2$  for a given propagation direction are the eigenvalues of the tensor  $Q_{jk} = S_{jk} / f_N^2$ . From Eqs. (3.12) and (4.7),

$$Q_{jk}(\mathbf{n}) = \tilde{A}^s_{jkpm} \frac{\partial X_r}{\partial a_p} \frac{\partial X_s}{\partial a_m} n_r n_s. \tag{4.8}$$

Truesdell<sup>8</sup> has called  $\mathbf{Q}(\mathbf{n})$  the *acoustical tensor* for the direction  $\mathbf{n}$  in an elastic material subject to the deformation gradient  $\partial X_k / \partial a_m$ . In one respect, the formula (4.8) is but a special case of Truesdell's general result, the specialization having been made to a hyperelastic material (material for which there exists a stored energy function). The loss of generality is unessential for the present purpose. Moreover, our inclusion of a non-mechanical variable (either temperature or entropy) in the internal energy function makes it possible to treat isentropic deformations superimposed on a state which is reached by an isothermal deformation from the natural unstrained state.

In showing that the speeds of propagation are independent of the rotation, the previous treatments<sup>7-9</sup> introduced a vector  $\mathbf{v}$  equal to the present  $\mathbf{N} / f_N$ . The above discussion and Fig. 1 clarify the geometrical significance of this vector. Its direction is the *natural* normal to the material plane containing the wave front, and its magnitude is the ratio of stressed to unstressed path length for propagation normal to this material plane.

5. VARIATION OF  $\rho_0 W^2$  WITH STATIC STRESS

In a typical experiment, the repetition frequency  $f$  is measured as a function of the applied stress at constant temperature. In all measurements on elastic crystals known to us,<sup>1,11-13</sup> this relation is linear to within experimental error. Hence its *slope* is of primary interest. Whereas one could readily evaluate the isothermal stress derivative for an arbitrary stress system, it seems sufficient to consider deformed states depending on a single scalar variable  $p$ . Ordinarily, though not necessarily,  $p$  will represent either the

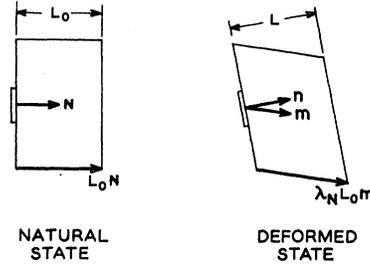


FIG. 1. Change of propagation direction  $\mathbf{n}$  and path length  $L$  with change of static deformation. (The propagation direction remains perpendicular to the reflecting faces of the specimen while the material line segment  $L_0\mathbf{N}$  is rotated and stretched into  $\lambda_N L_0\mathbf{m}$ . The perpendicular distance between the faces changes from  $L_0$  to  $L = \lambda_N L_0 \mathbf{m} \cdot \mathbf{n}$ .)

hydrostatic pressure, or the magnitude of a uniaxial load in some prescribed direction per unit of natural undeformed area. We refer the strain components to the natural unstressed state *at the temperature of the experiment*. Then strain components  $\eta_{ij}$  and thermodynamic tensions  $t_{ij}$  are functions of  $p$  which vanish at  $p=0$ . We wish to evaluate the quantity

$$(\rho_0 W^2)' \equiv [(\partial / \partial p)(\rho_0 W^2)]_T \tag{5.1}$$

at  $p=0$ .

By differentiation of Eq. (3.14), we obtain

$$(\rho_0 W^2)' U_j + \rho_0 W^2 U_j' = w_{jk}' U_k + w_{jk} U_k', \tag{5.2}$$

where the prime denotes the derivative with respect to  $p$  at constant temperature. We assume without loss of generality that the eigenvector  $\mathbf{U}$  is normalized, and hence

$$\mathbf{U} \cdot \mathbf{U} = 1, \quad \mathbf{U} \cdot \mathbf{U}' = 0. \tag{5.3}$$

