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# A Method for Determining the Elastic Constants of a Cubic Crystal from Velocity Measurements in a Single Arbitrary Direction; Application to $SrTiO_3$

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Three independent velocities of sound can be measured along any direction of propagation in a cubic crystal except the [100] and [111] directions. These three velocities suffice to determine the three elastic constants and for the [110] direction, the calculation of these constants is easy. For all other directions, the calculation is more difficult; the only existing method appears to be a perturbation technique developed by Neighbours.

The present paper presents a method using exact equations and an iterative procedure to solve these equations and to calculate both the elastic constants and their standard deviations from the sound velocities and their standard deviations. The method is illustrated with new data on $SrTiO_3$ which give $c_{11}=3.156\pm0.027$, $c_{12}=1.027\pm0.027$, $c_{44}=1.215\pm0.006\times10^{12}$ dynes/cm² at 25 °C. The importance of including covariance terms in calculations of the standard deviations is emphasized.

## 1. Introduction

The determination of the elastic constants of single crystals from measurements of the velocity of sound is an extensive and active field of research and several survey papers exist [*1, 2, 3, 4*].[1] For any direction in a single crystal three types of sound wave may be propagated: one quasi-longitudinal and two quasi-transverse waves. The three corresponding velocities are the roots of a cubic equation, sometimes called Christoffel's equation, whose coefficients are complicated functions of the elastic constants and the direction cosines for the direction of propagation of the sound. In the case of a cubic crystal, there are only three independent elastic constants so that velocity measurements in a single direction suffice to completely determine the elastic constants provided that no two velocities are required to be equal by crystal symmetry. Such equality is required for the [100] and [111] directions so that measurements in one of these directions alone do not provide sufficient information to determine the three elastic constants. It may happen that for some other direction two of the velocities are equal; the three velocities are still independent quantities, however, and measurements in such a direction would provide sufficient information to calculate the three elastic constants. We assume that the three velocities $v_1$, $v_2$, $v_3$, and their standard deviations $\sigma_1$, $\sigma_2$, $\sigma_3$, have been measured for some direction which is specified by direction cosines $l$, $m$, $n$ and which does not coincide with or closely neighbor [100] or [111]. We seek to calculate the three independent elastic constants $c_{11}$, $c_{12}$, $c_{44}$ and their standard deviations $\sigma_{11}$, $\sigma_{12}$, $\sigma_{44}$. The theory leads to a sixth degree algebraic equation of which $c_{11}$ must be a root. It may occur that more than one of the roots of this equation are of reasonable magnitude so that some test is needed to distinguish which of the roots is $c_{11}$. The direction of polarization of the quasi-transverse waves provides such a test and we therefore assume that the orientation of the transducer exciting each of the two quasi-transverse waves was also determined.

One would usually prefer to use the [110] direction for which the calculations are easy and well known and for which the present method is unnecessary. However, single crystals of many substances are available only in very limited sizes and shapes and it may occur that the only available crystals do not permit measurement along [110]. Also, even if [110] is accessible for measurement, it may be desired to check the results by measurements in other directions.

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[1] Italicized figures in brackets indicate the literature references at the end of this paper.

Neighbours and his collaborators [*5, 6, 7*], following a beginning by Ahrenberg [*8*], have developed an approximation method for calculating elastic constants from wave velocities and have applied it to the case of cubic crystals as well as several other crystal systems. In Neighbours' method, the equations relating the velocities and the elastic constants are expanded into infinite series. The first term of each equation is a simple linear combination of elastic constants and the first step in his self-consistent calculation is to solve for the elastic constants ignoring all other terms. The values so obtained are used to calculate the largest of the remaining terms of the infinite series and a second set of values of the elastic constants is then calculated considering only the elastic constants of the first term as variables. This process is repeated as often as necessary to obtain the desired degree of accuracy. Successive sets of elastic constants calculated in this manner converge to a set which satisfies the chosen finite portions of Neighbours' expanded form of the velocity equations.

Presumably the next order terms could be calculated if greater accuracy were desired, but they apparently have not been given. The present method which uses exact equations thus provides a desirable alternative to Neighbours' method. The propagation-of-error theory could presumably be applied to Neighbours' method to calculate standard deviations, but this has apparently not been worked out. The present method includes such a calculation and this is worthy of note because the calculation involves quantities which are not statistically independent and serious errors can arise if the elementary propagation-of-error equations, which do not include covariance terms, are used. Any comparison of Neighbours' method with the present work should note the great utility and generality of the former which can be applied to crystals of any symmetry (if sufficient measurements are available) while the latter is strictly limited to cubic crystals.

