EVALUATION OF TWO METHODS FOR THE DETERMINATION OF THE ELASTIC CONSTANTS OF TRIGONAL CRYSTALS

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ABSTRACT

Two procedures for the computation of the elastic constants (trigonal system) from measured values of elastic wave velocities are discussed. The simplified procedure first used by Bhimasenachar is incorrect in principle although, in very rare cases, it may lead to only small numerical errors. A new procedure is mentioned which simplifies the use of the Christoffel equations in an exact way.

INTRODUCTION

The velocity with which ultrasonic waves are propagated in various directions in a single crystal has been used repeatedly to determine the elastic constants and elastic moduli of various substances. Christoffel’s equations are ordinarily used to obtain the relationship between the velocities of the three possible waves in certain directions and the values of the elastic constants. In most cases, however, the mathematical formulation becomes rather involved, and possibilities to simplify the algebra have been considered in the past. Some simplifying expressions are given by Bhimasenachar\(^1,2\) which are based on a rotation of the co-ordinate system and on the assumption that small coupling terms can be neglected. Sundara Rao\(^3\) gives a set of simplified formulas for the trigonal system which reduces to Bhimasenachar’s formulation. Mayer and Hiedemann\(^4\) give a detailed description of the above-mentioned approach, and in a later communication\(^5\) they point out that the approximate approach is incorrect in principle.

Another simplifying method was given by Mayer and Parker\(^6\) for the trigonal system. This method of evaluation derives from the Christoffel equations but does not introduce approximations. The present communication indicates the reasons why, in general, the approximate method will not give reliable results and how the procedure proposed by Mayer and Parker can be used to test certain results obtained with the approximate method.
DISCUSSION

In the exact formulation of the problem one solves the Christoffel equation for the $C_{pq}$ from the measured values of the three roots $\rho V^2$. The approximate method uses a transformation, and one obtains values of $C_{33}'$ and $C_{44}'$ in terms of the constants $C_{pq}$ where one expression for $C_{33}'$ and two expressions for $C_{44}'$ are found corresponding to the three possible values of $\rho V^2$. However, since small coupling terms are neglected, the values of the elastic constants (for the trigonal system) $C_{12}$, $C_{13}$ and $C_{14}$, will only be approximations because the transformation is incomplete.* A specific example of the form of the resulting determinants is given in the Appendix.

The transformation used to obtain the approximate expressions gives mathematically correct results only for the case where a pure longitudinal and pure shear waves are present. There may, however, be very special cases where the approximate and the exact method give results in rather good agreement. The calculation of the elastic constants for sapphire from ultrasonic velocity measurements show good agreement, as shown in Table I.

<table>
<thead>
<tr>
<th>( C_{11} )</th>
<th>( C_{33} )</th>
<th>( C_{44} )</th>
<th>( C_{12} )</th>
<th>( C_{13} )</th>
<th>( C_{14} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approximation ..</td>
<td>( 4.96 )</td>
<td>( 5.02 )</td>
<td>( 1.41 )</td>
<td>( 1.36 )</td>
<td>( 1.20 )</td>
</tr>
<tr>
<td>Exact Method ..</td>
<td>( 4.96 )</td>
<td>( 5.02 )</td>
<td>( 1.41 )</td>
<td>( 1.35 )</td>
<td>( 1.17 )</td>
</tr>
</tbody>
</table>

However, the differences may be appreciably greater for other crystals with trigonal symmetry. In general, one cannot predict how great an error will be introduced in the $C_{pq}$ if the approximate method is used. It can be shown that the two determinants (exact and approximate method) are mathematically identical only with certain restrictions on the magnitudes of various constants as pointed out in the Appendix. These restrictions can be obtained if the determinants for certain propagation directions are compared.

The second condition is also quoted by Wachtman and co-workers.\(^7\) The last restriction is identical to the hypothetical condition given by Borgnis\(^8\); under this condition it would be possible to propagate pure longitudinal and

* A. J. deWitte, private communication.
TABLE II

Conditions for agreement of exact and approximate formulas

<table>
<thead>
<tr>
<th>l</th>
<th>m</th>
<th>n</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>none</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>(C_{14} = 0)</td>
</tr>
<tr>
<td>0</td>
<td>1/\sqrt{2}</td>
<td>±1/\sqrt{2}</td>
<td>(C_{14} = 0, C_{11} = C_{33})</td>
</tr>
<tr>
<td>1/\sqrt{2}</td>
<td>0</td>
<td>±1/\sqrt{2}</td>
<td>(C_{14} = 0, C_{11} = C_{33}, 2C_{44} = C_{11} - C_{13})</td>
</tr>
</tbody>
</table>

pure shear waves in an arbitrary direction (for the trigonal system), however, trigonal symmetry would no longer exist in such a hypothetical case.