Multiplying Eq. (5.2) by  $U_j$  and making use of Eq. (5.3), we find

$$(\rho_0 W^2)' = U_j w_{jk}' U_k + U_j w_{jk} U_k'. \tag{5.4}$$

Now at  $p=0$ ,  $w_{jk}$  is symmetric, being identically equal to  $S_{jk}$ . It follows that

$$(U_j w_{jk})_{p=0} = (\rho_0 W^2 U_k)_{p=0} \tag{5.5}$$

and hence when Eq. (5.4) is evaluated at  $p=0$ , the last term vanishes, leaving only

$$(\rho_0 W^2)'_{p=0} = (U_j w_{jk}' U_k)_{p=0}. \tag{5.6}$$

Equation (5.6) states that the derivative of an eigenvalue of the tensor  $w_{jk}$ , evaluated at  $p=0$ , is obtained from the corresponding eigenvector of the tensor  $w_{jk}$  and the components of  $w_{jk}'$ .

If  $w_{jk}$  has multiple eigenvalues at  $p=0$ , a precaution should be observed in the use of Eq. (5.6) because the direction of the eigenvector belonging to a multiple eigenvalue is not determined. It is implicit in the use of the relation  $\mathbf{U} \cdot \mathbf{U}' = 0$  that in this case one should use in Eq. (5.6) the limiting right eigenvector of  $w_{jk}(p)$  as

<sup>11</sup> H. J. McSkimin and P. Andreatch, J. Appl. Phys. 34, 651 (1963).

<sup>12</sup> H. J. McSkimin, measurements on quartz (private communication).

<sup>13</sup> J. R. Drabble, measurements of germanium and silicon (private communication).

TABLE I. Cubic crystals under hydrostatic pressure.<sup>a</sup>

Propagation direction	Displacement direction	$w \equiv (\rho_0 V^2)_{p=0}$	$(\rho_0 W^2)'_{p=0}$
[100]	[100]	$c_{11}^S$	$-1 - \frac{2w}{3B} - \frac{1}{3B}(C_{111} + 2C_{112})$
[100]	Any $\perp$ direction	$c_{44}$	$-1 - \frac{2w}{3B} - \frac{1}{3B}(C_{144} + 2C_{166})$
[110]	[110]	$\frac{1}{2}(c_{11}^S + c_{12}^S + 2c_{44})$	$-1 - \frac{2w}{3B} - \frac{1}{3B}(\frac{1}{2}C_{111} + 2C_{112} + C_{144} + 2C_{166} + \frac{1}{2}C_{123})$
[110]	[1 $\bar{1}$ 0]	$\frac{1}{2}(c_{11}^S - c_{12}^S)$	$-1 - \frac{2w}{3B} - \frac{1}{3B}(\frac{1}{2}C_{111} - \frac{1}{2}C_{123})$
[110]	[001]	$c_{44}$	$-1 - \frac{2w}{3B} - \frac{1}{3B}(C_{144} + 2C_{166})$

<sup>a</sup>  $B = 1/3(s_{11}^T + 2s_{12}^T) = \frac{1}{3}(c_{11}^T + 2c_{12}^T)$  = isothermal bulk modulus at  $p = 0$ .

$p \rightarrow 0$ , and not just any eigenvector of  $w_{jk}(0)$  belonging to the multiple eigenvalue.

Let us now evaluate  $w_{jk}'(0)$  for use in Eq. (5.6). Quantities dependent on the strain are differentiated in accordance with the formula

$$\left(\frac{\partial}{\partial p}\right)_T = \left(\frac{\partial t_{km}}{\partial p}\right)_T \left(\frac{\partial \eta_{ij}}{\partial t_{km}}\right)_T \left(\frac{\partial}{\partial \eta_{ij}}\right)_T = t_{km}' s^T_{ijkm} \left(\frac{\partial}{\partial \eta_{ij}}\right)_T. \quad (5.7)$$