## 2. Equations for Calculating Elastic Constants

The equations relating elastic constants to wave velocities are derived in many places; see, for example, Kolsky [*9*] for a treatment in conventional (matrix) notation and Farnell [*10*] for a brief sketch in tensor notation. The resulting secular equation can be written as an equation involving a $3 \times 3$ determinant using Farnell's notation as

$$|\Gamma_{jk}-\delta_{jk}x|=0 \tag{1}$$

where

$$x=\rho v^2 \tag{2}$$

$$\rho=\text{density},$$

$$v=\text{velocity},$$

and

$$\Gamma_{jk}=\frac{1}{2}\sum_{i,l}\alpha_i\alpha_l(c_{ijkl}+c_{ljki}) \tag{3}$$

In the last expression, the $\alpha_i$ are the direction cosines for the direction of propagation and the $c_{ijkl}$ are the elastic constants; both are referred to the crystal axes. Assuming cubic symmetry, writing $l$, $m$, $n$ for the direction cosines and using the conventional matrix notation for elastic constants, the $\Gamma_{jk}$ become

$$\Gamma_{11}=c_{11}l^2+c_{44}(m^2+n^2) \tag{4}$$

$$\Gamma_{22}=c_{11}m^2+c_{44}(l^2+n^2) \tag{5}$$

$$\Gamma_{33}=c_{11}n^2+c_{44}(l^2+m^2) \tag{6}$$

$$\Gamma_{12}=\Gamma_{21}=(c_{12}+c_{44})lm, \tag{7}$$

$$\Gamma_{13}=\Gamma_{31}=(c_{12}+c_{44})ln, \tag{8}$$

and

$$\Gamma_{23}=\Gamma_{32}=(c_{12}+c_{44})mn. \tag{9}$$

These values can be substituted into the secular equation to give a cubic equation in $x$. We assume that for a given direction $(l, m, n)$ the three velocities have been measured and the three corresponding values $x_1$, $x_2$, $x_3$, computed. Then for this direction the cubic equation obtained from the secular equation must factor into

$$(x-x_1)(x-x_2)(x-x_3)=0. \tag{10}$$

When this factored equation is multiplied out and the coefficients of each power of $x$ equated to the coefficient of the same power in the secular equation three simultaneous equations are obtained. To simplify these, let

$$\alpha=c_{11}, \tag{11}$$

$$\beta=c_{44}, \tag{12}$$

$$\gamma=c_{12}+c_{44}, \tag{13}$$

$$u=x_1+x_2+x_3, \tag{14}$$

$$v=x_1x_2+x_1x_3+x_2x_3, \tag{15}$$

and

$$w=x_1x_2x_3. \tag{16}$$

The three equations are

$$u=\alpha+2\beta, \tag{17}$$

$$\begin{aligned} v=&[\alpha l^2+\beta(l^2+m^2)][\alpha m^2+\beta(l^2+n^2)]\\ &+[\alpha l^2+\beta(l^2+m^2)][\alpha n^2+\beta(l^2+m^2)]\\ &+[\alpha m^2+\beta(l^2+n^2)][\alpha n^2+\beta(l^2+m^2)]\\ &-\gamma^2(l^2m^2+l^2n^2+m^2n^2), \end{aligned} \tag{18}$$

and

$$\begin{aligned} w=&[\alpha l^2+\beta(m^2+n^2)][\alpha m^2+\beta(l^2+n^2)][\alpha n^2+\beta(l^2+m^2)]\\ &+2\gamma^3l^2m^2n^2-\gamma^2\{l^2m^2[\alpha n^2+\beta(l^2+m^2)]\\ &+l^2n^2[\alpha m^2+\beta(l^2+n^2)]+m^2n^2[\alpha l^2+\beta(m^2+n^2)]\}. \end{aligned} \tag{19}$$

The problem is to solve for $\alpha$, $\beta$, and $\gamma$ from a known set of values of $u$, $v$, $w$, $l$, $m$, and $n$. The procedure is to use eq (17) to eliminate $\beta$ from eqs (18) and (19). Then use (18) to eliminate the $\gamma^2$ term from (19). This leaves one equation, derived from (18), which can be solved for $\gamma^2$ and one equation, derived from (19), which can be solved for $\gamma^3$. Cubing the first of these two equations and squaring the second allows the elimination of $\gamma$ and gives a 6th degree equation in $\alpha$. The coefficients in this equation are very long expressions when written out in full and it is much more convenient to define various functions of the starting quantities $(l, m, n, u, v, w)$ and so simplify the algebraic manipulations. We thus define

