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Method for the Determination of Elastic Constants for Some Crystallographic Groups*

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Expressions are given relating the velocities with which mechanical vibrations are propagated in single crystals of various symmetries to the appropriate elastic constants. Symmetries considered are: trigonal (seven elastic constants), trigonal (six elastic constants), hexagonal, tetragonal (seven elastic constants), tetragonal (six elastic constants), and cubic. The expressions given derive from the Christoffel equations without introduction of approximations.

In a previous communication Mayer & Parker (1961) have described a method which, in principle, allows evaluation of the elastic constants of single crystals belonging to the trigonal group (six elastic constants) from ultrasonic velocity measurements along a set of selected crystallographic directions. In the present paper we extend this method to other crystallographic groups; we use the general theory and notation established in the previous paper. As before, $S_1 = \varrho(V_1^2+V_2^2+V_3^2)$, $S_2=\varrho^2(V_1^4+V_2^4+V_3^4)$, where ϱ is the density, and V_1, V_2, V_3 are the possible velocities of propagation of mechanical waves along a given direction.

1. Trigonal system (seven elastic constants)

For trigonal systems whose first order elastic properties are described by seven independent elastic constants $C_{11}, C_{33}, C_{44}, C_{66}, C_{13}, C_{14}, C_{25}$ with $C_{66}=\frac{1}{2}(C_{11}-C_{12})$, we find

$$S_1=C_{11}+C_{44}+C_{66}+n^2(C_{33}+C_{44}-C_{11}-C_{66}) . \quad (1)$$

$$S_2=n^4C_{33}^2+(1+n^4)C_{44}^2+(1-n^2)^2A+2n^2(1-n^2)B -4mn(m^2-3l^2)D-4\,ln\,(l^2-3m^2)E\,, \quad (2)$$

where

$$A = (C_{11}+C_{66})^2-2C_{11}C_{66}+2(C_{14}^2+C_{25}^2)\,, \quad (3)$$

$$B = C_{13}^2+4(C_{14}^2+C_{25}^2)+C_{44}(C_{11}+C_{66}+C_{33}+2C_{13}), \quad (4)$$

$$D = C_{14}(C_{11}+C_{44}+C_{13}-C_{66})\,, \quad (5)$$

$$E = C_{25}(C_{11}+C_{44}+C_{13}-C_{66})\,. \quad (6)$$

There are many ways in which information about the elastic constants may be obtained from (1) and (2). A *possible* procedure is as follows: for direction $[l, m, n]=[0, 0, 1]$ the Christoffel determinant is diagonal and immediately gives C_{33} and C_{44}. For any direction for which $n=0$, e.g., for $[1, 0, 0]$ or for $[0, 1, 0]$, equation (1) gives the numerical value of $(C_{11}+C_{66})$, and equation (2) gives the numerical value of A. Then, equation (2) applied to two different directions for which $l=m\neq0$, $n\neq0$ yields B.† Next, equation (2) applied to a direction such that $l=0$, $m\neq0$, $n\neq0$ gives D; and equation (2) applied to a direction such that $l\neq0$, $m=0$, $n\neq0$ gives E. With A, B, D, and E known, and with the value of $(C_{11}+C_{66})$ known, we have five relations among five elastic constants from which these constants can be determined. Unfortunately, these relations are relatively complicated, and it is perhaps of advantage to consider the following auxiliary procedure. From theory of equations it is known that the product of the three roots of the Christoffel determinant, namely, $\varrho^3V_1^2V_2^2V_3^2$ is equal to the constant term of the secular equation (if the coefficient of the $(\varrho V^2)^3$ term is -1). Application of this theorem shows that

$$\varrho^3V_1^2V_2^2V_3^2=C_{11}C_{44}C_{66}-C_{25}^2C_{66}-C_{14}^2C_{11}\,, \quad \text{for direction } [1, 0, 0] \quad (7)$$

and

$$\varrho^3V_1^2V_2^2V_3^2=C_{11}C_{44}C_{66}-C_{25}^2C_{11}-C_{14}^2C_{66}\,, \quad \text{for direction } [0, 1, 0]\,. \quad (8)$$

The sum of these relations is

$$\sigma=2C_{44}(C_{11}C_{66})-(C_{14}^2+C_{25}^2)(C_{11}+C_{66}) \quad (9)$$

in which C_{44} and $(C_{11}+C_{66})$ are known quantities, and σ can be determined from experiment. Solution of equation (9) for $(C_{14}^2+C_{25}^2)$ and substitution into equation (3) yields an equation from which the numerical value of $C_{11}C_{66}$ can be determined. Since $C_{11}+C_{66}$ is known, C_{11} and C_{66} can now be found. These can be determined uniquely, since $C_{11}>0$, $C_{66}>0$. Furthermore, $C_{14}^2+C_{25}^2$ now follows from equation (3), and the ratio C_{14}/C_{25} follows from equa-

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† Equation (2) applied to two different directions for which $l=-m\neq0$, $n\neq0$ will also yield B.

tions (5) and (6). This allows calculation of C_{14} and C_{25} apart from an ambiguity in sign. Also, equation (4) is now a quadratic equation in C_{13} which yields two possible values for C_{13}. Returning to equations (5) and (6), that root of C_{13} and those signs of C_{14} and C_{25} are chosen which make equations (5) and (6) self-consistent. With the constants determined in this manner, one may now return to equations (3) through (6) and calculate the values of the constants without the use of the auxiliary equation (9). This will improve the accuracy of the result, since the experimental error range affects equation (9) more seriously than equation (2).