Recalling that  $\mathbf{N}$  is independent of  $p$ , we obtain, by differentiation of Eq. (3.15),

$$w_{jk}'(0) = N_r N_s [\delta_{jk} t_{rs}'(0) + t_{ab}'(0) \times (2s^T_{qkab} c^S_{jrs} + s^T_{ipab} C_{jrkspi})], \quad (5.8)$$

where all quantities are evaluated at  $p = 0$  and

$$C_{jrkspi} \equiv \left(\frac{\partial c^S_{jrkps}}{\partial \eta_{ip}}\right)_{T; p=0}. \quad (5.9)$$

The derivatives  $t_{rs}'(0)$  are easily evaluated for hydrostatic pressure and uniaxial compression. From Eq. (2.2),

$$t_{rs}' = J \frac{\partial a_r}{\partial X_k} \frac{\partial a_s}{\partial X_j} \tau_{kj}. \quad (5.10)$$

For hydrostatic pressure,  $\tau_{kj} = -p\delta_{kj}$ , and hence

$$t_{rs}'(0) = -\delta_{kj} \left( J \frac{\partial a_r}{\partial X_k} \frac{\partial a_s}{\partial X_j} \right)_{p=0} = -\delta_{rs}. \quad (5.11)$$

For uniaxial compression in the direction of a unit vector  $M$ ,

$$\tau_{kj} = -\sigma M_k M_j = -p(A_0/A) M_k M_j,$$

where  $\sigma$  is the actual magnitude of the compressive stress, i.e., force per unit of actual area  $A$ , and  $p$  is the compressive force per unit of original area  $A_0$ . By substitution into Eq. (5.10), and differentiation with respect to  $p$ , we find

$$t_{rs}'(0) = -M_k M_j \left( J \frac{A_0}{A} \frac{\partial a_r}{\partial X_k} \frac{\partial a_s}{\partial X_j} \right)_{p=0} = -M_r M_s. \quad (5.12)$$

Now let  $\mathbf{U}^0$  denote a limiting eigenvector of  $w_{jk}(p)$  as  $p \rightarrow 0$ , and  $w$  the corresponding eigenvalue, i.e.,

$$w \equiv (\rho_0 W^2)_{p=0} = (\rho_0 V^2)_{p=0}. \quad (5.13)$$

It follows easily from Eqs. (3.14)–(3.16) that

$$w_{jk}(0) = N_r N_s c^S_{jrkps}, \quad w_{jk}(0) U_j^0 = w U_k^0, \quad (5.14)$$

where the elastic coefficients are now understood to be

TABLE II. Cubic crystals under uniaxial compression along [001].<sup>a</sup>

Propagation direction	Displacement direction	$w \equiv (\rho_0 V^2)_{p=0}$	$F_U^0$	$(\rho_0 W^2)'_{p=0}$
[100]	[100]	$c_{11}^S$	$a$	$2wF_U^0 + aC_{111} + C_{112}(a-b)$
[100]	[010]	$c_{44}$	$a$	$2wF_U^0 - bC_{144} + 2aC_{166}$
[100]	[001]	$c_{44}$	$\frac{1}{2}(a-b)$	$2wF_U^0 + aC_{144} + C_{166}(a-b)$
[110]	[110]	$\frac{1}{2}(c_{11}^S + c_{12}^S + 2c_{44})$	$a$	$2wF_U^0 + \frac{1}{2}aC_{111} + \frac{1}{2}C_{112}(3a-b) + 2aC_{166} - bC_{144} - \frac{1}{2}bC_{123}$
[110]	[110]	$\frac{1}{2}(c_{11}^S - c_{12}^S)$	$a$	$2wF_U^0 + \frac{1}{2}aC_{111} - \frac{1}{2}C_{112}(a+b) + \frac{1}{2}bC_{123}$
[110]	[001]	$c_{44}$	$\frac{1}{2}(a-b)$	$2wF_U^0 + aC_{144} + C_{166}(a-b)$

<sup>a</sup>  $a = -s_{12}^T = c_{12}^T/3B(c_{11}^T - c_{12}^T)$ .  $b = s_{11}^T = (c_{11}^T + c_{12}^T)/3B(c_{11}^T - c_{12}^T)$ .  $B = \frac{1}{3}(c_{11}^T + 2c_{12}^T)$ .