$$l_1=1-l^2, \tag{20}$$

$$m_1=1-m^2, \tag{21}$$

$$n_1=1-n^2, \tag{22}$$

$$l_2=3l^2-1, \tag{23}$$

$$m_2=3m^2-1, \tag{24}$$

$$n_2=3n^2-1, \tag{25}$$

$$e=l^2m^2+l^2n^2+m^2n^2, \tag{26}$$

$$f=l^2m^2n_2+l^2n^2m_2+m^2n^2l_2, \tag{27}$$

$$g=l_2m_2+l_2n_2+m_2n_2, \tag{28}$$

$$h=l_2m_2n_1+l_2n_2m_1+m_2n_2l_1, \tag{29}$$

$$j = l_2 m_1 + l_1 m_2 + l_2 n_1 + l_1 n_2 + m_2 n_1 + m_1 n_2, \tag{30}$$

$$k = l^2 m^2 n_1 + l^2 n^2 m_1 + m^2 n^2 l_1, \tag{31}$$

$$p = l_2 m_1 n_1 + l_1 m_2 n_1 + l_1 m_1 n_2, \tag{32}$$

$$q = l_1 m_1 + l_1 n_1 + m_1 n_1, \tag{33}$$

$$r = 2 l^2 m^2 n^2, \tag{34}$$

$$s = l_1 m_1 n_1, \tag{35}$$

$$s_1 = l_2 m_2 n_2, \tag{36}$$

$$g_1 = gf/e - s_1, \tag{37}$$

$$h_1 = (ugk + ujf)/e - hu, \tag{38}$$

$$j_1 = (u^2 jk + u^2 qf - 4vf)/e - u^2 p, \tag{39}$$

$$k_1 = uk(u^2 q - 4v)/e - u^3 s + 8w, \tag{40}$$

and

$$p_1 = u^2 q - 4v. \tag{41}$$

When (17) is used to eliminate $\beta$, eq (18) becomes

$$v = \alpha^2 g/4 + \alpha uj/4 + u^2 q/4 - \gamma^2 e, \tag{42}$$

and eq (19) becomes

$$w = \alpha^3 s_1/8 + \alpha^2 uh/8 + \alpha u^2 p/8 + u^3 s/8 + r\gamma^3 - \gamma^2(\alpha f + uk)/2. \tag{43}$$

Substituting for $\gamma^2$ from (42) into (43) gives

$$w = \alpha^3(s_1 e - gf)/8e + \alpha^2(ueh - ugk - ujf)/8e + \alpha(u^2 ep - u^2 jk - u^2 qf + 4vf)/8e + (u^3 es - u^3 kq + 4uvk)/8e + r\gamma^3. \tag{44}$$

Computing $64r^2\gamma^6/e^2$ from (42) and equating to the same quantity computed from (44) gives

$$a_6\alpha^6 + a_5\alpha^5 + a_4\alpha^4 + a_3\alpha^3 + a_2\alpha^2 + a_1\alpha + a_0 = 0 \tag{45}$$

where

$$a_0 = r^2 p_1^3/e^3 - k_1^2, \tag{46}$$

$$a_1 = 3ur^2 j p_1^2/e^3 - 2j_1 k_1, \tag{47}$$

$$a_2 = 3r^2(g p_1^2 + u^2 j^2 p_1)/e^3 - 2h_1 k_1 - j_1^2, \tag{48}$$

$$a_3 = r^2(6ugjp_1 + u^3 j^3)/e^3 - 2(g_1 k_1 + h_1 j_1), \tag{49}$$

$$a_4 = 3r^2(u^2 g j^2 + g^2 p_1)/e^3 - (2g_1 j_1 + h_1^2), \tag{50}$$

$$a_5 = 3ur^2 g^2 j/e^3 - 2g_1 h_1, \tag{51}$$

and

$$a_6 = r^2 g^3/e^3 - g_1^2. \tag{52}$$

The procedure for determining the elastic constants is thus as follows: Starting with the density, $\rho$, the velocities $v_1$, $v_2$, $v_3$ and the direction cosines $l$, $m$, $n$ first compute $x_1$, $x_2$, $x_3$ from (2), next compute $u$, $v$, $w$ from eqs (14) through (16), next compute the quantities defined in eqs (20) through (41), then compute the coefficients given by eqs (46) through (52). Using these coefficients plot eq (45) to determine the real, positive roots in the region of physical interest; if there is more than one such root choose the correct one, which is $\alpha = c_{11}$, as described below. Equation (45) can be plotted and the chosen root determined as accurately as desired by routine automatic computer techniques to save laborious hand computation. Then compute $c_{44}$ from

$$c_{44} = (u - c_{11})/2. \tag{53}$$

Use eq (42) to compute $\gamma^2=(c_{12}+c_{44})^2$ and obtain $\gamma$. The sign of the square root is determined by the $\gamma^3$ term in eq (43). Then compute $c_{12}$ from

$$c_{12}=\gamma-c_{44}. \tag{54}$$

The only ambiguity which arises in this calculation results from the fact that more than one physically reasonable root of eq (45) may occur and each such root may lead to a set of three elastic constants, none of which can be ruled out by the inequalities of Alers and Neighbours [*11*] or by any general physical argument. In this case, one can take one set and compute the polarization of each of the two quasi-transverse waves (the procedure for computing the polarization is given, for example, by Farnell [*10*]) and compare with the polarization of the transducer used to excite the waves. The results should agree for only one set of elastic constants so that the correct choice of root for $c_{11}$ can be made in this way. A second way is to measure velocities in a second direction in the crystal and compare the elastic constants so determined. Although more than one set of elastic constants may give the correct velocities for one direction (but not the correct polarizations) only one set should give the correct velocities for both directions. This second way of choosing $c_{11}$ avoids the need to consider the direction of polarization.