As remarked in our previous paper, the numerical values of some of the elastic constants determined in the above way are rather sensitive to the accuracy of velocity data. It is, therefore, advantageous, in general, to overdetermine the elastic constants by making measurements in more than the minimum number of directions required, and thus to reduce the error range.

2. Trigonal system (six elastic constants)

This is the system treated in the previous paper. We include it here for the sake of completeness, and also because the procedure for the evaluation of the elastic constants previously given was necessarily limited by the nature of the data of Wachtman *et al.* (1960). A set of independent elastic constants is C_{11}, C_{33}, C_{44}, C_{66}, C_{13}, C_{14}. Equations (1) through (6) apply with $C_{25}=0$. A possible procedure is as follows: for directions [1, 0, 0], [0, 1, 0], and [0, 0, 1] the Christoffel determinant yields directly C_{11}, C_{33}, C_{44}, and C_{66}. From the S_2 equation, and with $l=1$ or $m=1$ one obtains the value of C_{14}^2. Then, the S_2 equation applied to a direction for which $l\neq 0$, $m=0$, $n\neq 0$ gives the value of B, and subsequently, the S_2 equation applied to a direction for which $l=0$, $m\neq 0$, $n\neq 0$ gives the value of D. Equation (4) is then quadratic in C_{13}. With C_{13} known, equation (5) yields C_{14}. That value of C_{13} is used which gives a C_{14} whose square is the one determined previously.

3. Hexagonal system

A set of independent elastic constants is C_{11}, C_{33}, C_{44}, C_{66}, C_{13}. Equations (1) through (6) apply with $C_{25}=C_{14}=0$, i.e.,

$$S_1=C_{11}+C_{44}+C_{66}+n^2(C_{33}+C_{44}-C_{11}-C_{66})\ , \qquad (10)$$

$$S_2=n^4C_{33}^2+(1+n^4)C_{44}^2+(1-n^2)^2(C_{11}^2+C_{66}^2) +2n^2(1-n^2)B\ , \qquad (11)$$

where

$$B=C_{13}^2+C_{44}(C_{11}+C_{33}+C_{66}+2C_{13})\ . \qquad (12)$$

A possible procedure is as follows: directions [0, 0, 1] and [0, 1, 0] or [1, 0, 0] yield C_{11}, C_{33}, C_{44}, and C_{66} from the diagonal form of the Christoffel determinant. Then, any direction for which $n\neq 0$, $n\neq 1$ yields the numerical value of B from the S_2 equation. A quadratic equation in C_{13} results which gives two possible values for C_{13}. We encounter here the troublesome problem of extraneous calculated values for some of the elastic constants. This problem has been discussed by Alers & Neighbours (1957) and by Fisher & McSkimin (1958). As discussed there it is sometimes but not always possible to discard extraneous values on the grounds of stability criteria. Our *general* treatment here fails in this respect, although for a given crystal it may be feasible to make a reasonable choice between the two possibilities. It may be thought that consideration of the quantity $S_3=\varrho^3(V_1^6+V_2^6+V_3^6)$, for whose computation all three coefficients a_1, a_2, a_3 of the secular equation are utilized, may resolve the ambiguity in C_{13}. However, computation of S_3 shows that this is not so.

4. Tetragonal system (seven elastic constants)

A set of independent elastic constants is C_{11}, C_{33}, C_{44}, C_{66}, C_{12}, C_{13}, C_{16}; one finds

$$S_1=C_{11}+C_{44}+C_{66}+n^2(C_{33}+C_{44}-C_{11}-C_{66})\ , \qquad (13)$$

$$S_2=n^4C_{33}^2+(1+n^4)C_{44}^2+2n^2(1-n^2)A+(1-n^2)^2B +2l^2m^2D-2(l^4+m^4)E-4lm(m^2-l^2)F\ , \qquad (14)$$

where

$$A = C_{13}^2+C_{44}(C_{11}+C_{33}+C_{66}+2C_{13})\ , \qquad (15)$$

$$B = (C_{11}+C_{66})^2+2C_{16}^2\ , \qquad (16)$$

$$D = C_{12}^2-C_{11}^2+2C_{12}C_{66}\ , \qquad (17)$$

$$E = C_{11}C_{66}\ , \qquad (18)$$

$$F = C_{16}(C_{11}+C_{12})\ . \qquad (19)$$

From the principal directions [1, 0, 0], [0, 1, 0], and [0, 0, 1] one finds C_{33}, C_{44}, from equation (13) one finds $(C_{11}+C_{66})$. Since A, B, D, E, and F have different coefficients in equation (14), they can be found from the S_2 equation, again by making measurements along a number of properly chosen directions. (We give here no detailed procedure since there is no 'obvious' choice of directions in preference to others.) With A, B, D, E, and F known, and since $C_{11}>0$, $C_{66}>0$, E gives C_{11} and C_{66}. Then, from B, D, and F a self-consistent set of values for C_{12} and C_{16} can be determined. Finally, A yields the value of C_{13} (two roots). This ambiguity cannot be resolved by consideration of S_3.