TABLE III. Cubic crystals under uniaxial compression along [110].<sup>a</sup>

Propagation direction	Displacement direction	$w \equiv (\rho_0 V^2)_{p=0}$	$F_U^0$	$(\rho_0 W^2)'_{p=0}$
[001]	[001]	$c_{11}^S$	$a$	$2wF_U^0 + aC_{111} + (a-b)C_{112}$
[001]	[110]	$c_{44}$	$\frac{1}{2}(a-b-2c)$	$2wF_U^0 + \frac{1}{2}(a-b)C_{144} + \frac{1}{2}C_{166}(3a-b) - 2cC_{456}$
[001]	[110]	$c_{44}$	$\frac{1}{2}(a-b+2c)$	$2wF_U^0 + \frac{1}{2}(a-b)C_{144} + \frac{1}{2}C_{166}(3a-b) + 2cC_{456}$
[110]	[110]	$\frac{1}{2}(c_{11}^S + c_{12}^S + 2c_{44})$	$\frac{1}{2}(a-b+2c)$	$\left\{ \begin{aligned} &2wF_U^0 + \frac{1}{2}(a-b)C_{111} + \frac{1}{2}C_{112}(5a-3b) \\ &+ C_{166}(a-b+4c) + aC_{144} + \frac{1}{2}aC_{123} \end{aligned} \right.$
[110]	[110]	$\frac{1}{2}(c_{11}^S - c_{12}^S)$	$\frac{1}{2}(a-b-2c)$	$2wF_U^0 + \frac{1}{2}(a-b)C_{111} + \frac{1}{2}C_{112}(a+b) - \frac{1}{2}aC_{123}$
[110]	[001]	$c_{44}$	$a$	$2wF_U^0 + \frac{1}{2}(a-b)C_{144} + \frac{1}{2}C_{166}(3a-b) + 2cC_{456}$

<sup>a</sup>  $c = \frac{1}{2}s_{44} = 1/4c_{44}$ .  $a, b$  as in Table II.

evaluated at  $p=0$ . When Eqs. (5.8) and (5.14) are substituted into Eq. (5.6), we obtain

$$(\rho_0 W^2)'_{p=0} = t_{ab}'(0) [N_a N_b + U_j^0 U_k^0 \times (2w s^T_{jkab} + N_r N_s s^T_{ipab} C_{jrstip})]. \quad (5.15)$$

The reduction of Eq. (5.15) to obtain special formulas for given directions of wave propagation and stress can be quickly carried out by hand only for simple directions in crystals of high symmetry. However, such algebraic reduction can be done automatically by computer. The special results for cubic crystals in Tables I-III have in fact been checked by a computer program using ALPAK.<sup>4</sup>

In experimental investigations, the "natural" direction of propagation  $\mathbf{N}$  is frequently chosen such that  $\mathbf{U}^0$  is along a principal axis of the second-rank symmetric tensor

$$F^0_{qk} \equiv \left( \frac{d\eta_{qk}}{dp} \right)_{p=0} = s^T_{qkab} t_{ab}'(0). \quad (5.16)$$

Then

$$F^0_{qk} U_k^0 = F_U^0 U_q^0, \quad (5.17)$$

where  $F_U^0$  is the eigenvalue of  $F^0_{qk}$  belonging to  $\mathbf{U}^0$ . In this case, the middle term in Eq. (5.15) can be simplified as follows:

$$2w s^T_{jkab} t_{ab}'(0) U_k^0 U_j^0 = 2w F_U^0. \quad (5.18)$$

Thus, whenever the particle displacement direction  $\mathbf{U}^0$  is an eigenvector of  $F^0_{qk}$ , we obtain the following simpler version of Eq. (5.15):

$$(\rho_0 W^2)'_{p=0} = 2w F_U^0 + N_r N_s [t_{rs}'(0) + U_j^0 U_k^0 s^T_{ipab} t_{ab}'(0) C_{jrstip}]. \quad (5.19)$$

In addition,  $N_r N_s t_{rs}'(0)$  is easily simplified for hydrostatic pressure and for uniaxial compression along  $M$ .

$$N_r N_s t_{rs}'(0) = -1 \text{ for hydrostatic pressure,} \\ = -(\mathbf{N} \cdot \mathbf{M})^2 \text{ for uniaxial compression.} \quad (5.20)$$

This term is therefore zero when the propagation direction is perpendicular to the direction of uniaxial stress.