## 3. Equations for Computing Standard Deviations of the Elastic Constants

It is assumed that uncertainty in the density and the direction cosines may be ignored and that the principal uncertainty in the data is expressed by the three statistically independent standard deviations $\sigma_1$, $\sigma_2$, $\sigma_3$ of the velocities $v_1$, $v_2$, $v_3$. It is easiest to divide the calculation of the standard deviations $\sigma_{11}$, $\sigma_{12}$, $\sigma_{44}$ (of $c_{11}$, $c_{12}$, $c_{44}$ respectively) into two parts. First, propagation-of-error theory is used to calculate the variances and covariances of $u$, $v$, $w$. Second, these results are then used to calculate $\sigma_{11}$, $\sigma_{12}$, and $\sigma_{13}$.

The following result [12] from propagation-of-error theory is needed: Let $x$ and $y$ be statistically independent variables with known variances (variance=square of standard deviation). Let $u$ and $v$ be defined as functions of $x$ and $y$ and let $F$ be defined as a function of $u$ and $v$. Then

$$\sigma_F^2=\left(\frac{\partial F}{\partial u}\right)^2\sigma_u^2+\left(\frac{\partial F}{\partial v}\right)^2\sigma_v^2+2\left(\frac{\partial F}{\partial u}\right)\left(\frac{\partial F}{\partial v}\right)\operatorname{cov}(u,v), \tag{55}$$

where

$$\sigma_u^2=\left(\frac{\partial u}{\partial x}\right)^2\sigma_x^2+\left(\frac{\partial u}{\partial y}\right)^2\sigma_y^2, \tag{56}$$

$$\sigma_v^2=\left(\frac{\partial v}{\partial x}\right)^2\sigma_x^2+\left(\frac{\partial v}{\partial y}\right)^2\sigma_y^2, \tag{57}$$

and

$$\operatorname{cov}(u,v)=\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial v}{\partial x}\right)\sigma_x^2+\left(\frac{\partial u}{\partial y}\right)\left(\frac{\partial v}{\partial y}\right)\sigma_y^2. \tag{58}$$

In some textbooks it is implicitly assumed that quantities such as $u$ and $v$ are statistically independent so that their covariance is zero and equations such as (56) and (57) with no covariance terms are given instead of the complete eq (55). The use of the complete equation is important in the present case; the extension of these equations from two to three variables is obvious.

Application of eqs (56) through (58) gives

$$\sigma_u^2=\sigma_{x_1}^2+\sigma_{x_2}^2+\sigma_{x_3}^2, \tag{59}$$

$$\sigma_v^2=(x_2+x_3)^2\sigma_{x_1}^2+(x_1+x_3)^2\sigma_{x_2}^2+(x_1+x_2)^2\sigma_{x_3}^2, \tag{60}$$

$$\sigma_w^2=(x_2x_3)^2\sigma_{x_1}^2+(x_1x_3)^2\sigma_{x_2}^2+(x_1x_2)^2\sigma_{x_3}^2, \tag{61}$$

$$\operatorname{Cov}(u,v)=(x_2+x_3)\sigma_{x_1}^2+(x_1+x_3)\sigma_{x_2}^2+(x_1+x_2)\sigma_{x_3}^2, \tag{62}$$

$$\operatorname{Cov}(u,w)=x_2x_3\sigma_{x_1}^2+x_1x_3\sigma_{x_2}^2+x_1x_2\sigma_{x_3}^2, \tag{63}$$

and

$$\mathrm{Cov}\,(v, w)=(x_2+x_3)x_2x_3\sigma_{x1}^2+(x_1+x_3)x_1x_3\sigma_{x2}^2+(x_1+x_2)x_1x_2\sigma_{x3}^2, \tag{64}$$

where

$$\sigma_{x1}=2\rho v_1\sigma_1,\ \sigma_{x2}=2\rho v_2\sigma_2,\ \sigma_{x3}=2\rho v_3\sigma_3.$$