5. Tetragonal system (six elastic constants)

A set of independent elastic constants is C_{11}, C_{33}, C_{44}, C_{66}, C_{12}, C_{13}. Equations (13) through (19) apply with $C_{16}=0$. For directions [1, 0, 0], [0, 1, 0], and [0, 0, 1] the diagonal forms of the Christoffel determinant give C_{11}, C_{33}, C_{44}, and C_{66}. For a direction $l \neq 0$, $m \neq 0$, $n=0$, the S_2 equation yields D, from which C_{12} can be determined (two roots). Subsequent application of the S_2 equation to any direction $n \neq 0$, $\neq 1$ yields the value of A from which C_{13} can be determined (two roots). Consideration of the S_3 equation shows that the ambiguity in C_{12} can be resolved, but not the ambiguity in C_{13}. To be specific, in the S_3 equation there occurs a term $l^2m^2n^2(C_{12}+C_{66})(C_{13}+C_{44})^2$. Since $(C_{13}+C_{44})^2$ is known from A, a unique value of C_{12} can be found. However, the only combination in which C_{13} occurs in S_3 is $(C_{13}+C_{44})^2$ so that no further information about C_{13} beyond that contained in equation (14) is obtained. The ambiguity in C_{13} remains.

6. Cubic system and isotropic substances

For the cubic system a set of independent elastic constants is C_{11}, C_{44}, C_{12}. The evaluation of these constants from velocity measurements is rather straightforward; the Christoffel equations yield them readily. Nevertheless, we include here the S_1 and S_2 equations. Equations (13) through (19) apply with $C_{33}=C_{11}$, $C_{66}=C_{44}$, $C_{13}=C_{12}$, and $C_{16}=0$. After some rearrangement,

$$S_1=C_{11}+2C_{44}\,, \tag{20}$$

$$S_2=C_{11}^2+2C_{44}^2+2[n^2(1-n^2)+l^2m^2] \times[(C_{12}+C_{44})^2-(C_{11}-C_{44})^2]\,. \tag{21}$$

For C_{12} two roots are obtained from equation (21). The S_3 equation contains a term in $(C_{12}+C_{44})^3$, hence the ambiguity in C_{12} is resolvable.

The approach given here must also be correct for isotropic substances. Setting $C_{11}=\lambda+2\mu$, $C_{44}=\mu$, $C_{12}=\lambda$, it is seen that

$$S_1=\lambda+4\mu\,, \tag{22}$$

$$S_2=\lambda^2+6\mu^2+4\lambda\mu\,, \tag{23}$$

which is consistent with $\varrho V_1^2=\lambda+2\mu$, $\varrho V_2^2=\mu=\varrho V_3^2$.

7. Concluding remarks

Implications arising from the form of S_1 for a number of crystallographic groups have already been discussed by Haussühl (1956, 1957, 1957*a*). Our discussion here is along the lines of Haussühl's observations.

It is well known that V_1 and V_2 are independent of direction of propagation in isotropic media. Therefore, neither S_1 nor S_2 contain direction cosines l, m, n. In the cubic system V_1, V_2 and V_3 are not independent of direction of propagation. Yet the expression for S_1 does not contain l, m or n. This implies that the sum of the squares of the velocities $(V_1^2+V_2^2+V_3^2)$ is a constant for any direction of propagation despite the fact that the individual values of the velocities vary with direction. For more complicated systems (up to but not including rhombic) the sum of the squares of the velocities is constant only for a given direction cosine $\pm n$. Therefore, for the cubic system the sum of the propagation velocities is an invariant, and the end point of the propagation vector may lie anywhere on a sphere around the origin (i.e. any possible combination of l, m, n) for the sum of the squares of the velocities to be an invariant. For the other systems discussed here the wave propagation vector may describe cones around the Z axis (i.e. a given $|n|$ regardless of the possible l and m) for the sum of the squares of the velocities to remain constant.

These properties can be helpful from the experimental point of view. If the three velocities are determined in a certain direction, only two velocities have to be measured in a direction described by the same $|n|$ in order to compute the third velocity. For the cubic system this scheme may be used for any direction whatsoever, either as a means of finding an undetermined velocity or simply as a check for consistency. For more complicated symmetries the expressions for S_1 depend on l, m and n, and the sum of the squares of the velocities is no longer constant for a given $|n|$.

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