### 6. VARIATION OF $\rho_0 V^2$ WITH STATIC STRESS

The formula for  $(\rho_0 V^2)'$  is in general more complicated than that for  $(\rho_0 W^2)'$  because of the variation of

$$(V/W)^2 = (L/L_0)^2 = 1/f_N^2. \quad (6.1)$$

By straightforward evaluation, using Eqs. (4.3), (3.16), and (5.7),

$$\left[ \frac{\partial}{\partial p} \left( \frac{1}{f_N} \right)^2 \right]_{T; p=0} = 2N_k N_m s^T_{kmpq} t_{pq}'(0) \\ = 2N_k N_m F^0_{km}. \quad (6.2)$$

It follows that

$$[(\rho_0 V^2)' - (\rho_0 W^2)']_{p=0} = 2N_k N_m F^0_{km} w. \quad (6.3)$$

In view of Eqs. (5.14) and (5.15), the general result (6.3) can be expanded to the form

$$(\rho_0 V^2)'_{p=0} = N_r N_s U_j^0 U_k^0 [\delta_{jk} t_{rs}'(0) + 2N_i N_m F^0_{im} C^S_{jrst} \\ + 2F^0_{qk} C^S_{jrqs} + F^0_{ip} C_{jrstip}], \quad (6.4)$$

where, as before, all quantities are evaluated at  $p=0$ .

Equation (6.4) differs from a formula published previously<sup>7</sup> because the previous formula is for propagation along a given material line, whereas the present formula is for propagation normal to a given material plane. The two formulas give the same result whenever the normal direction to the material plane continues to lie along the same material line, or when  $\mathbf{N}$  is an eigenvector of the second rank tensor  $F^0_{im}$  defined in Eq. (5.16). This is true for all of the special cases previously worked out, and will frequently be true in future experiments. In this case, Eq. (6.3) can be simplified:

TABLE IV. Isotropic medium.

Type of stress	Propagation direction N	Mode <sup>a</sup>	Displacement direction U	$w \equiv (\rho_0 V^2)_{p=0}$	$(\rho_0 W^2)'$
Hydrostatic pressure	arbitrary	L	to N	$c_{11}^S = \lambda^S + 2\mu$	$-1 - \frac{1}{3B}(2w + 3\nu_1 + 10\nu_2 + 8\nu_3)$
Hydrostatic pressure	arbitrary	S	⊥ to N	$c_{44} = \mu$	$-1 - \frac{1}{3B}(2w + 3\nu_2 + 4\nu_3)$
Uniaxial compression	⊥ to stress	L	to N	$c_{11}^S = \lambda^S + 2\mu$	$\frac{1}{E}[\sigma(2w + 8\nu_3) + \nu_1(2\sigma - 1) + \nu_2(8\sigma - 2)]$
Uniaxial compression	⊥ to stress	S	to stress	$c_{44} = \mu$	$\frac{1}{E}[-2w + \nu_2(2\sigma - 1) + 2\nu_3(\sigma - 1)]$
Uniaxial compression	⊥ to stress	S	⊥ to stress	$c_{44} = \mu$	$\frac{1}{E}[\sigma(2w + 4\nu_3) + \nu_2(2\sigma - 1)]$

<sup>a</sup> L = longitudinal, S = shear;  $B = \lambda^T + \frac{2}{3}\mu$  = isothermal bulk modulus;  $E = 1/s_{11}^T = 3\mu B/(\lambda^T + \mu)$  = isothermal Young's modulus;  $\sigma = -s_{12}^T/s_{11}^T = \lambda^T/2(\lambda^T + \mu)$  = isothermal Poisson's ratio.