To use eq (55) for the standard deviations of the elastic constants one must compute the partial derivatives of these constants with respect to $u$, $v$, $w$. These partials of $c_{11}$ can be obtained by taking derivatives of eq (45). The resulting expressions involve partials of the coefficients $a_i$ and these in turn involve partials of the quantities defined in eqs (38) through (41). Let subscripts $u$, $v$, $w$ denote partial differentiation with respect to $u$, $v$, $w$ respectively. Then from eqs (38) through (41)

$$h_{1u}=(gk+jf)/e-h, \tag{65}$$

$$j_{1u}=2u[(jk+gf)/e-p], \tag{66}$$

$$k_{1u}=k(3u^2q-4v)/e-3u^2s, \tag{67}$$

$$p_{1u}=2uq, \tag{68}$$

$$j_{1v}=-4f/e, \tag{69}$$

$$k_{1v}=-4uk/e, \tag{70}$$

$$p_{1v}=-4 \tag{71}$$

$$k_{1w}=8 \tag{72}$$

and the following are all zero: $h_{1v}$, $h_{1w}$, $j_{1w}$, and $p_{1w}$. We shall next require the partial derivatives of the $a_i$ which are given by differentiating eqs (46) through (52) with the result for the $u$ derivatives

$$a_{0u}=3r^2p_1^2p_{1u}/e^3-2k_1k_{1u}, \tag{73}$$

$$a_{1u}=3r^2(jp_1^2+2ujp_1p_{1u})/e^3-2j_1k_{1u}-2k_1j_{1u}, \tag{74}$$

$$a_{2u}=3r^2(2gp_1p_{1u}+2uj^2p_1+u^2j^2p_{1u})/e^3-2h_1k_{1u}-2k_1h_{1u}-2j_1j_{1u}, \tag{75}$$

$$a_{3u}=r^2(6gjp_1+6ugjp_{1u}+3u^2j^3)/e^3-2(g_1k_{1u}+h_1j_{1u}+j_1h_{1u}), \tag{76}$$

$$a_{4u}=3r^2(2ugj^2+g^2p_{1u})/e^3-2g_1j_{1u}-2h_1h_{1u}, \tag{77}$$

$$a_{5u}=3r^2g^2j/e^3-2g_1h_{1u}, \tag{78}$$

and with $a_{6u}$ equal to zero. For the $v$ derivatives the result is

$$a_{0v}=-12r^2p_1^2/e^3-2k_1k_{1v}, \tag{79}$$

$$a_{1v}=-24r^2ujp_1/e^3-2j_1k_{1v}-2k_1j_{1v}, \tag{80}$$

$$a_{2v}=-12r^2(2gp_1+u^2j^2)/e^3-2h_1k_{1v}-2j_1j_{1v}, \tag{81}$$

$$a_{3v}=-24r^2ugj/e^3-2(g_1k_{1v}+h_1j_{1v}), \tag{82}$$

$$a_{4v}=-12r^2g^2/e^3-2g_1j_{1v}, \tag{83}$$

and with $a_{5v}$ and $a_{6v}$ equal to zero. For the $w$ derivatives the result is

$$a_{0w}=-16k_1, \tag{84}$$

$$a_{1w}=-16j_1, \tag{85}$$

$$a_{2w}=-16h_1, \tag{86}$$

$$a_{3w}=-16g_1, \tag{87}$$

and with $a_{4w}$, $a_{5w}$, and $a_{6w}$ equal to zero. Define

$$D=6a_6c_{11}^5+5a_5c_{11}^4+4a_4c_{11}^3+3a_3c_{11}^2+2a_2c_{11}+a_1 \tag{88}$$

then differentiation of eq (45) gives

$$c_{11u} = -(a_{5u}c_{11}^5 + a_{4u}c_{11}^4 + a_{3u}c_{11}^3 + a_{2u}c_{11}^2 + a_{1u}c_{11} + a_{0u})/D, \tag{89}$$

$$c_{11v} = -(a_{4v}c_{11}^4 + a_{3v}c_{11}^3 + a_{2v}c_{11}^2 + a_{1v}c_{11} + a_{0v})/D, \tag{90}$$

and

$$c_{11w} = -(a_{3w}c_{11}^3 + a_{2w}c_{11}^2 + a_{1w}c_{11} + a_{0w})/D, \tag{91}$$

where we have assumed $D \neq 0$. For the [110] direction $D=0$ and a different treatment, described below, is required. The derivatives of $c_{44}$ are obtained from (53) and are

$$c_{44u} = (1 - c_{11u})/2, \tag{92}$$

$$c_{44v} = -c_{11v}/2, \tag{93}$$

and

$$c_{44w} = -c_{11w}/2. \tag{94}$$

The derivatives of $c_{12}$ are obtained from eq (54) and so involve derivatives of $\gamma$. From (42) we have

$$\gamma^2 = (gc_{11}^2 + ujc_{11} + p_1)4e, \tag{95}$$

so that

$$(\gamma^2)_u = (2c_{11}gc_{11u} + jc_{11} + ujc_{11u} + p_{1u})/4e, \tag{96}$$

$$(\gamma^2)_v = (2c_{11}gc_{11v} + ujc_{11v} - 4)/4e, \tag{97}$$

and

$$(\gamma^2)_w = (2c_{11}g + uj)c_{11w}/4e. \tag{98}$$

Now use $\gamma_u = (\gamma^2)_u/2\gamma$ and eq (54) to obtain

$$c_{12u} = (\gamma^2)_u/2\gamma - c_{44u}, \tag{99}$$

$$c_{12v} = (\gamma^2)_v/2\gamma - c_{44v}, \tag{100}$$

and

$$c_{12w} = (\gamma^2)_w/2\gamma - c_{44w}. \tag{101}$$

The expression for $\sigma_{11}^2$ is then

$$\sigma_{11}^2 = c_{11u}^2\sigma_u^2 + c_{11v}^2\sigma_v^2 + c_{11w}^2\sigma_w^2 + 2c_{11u}c_{11v}\,\mathrm{cov}\,(u, v) + 2c_{11u}c_{11w}\,\mathrm{cov}\,(u, w) + 2c_{11v}c_{11w}\,\mathrm{cov}\,(v, w). \tag{102}$$

