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Method for the Determination of Elastic Constants of Trigonal Crystal Systems*

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Expressions are given which relate the propagation velocities of mechanical waves to the elastic constants in single crystals of trigonal symmetry (characterized by six elastic constants). These expressions derive from the Christoffel equations without introduction of approximations. It is also shown how the expressions can be employed to evaluate the elastic constants in a relatively simple, straightforward manner from ultrasonic measurements.

1. Introduction

A number of experimental methods exists for the determination of the elastic constants and elastic moduli of single crystals. The velocities with which ultrasonic waves are propagated along certain crystallographic directions are frequently used to deduce the elastic constants. The relationship between measured velocities and elastic constants is given by the Christoffel equations. The general form of these equations is applicable to any crystalline system; however, manipulation of the equations is quite involved for all but the most simple crystallographic groups. Therefore, various simplifying schemes have been developed to deal with the Christoffel equations. Bhimasenachar (1945) describes a method which, when applied to the trigonal system, gives approximate values for some of the elastic constants because small coupling terms in the Christoffel equations are omitted. Another method is described by Arenberg (1950) who makes use of a perturbation expansion which is exact in the limit and applies to any crystallographic direction. This approach is further investigated by Neighbours & Smith (1950).

In this communication we develop for the trigonal group (six elastic constants) relatively simple expressions which derive from the Christoffel equations without introduction of approximations. We also show how these expressions can be employed for the evaluation of the elastic constants from ultrasonic measurements.

2. Theory

Three displacement vectors can be associated with an elastic wave propagated in an anisotropic medium. These vectors relate to three different modes of vibration which are propagated with three distinct velocities. In general, one of these modes represents a predominantly longitudinal wave whereas the other two represent predominantly shear waves. Pure waves can be propagated only in very special crystallographic directions.

Let the direction of wave propagation in a single crystal have direction cosines l, m, n with respect to a Cartesian coordinate system attached to the crystal in the usual way, as described by Cady (1946). The three possible wave velocities V can, in principle, be found in terms of the elastic constants C_{pq} from the roots of the secular polynomial of the Christoffel equations

$$\begin{vmatrix} \varphi_{11}-\varrho V^2 & \varphi_{12} & \varphi_{13} \\ \varphi_{12} & \varphi_{22}-\varrho V^2 & \varphi_{23} \\ \varphi_{13} & \varphi_{23} & \varphi_{33}-\varrho V^2 \end{vmatrix} = 0 \qquad (1)$$

where ϱ is the density, and where the φ_{ab} are defined as

$$\varphi_{ab} = l^2 C_{1a1b} + m^2 C_{2a2b} + n^2 C_{3a3b} + lm(C_{1a2b} + C_{2a1b}) + ln(C_{1a3b} + C_{3a1b}) + mn(C_{2a3b} + C_{3a2b}) . \qquad (2)$$

The constants C_{ijkl} can be written in the usual form C_{pq} by replacing the suffixes $ij, kl = 11, 22, 33, 23, 13, 12$ by $p, q = 1, 2, \ldots, 6$. Expressions for the φ_{ab} for a particular crystal group can be written down by substituting the C_{pq} from the appropriate matrix of elastic constants given in standard reference treatises.

For a number of crystallographic systems, some of the φ_{ab} vanish if two of the direction cosines equal zero. Some of the C_{pq} can then be obtained quite readily. However, the determination of the remaining C_{pq} is possible only if additional velocity measurements are made in directions for which at least two of the direction cosines are different from zero. In this case, (1) usually becomes quite difficult to deal with directly.

Now, the secular determinant equation (1), if expanded, is of the form

$$F^3 + a_1 F^2 + a_2 F + a_3 = 0 , \qquad (3)$$

where $F = \varrho V^2$. It is known from theory of equations* that

$$a_1 = -S_1 \qquad (4)$$

and

$$a_2 = -\tfrac{1}{2}S_2 + \tfrac{1}{2}S_1^2 , \qquad (5)$$

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* See, for example, L. E. Dickson, *First Course in the Theory of Equations* (John Wiley & Sons, Inc., New York, 1931).

where

$$S_1 = \varrho(V_1^2 + V_2^2 + V_3^2)\ , \tag{6}$$

and

$$S_2 = \varrho^2(V_1^4 + V_2^4 + V_3^4)\ . \tag{7}$$

It remains to solve (4) and (5) for S_1 and S_2 in terms of a_1 and a_2, and to compute a_1 and a_2 for a given crystal group from (1). There results then a relationship between quantities which can be determined from experiment (namely, S_1 and S_2) and the elastic constants C_{pq}.