When N is an eigenvector of  $F_{km}^0$ ,

$$[(\rho_0 V^2)' - (\rho_0 W^2)']_{p=0} = 2F_{N^0} w, \quad (6.5)$$

where  $F_{N^0}$  is the eigenvalue of  $F_{km}^0$  belonging to N.

Because early workers<sup>1,2</sup> have reported values of  $(\rho V^2)'$ , we note that at  $p=0$ ,

$$\begin{aligned} (\rho V^2)' - (\rho_0 V^2)' &= -\left(\rho_0 V^2 \frac{dJ}{dp}\right)_{p=0} \\ &= -(\rho_0 V^2 s^T_{iia b' a b'})_{p=0}. \end{aligned}$$

Of course the same formula also holds with  $V$  replaced by  $W$ .

### 7. RELATIONS FOR CUBIC CRYSTALS AND ISOTROPIC MEDIA

The elastic coefficients of the  $n$ th order are tensors of order  $2n$ . They must be invariant under the symmetry operations of the point group of the crystal. This condition requires certain coefficients to vanish and supplies relations among some of the remaining ones. The second- and third-order coefficients have been exhaustively treated and the results are tabulated for all point groups.<sup>14</sup> For the cubic point groups  $O$ ,  $O_h$  and  $T_d$ , one has in the abbreviated notation of the following paper<sup>5</sup> for the second order:

$$\begin{aligned} c_{11} &= c_{22} = c_{33}, \\ c_{12} &= c_{23} = c_{13}, \\ c_{44} &= c_{55} = c_{66}, \end{aligned} \quad (7.1)$$

and all others zero,

<sup>14</sup> See for example, W. P. Mason, *Piezoelectric Crystals and Their Application to Ultrasonics* (D. Van Nostrand Company, Inc., New York, 1950) for second-order coefficients; and R. F. S. Hearman, *Acta Cryst.* **6**, 331 (1953) for third-order stiffnesses.

and for the third order:

$$\begin{aligned} C_{111} &= C_{222} = C_{333}, \\ C_{144} &= C_{255} = C_{366}, \\ C_{112} &= C_{223} = C_{133} = C_{113} = C_{122} = C_{233}, \\ C_{155} &= C_{244} = C_{344} = C_{166} = C_{266} = C_{355}, \\ C_{123}, \\ C_{456}, \end{aligned} \quad (7.2)$$

and all others zero.

For isotropic media, the above three second-order coefficients and six third-order coefficients have the following representation in terms of the Lamé coefficients of second order  $(\lambda, \mu)$ , and third order<sup>9</sup>  $(\nu_1, \nu_2, \nu_3)$ :

$$\begin{aligned} c_{11} &= \lambda + 2\mu, & c_{12} &= \lambda, & c_{44} &= \mu, \\ C_{123} &= \nu_1, & C_{144} &= \nu_2, & C_{456} &= \nu_3, \\ C_{112} &= \nu_1 + 2\nu_2, & C_{155} &= \nu_2 + 2\nu_3, & C_{111} &= \nu_1 + 6\nu_2 + 8\nu_3. \end{aligned} \quad (7.3)$$

Values of  $w$  and  $(\rho_0 W^2)'_{p=0}$  for various cases in cubic crystals belonging to the point groups  $O$ ,  $O_h$ , and  $T_d$  are given in Tables I–III. The corresponding formulas for  $(\rho_0 V^2)'$  and  $(\rho V^2)'$  are consistent with formulas already in the literature.<sup>1,2,7</sup> The new definitions should be noted.<sup>5</sup>

Special formulas for isotropic media are given in Table IV. The corresponding formulas for  $(\rho_0 V^2)'$  agree with those given by Toupin and Bernstein<sup>9</sup> if one sets  $\lambda^T = \lambda^S = \lambda$ .

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