The equations for $\sigma_{44}^2$ and $\sigma_{12}^2$ are the same with the subscripts on $c_{11}$ changed to 44 and 12 respectively.

The procedure for obtaining the desired standard deviations is thus straightforward although tedious. One begins by calculating the variances and covariances of $u, v, w$ from eqs (59) through (64). Then compute in succession the quantities given by eqs (65) through (102).

Following eq (91) we noted that $D=0$ for the [110] direction. This can be seen as follows: For the [110] direction $r$ is zero by eq (34) and the $\gamma^3$ term drops out of eq (43). Then eq (45) simply consists of the square of all the terms in (43) except $r\gamma^3$. Let

$$B = \alpha^4 s_1/8 + \alpha^2 uh/8 + \alpha u^2 p/8 + u^3 s/8 - \gamma^2(\alpha f + uk)/2 - w. \tag{103}$$

Then eq (45) for the [110] direction is $B^2=0$, and $D$ is then $D = 2B\dfrac{dB}{d\alpha}$, and therefore $D=0$.

The foregoing statistical treatment thus fails for any direction for which $c_{11}$ is a double root of eq (45). This appears to be true only for the [110] direction (we have already noted that the [100] and [111] directions are not suitable for the method of this paper) but the writers have not been able to construct a proof.

For the [110] direction the following results are well known and easily obtained from the treatment of Kolsky [9], for example. If $x_1$ corresponds to the longitudinal wave, $x_2$ to the transverse wave with displacement parallel to [001], and $x_3$ to the transverse wave with displacement parallel to [1̄10], then

$$c_{11}=x_1-x_2+x_3, \tag{104}$$

$$c_{12}=x_1-x_2-x_3, \tag{105}$$

and

$$c_{44}=x_2. \tag{106}$$

These give

$$\sigma_{11}^2=\sigma_{12}^2=\sigma_{x1}^2+\sigma_{x2}^2+\sigma_{x3}^2, \tag{107}$$

and

$$\sigma_{44}=\sigma_{x2}. \tag{108}$$

We have assumed throughout this paper that errors in thickness and density can be neglected in comparison with errors in transit time $t$. If standard deviations were assigned to the thickness and density as well, the quantities $x_i$ would not be statistically independent and two modifications of the foregoing treatment would be required. First, eqs (56) through (58) would have to be used with the thickness, density, and transit times as independent variables to give the variances and covariances of $u$, $v$, $w$. The calculations using eqs (65) through (102) would then go as before. Second, eqs (107) and (108) would have to be replaced by appropriate expressions in terms of the standard deviations of the thickness, density, and transit times derived from (56) through (58) and (104) through (106). No attempt has been made to allow for uncertainties in the orientation; such allowance should probably be made but appears to be an exceedingly difficult problem.

## 4. Procedure for Computing the Elastic Compliances and Their Standard Deviations

The foregoing results form a complete unit, giving the elastic constants, $c_{ij}$, and their standard deviations. The present section may be skipped unless it is desired to put the results in terms of the elastic compliances, $s_{ij}$. The calculation of the $s_{ij}$ from the $c_{ij}$ is trivial but the calculation of the standard deviations of the $s_{ij}$ is more difficult and serious errors can result if the covariance terms are not taken into account. There appears to be no discussion of this problem in the literature on elastic constants, so we present the method for the cubic case.

The well-known equations for the elastic compliances of a cubic crystal in terms of the elastic constants are

$$s_{11}=(c_{11}+c_{12})/c, \tag{109}$$

$$s_{12}=-c_{12}/c, \tag{110}$$

and

$$s_{44}=1/c_{44}, \tag{111}$$

where

$$c=(c_{11}-c_{12})(c_{11}+2c_{12}). \tag{112}$$

To compute the standard deviations of the $s_{ij}$ one can apply eq (55) which requires the covariances of the $c_{ij}$. To compute these covariances one might try to use eq (58) which would be wrong because $x$ and $y$ were assumed to be statistically independent. We require the more general formula