For crystals with trigonal symmetry (six elastic constants) one has

$$\begin{aligned}
\varphi_{11} &= l^2C_{11} + m^2C_{66} + n^2C_{44} + 2mnC_{14}\\
\varphi_{22} &= l^2C_{66} + m^2C_{11} + n^2C_{44} - 2mnC_{14}\\
\varphi_{33} &= l^2C_{44} + m^2C_{44} + n^2C_{33}\\
\varphi_{12} &= 2lnC_{14} + lm(C_{11} - C_{66})\\
\varphi_{13} &= ln(C_{13} + C_{44}) + 2lmC_{14}\\
\varphi_{23} &= (l^2 - m^2)C_{14} + mn(C_{13} + C_{44})\ .
\end{aligned} \tag{8}$$

Proceeding as outlined above, we find for the trigonal group that

$$S_1 = C_{11} + C_{44} + C_{66} + n^2(C_{33} + C_{44} - C_{11} - C_{66}) \tag{9}$$

and

$$\begin{aligned}
S_2 = {} & n^4C_{33}^2 + (1 + n^4)C_{44}^2 + (1 - n^2)^2(C_{11}^2 + C_{66}^2 + 2C_{14}^2)\\
& + 2n^2(1 - n^2)[C_{13}^2 + 4C_{14}^2 + C_{44}(C_{11} + C_{33} + C_{66} + 2C_{13})]\\
& - 4mn(m^2 - 3l^2)C_{14}(C_{11} + C_{44} + C_{13} - C_{66})\ .
\end{aligned} \tag{10}$$

3. Application

As an example of the use of (9) and (10) we calculate the elastic constants of sapphire from a set of velocity measurements reported by Wachtman *et al.* (1960). These measurements were made in the directions specified by the direction cosines l, m, n, given in Table 1.

Table 1. *Direction cosines of measurements by Wachtman et al.*

Direction of measurements	Direction cosines l	m	n
(X)	1	0	0
(Y)	0	1	0
(Z)	0	0	1
(45)	0	$1/\sqrt{2}$	$1/\sqrt{2}$
(135)	0	$1/\sqrt{2}$	$-1/\sqrt{2}$

For direction (Z), (9) reduces to

$$S_1(Z) = C_{33} + 2C_{44} = \varrho[V_1^2(Z) + V_2^2(Z) + V_3^2(Z)]\ . \tag{11}$$

Since for direction (Z), equation (1) is diagonal, one finds immediately that $V_2(Z) = V_3(Z)$, $C_{33} = \varrho V_1^2(Z)$, $C_{44} = \varrho V_2^2(Z)$. Also,

$$S_1(X) = C_{11} + C_{44} + C_{66} = \varrho[V_1^2(X) + V_2^2(X) + V_3^2(X)]\ , \tag{12}$$

and $C_{11} = \varrho V_1^2(X)$. With C_{11} and C_{44} known, C_{66} follows from (12). Now C_{13} and C_{14} still need to be determined. It follows from (10) that

$$S_2(X) = S_2(Y) = C_{44}^2 + 2C_{14}^2 + C_{11}^2 + C_{66}^2\ , \tag{13}$$

and in this expression only C_{14}^2 is unknown. To infer the sign of C_{14} one may consider

$$S_2(45) - S_2(135) = -2C_{14}(C_{11} + C_{44} + C_{13} - C_{66})\ , \tag{14}$$

where

$$\begin{aligned}
S_2(45) - S_2(135) = {} & \varrho^2[V_1^4(45) + V_2^4(45) + V_3^4(45)]\\
& - \varrho^2[V_1^4(135) + V_2^4(135) + V_3^4(135)]\ .
\end{aligned} \tag{15}$$

From the data one finds whether $S_2(45) > S_2(135)$ or $S_2(45) < S_2(135)$, i.e. whether the right-hand side of (14) is positive or negative. Considering the possible magnitudes of the constants one sees that the terms in brackets of the right-hand side of (14) usually represent a positive quantity.* Therefore, if $S_2(45) < S_2(135)$, $C_{14} > 0$, and if $S_2(45) > S_2(135)$, $C_{14} < 0$. With C_{14} determined, the value of C_{13} follows from (14).

Numerical evaluation is thus straightforward. From (11) one obtains $C_{33} = 4{\cdot}981$ and $C_{44} = 1{\cdot}474$. (These and subsequent values of the elastic constants are in units of 10^{12} dynes/cm.^{2}). Equation (12) yields $C_{11} = 4{\cdot}968$ and $C_{66} = 1{\cdot}666$. From (13) one finds $C_{14} = \pm 0{\cdot}22$, and since $S_2(45) = 28{\cdot}279$ and $S_2(135) = 25{\cdot}484$, it follows that $C_{14} = -0{\cdot}22$. From (14) the value of C_{13} is then 1·57. The results agree satisfactorily with those cited by Wachtman *et al.* The value of C_{13} given here is higher than that quoted by Wachtman, $C_{13} = 1{\cdot}109 \pm 0{\cdot}022$. However, changing the appropriate values of 'calculated velocities' cited by Wachtman by approximately 0·1% yields $C_{13} = 1{\cdot}05$. Thus it must be noted that the values of C_{13} and C_{14} are rather sensitive to the accuracy of velocity data.

The general method given here can be applied to other crystal systems as well. A note giving appropriate equations is in preparation.

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* It is conceivable that the terms in brackets of the right-hand side of (14) represent a negative quantity rather than a positive quantity. However, if both possibilities are considered numerically, one possibility usually leads to inconsistencies and can be discarded. See, for example, Alers & Neighbours (1957). *J. Appl. Phys.* **28**, 1514; Fisher & McSkimin (1958). *J. Appl. Phys.* **29**, 1473.