It is therefore necessary to compare the results of the approximate method with those of exact equations. This procedure eliminates the usefulness of the approximate method.

The appropriate relations between velocities and elastic constants can be obtained quite readily by applying the method proposed by Parker and Mayer\(^6\) which, for the trigonal system yields\(^6\)

\[
S_1 = \rho (V_1^2 + V_2^2 + V_3^2) = C_{11} + C_{44} + C_{66} + n^2 (C_{33} + C_{44}) - C_{11} - C_{66}). \tag{1}
\]

A similar equation for \(\rho^2 (V_1^4 + V_2^4 + V_3^4)\) contains the missing constants.

These equations are sufficient to obtain the elastic constants from the necessary set of velocity measurements. Moreover, they can also be used to verify the accuracy of the values of \(C_{pq}\) obtained by other techniques. If one substitutes the elastic constants into these equations together with the values for \(V\) measured in a particular direction, one must be able to balance Eq. (1).

It is also obvious from Eq. (1) that \(S_1\) depends only on one variable quantity, \(n^2\). Therefore the value of \(\rho (V_1^2 + V_2^2 + V_3^2)\) is fixed for any \(k\) on a given cone described by \(|n|\) as shown in Fig. 1. Although the individual
velocities may differ for the various propagation directions with a given $|n|$, the sum of their squares must be equal, regardless of the value of $l$ or $m$.

**Fig. 1**

**CONCLUSION**

It is shown why, in general, the approximate method cannot be expected to yield valid results for the elastic constants of trigonal crystals despite the fact that in very special cases the results may be sufficiently accurate. A new, simplified yet exact procedure is mentioned which not only gives the elastic constants but allows certain consistency tests concerning the accuracy of ultrasonic velocity measurements.

**ACKNOWLEDGMENT**

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**REFERENCES**


APPENDIX

The Christoffel determinant for the trigonal system with the wave vector $k$ in the XZ plane for the direction cosines $l = n = 1/\sqrt{2}$, $m = 0$ is given by

$$\begin{vmatrix}
\frac{1}{2} (C_{11} + C_{44}) - \rho V^2 & C_{14} & \frac{1}{2} (C_{13} + C_{44}) \\
C_{14} & \frac{1}{2} (C_{44} + C_{66}) - \rho V^2 & \frac{1}{2} C_{14} \\
\frac{1}{2} (C_{13} + C_{44}) & \frac{1}{2} C_{14} & \frac{1}{2} (C_{33} + C_{44}) - \rho V^2
\end{vmatrix} = 0. \quad (1)$$

For the same crystallographic direction the approximate method yields the three values

$$\rho V^2 = C_{33}' = \frac{1}{4} (C_{11} + C_{33} + 4C_{44} + 2C_{13}),$$

$$\rho V^2 = C_{44}' = \frac{1}{4} (C_{44} + C_{66}),$$

$$\rho V^2 = C_{66}' = \frac{1}{4} (C_{11} + C_{33} - 2C_{13}). \quad (2a, b, c)$$

which results in the approximate determinant

$$\begin{vmatrix}
\frac{1}{4} (C_{11} + C_{33} + 4C_{44} + 2C_{13}) - \rho V^2 & 0 & 0 \\
0 & \frac{1}{2} (C_{44} + C_{66}) - \rho V^2 & 0 \\
0 & 0 & \frac{1}{4} (C_{33} + C_{44} - 2C_{13}) - \rho V^2
\end{vmatrix} = 0. \quad (3)$$

If Equations (1) and (3) are compared one finds that the two determinants are equal only if certain restrictions are placed on some $C_{pq}$. Equation (3) is equivalent to Equation (1) if

$$C_{11} = C_{33}; \quad 2C_{44} = C_{11} - C_{13}; \quad C_{14} = 0.$$ 

Comparing the two determinants for other directions yields restrictions on some $C_{pq}$ which are listed in Table II above. Of the directions listed only one ($l = m = 0$, $n = 1$) yields the same determinant for both the exact and the approximate method. This one would expect since the off-diagonal terms vanish in either case.