$$\operatorname{cov}(F,G)=\frac{\partial F}{\partial u}\frac{\partial G}{\partial u}\sigma_u^2+\frac{\partial F}{\partial v}\frac{\partial G}{\partial v}\sigma_v^2+\left(\frac{\partial F}{\partial u}\frac{\partial G}{\partial v}+\frac{\partial F}{\partial v}\frac{\partial G}{\partial u}\right)\operatorname{cov}(u,v) \tag{113}$$

for the covariance [12] of $F$ and $G$ which are defined in terms of quantities $u$ and $v$ which are not statistically independent. Writing cov (11, 12) for the covariance of $c_{11}$ and $c_{12}$ we have

$$\operatorname{cov}(11,12)=c_{11u}c_{12u}\sigma_u^2+c_{11v}c_{12v}\sigma_v^2+c_{11w}c_{12w}\sigma_w^2+(c_{11u}c_{12v}+c_{11v}c_{12u})\operatorname{cov}(u,v)$$
$$+(c_{11u}c_{12w}+c_{11w}c_{12u})\operatorname{cov}(u,w)+(c_{11v}c_{12w}+c_{11w}c_{12v})\operatorname{cov}(v,w) \tag{114}$$

The expressions for cov (11, 44) and cov (12, 44) are identical except for the appropriate changes of subscripts, but we shall not need to calculate these latter two covariances. Writing $s_{11,11}$ for $\frac{\partial s_{11}}{\partial c_{11}}$ and similarly for other partials we have

$$s_{11,11}=c-\frac{(c_{11}+c_{12})(2c_{11}+c_{12})}{c^2}, \tag{115}$$

$$s_{11,12}=c+\frac{(c_{11}+c_{12})(4c_{12}+c_{11})}{c^2}, \tag{116}$$

$$s_{12,11}=\frac{c_{12}(2c_{11}+c_{12})}{c^2}, \tag{117}$$

$$s_{12,12}=-\frac{(c_{11}+c_{12})(4c_{12}-c_{11})}{c^2}, \tag{118}$$

$$s_{44,44}=-1/c_{44}^2, \tag{119}$$

and with $s_{11,44}$, $s_{12,44}$, $s_{44,11}$, $s_{44,12}$ all zero. Letting $\sigma s_{11}$ represent the standard deviation of $s_{11}$ and similarly for the other $s_{ij}$,

we have

$$\sigma_{s_{11}}^2=s_{11,11}^2\sigma_{11}^2+s_{11,12}^2\sigma_{12}^2+2s_{11,11}s_{11,12}\operatorname{cov}(11,12) \tag{120}$$

$$\sigma_{s_{12}}^2=s_{12,11}^2\sigma_{11}^2+s_{12,12}^2\sigma_{12}^2+2s_{12,11}s_{12,12}\operatorname{cov}(11,12), \tag{121}$$

and

$$\sigma_{s_{44}}=\sigma_{44}/c_{44}^2. \tag{122}$$

For the [110] direction the covariances of $c_{11}$ and $c_{12}$ is best calculated directly from (104) and (105) using (58). The result is

$$\operatorname{cov}(11,12)=\sigma_{x1}^2+\sigma_{x2}^2+\sigma_{x3}^2. \tag{123}$$

Thus, the procedure for calculating the standard deviation of the $s_{ij}$ for any direction, including the [100] and [111], is to use eqs (120) through (122) evaluating the partial derivations from eqs (115) through (119). The situation considered in the present paper, using only information obtainable from measurements in a single direction, compels us to exclude [100] and [111] from the present considerations. For [110] cov (11, 12) is given by (123); for any other direction, it is given by (114).

## 5. Measurements on $SrTiO_3$

The writers carried out a series of measurements on a boule of strontium titanate, kindly supplied by the National Lead Company, to check the method. The density value [*13*] of 5.116 g/cm³ was used. Flats were first ground to give the maximum thickness between parallel faces permitted by the shape of the crystal. A series of measurements was taken and analyzed. The crystal was then recut normal to the [110] direction and a second series of measurements was then made. The measurements were all made with 10 Mc/s X-cut and AC-cut quartz crystals 0.25 in. in diameter. A commercial pulsed oscillator was used to drive these transducers. The echoes were observed on a dual trace oscilloscope simultaneously with a 1 Mc/s standard frequency signal. The results are sumarized in table 1.

TABLE 1. *Data on $SrTiO_3$ at 25° C*

| Parameter | Symbol | First direction | Second direction, [110] |
|---|---|---|---|
| Direction | $l$ | 0.67905 | 0.70711 |
| Cosines | $m$ | .27160 | .70711 |
| | $n$ | .68300 | .00000 |
| Length, cm | | 5.3045 | 4.6670 |
| Transit times, $10^{-6}$ sec | $t_1$ | 13.16±0.10 | 11.38±0.05 |
| | $t_2$ | 22.09±.05 | 18.72±.07 |
| | $t_3$ | 23.15±.07 | 20.12±.08 |
| $x_i$, $10^{12}$ dyne/cm² | $x_1$ | 3.330±.051 | 3.308±.029 |
| | $x_2$ | 1.181±.005 | 1.219±.009 |
| | $x_3$ | 1.074±.008 | 1.064±.010 |

## 6. Results

The data are summarized in table 1. The calculation of $c_{11}$ by the method of eqs (20) through (52) was programmed for an automatic computer using an iterative procedure of solving eq (45) which gives the real roots to four places in the interval 0.0 to $5.0\times 10^{12}$ dynes/cm². For the first direction, there is a single root at $\alpha=3.162$ and a single root at $\alpha=3.497\times 10^{12}$ dynes/cm². For the second direction there is a double root at $\alpha=3.153$ and a double root at $\alpha=3.462\times 10^{12}$ dynes/cm². A complete set of elastic constants was computed for each of these possible choices of $c_{11}$ and the results are compared in table 2. The choice of 3.497 and 3.462 leads to a disagreement in $c_{12}$ which is outside the experimental error. The choice of 3.162 and 3.153 gives consistent sets of constants. The latter choice is also known to be correct because 3.153 is obtained from eq (104) when $x_2$ and $x_3$ are properly distinguished by the polarization of the corresponding sound waves.

For the first direction, the standard deviations of the $c_{ij}$ were determined by the method of eqs (59) through (102) using an automatic computer. Equations (107) and (108) were used for the second direction. The final values for the $c_{ij}$ were computed by averaging the results for the two directions weighted by the reciprocals of the squares of the standard deviations. The $s_{ij}$ values were then computed from eqs (109) through (112) and their standard deviations from eqs (113) through (123).

TABLE 2. *Comparison of possible sets of elastic constants*

| Constants | First direction | Second direction |
|---|---|---|
| Computed from correct choice of root for $c_{11}$ | | |
| $c_{11}$ | 3.162±0.052 | 3.153±0.032 |
| $c_{12}$ | 1.035±.052 | 1.024±.032 |
| $c_{44}$ | 1.212±.007 | 1.219±.009 |
| Computed from incorrect choice of root for $c_{11}$ | | |
| $c_{11}$ | 3.497 | 3.462±0.032 |
| $c_{12}$ | 1.200 | 1.024±.032 |
| $c_{44}$ | 1.044 | 1.064±.010 |

The $c_{11}$ and $c_{12}$ values of Bell and Rupprecht [*14*] agree within experimental error with the results of the present work as shown in table 3; the $c_{12}$ value of Poindexter and Giardini [*15*] also agrees within experimental error, but their $c_{11}$ value differs from the present result by much more than twice the standard deviation and so is significantly different from our result. The other workers' $c_{44}$ values lie on either side by slightly more than twice the standard deviation of our value, but are probably within the combined experimental error of their determination and ours. The writers feel that the $c_{11}$ values of Poindexter and Giardini should be rejected and that the remaining data show reasonable agreement.

The anisotropy of a cubic crystal depends on the quantity $\delta$ defined by

$$\delta=2s_{11}-2s_{12}-s_{44}. \tag{124}$$

The Young's modulus, $Y_f$, and shear modulus, $G_f$, are given as a function of the usual spherical polar angles by

$$\frac{1}{Y_f}=s_{11}-\delta \sin^2\theta\cos^2\theta-(\delta/4)\sin^4\theta\sin^2 2\phi, \tag{125}$$

and

$$\frac{1}{G_f}=s_{44}+2\delta \sin^2\theta\cos^2\theta+(\delta/2)\sin^4\theta\sin^2 2\phi. \tag{126}$$

These quantities are plotted in figure 1 which shows that $SrTiO_3$ comes close to being isotropic; Young's modulus varies by only 10 percent and the shear modulus by 5 percent.

TABLE 3. *Comparison with elastic constants of $SrTiO_3$ at 25 °C determined by other workers*

| Constants | Poindexter and Giardini [a] | Bell and Rupprecht [b] | Present work [b] | Percent difference, last two columns |
|---|---|---|---|---|
| $c_{11}$ | 3.48 | 3.181 | 3.156 ± 0.027 | 0.79 |
| $c_{12}$ | 1.01 | 1.025 | 1.027 ± .027 | 0.19 |
| $c_{44}$ | 1.19 | 1.236 | 1.215 ± .006 | 1.73 |
| $s_{11}$ | 3.3 | 3.729 | 3.772 ± .023 | 1.14 |
| $s_{12}$ | −0.74 | −0.909 | −0.926 ± .010 | 1.84 |
| $s_{44}$ | 8.4 | 8.091 | 8.233 ± .040 | 1.73 |

All $c_{ij}$ in units of $10^{12}$ dyne/cm²; $s_{ij}$ in units of $10^{-13}$ cm²/dyne.
[a] $s_{ij}$ determined by resonance method and $c_{ij}$ by matrix inversion.
[b] $c_{ij}$ determined by pulse velocity method and $s_{ij}$ by matrix inversion.

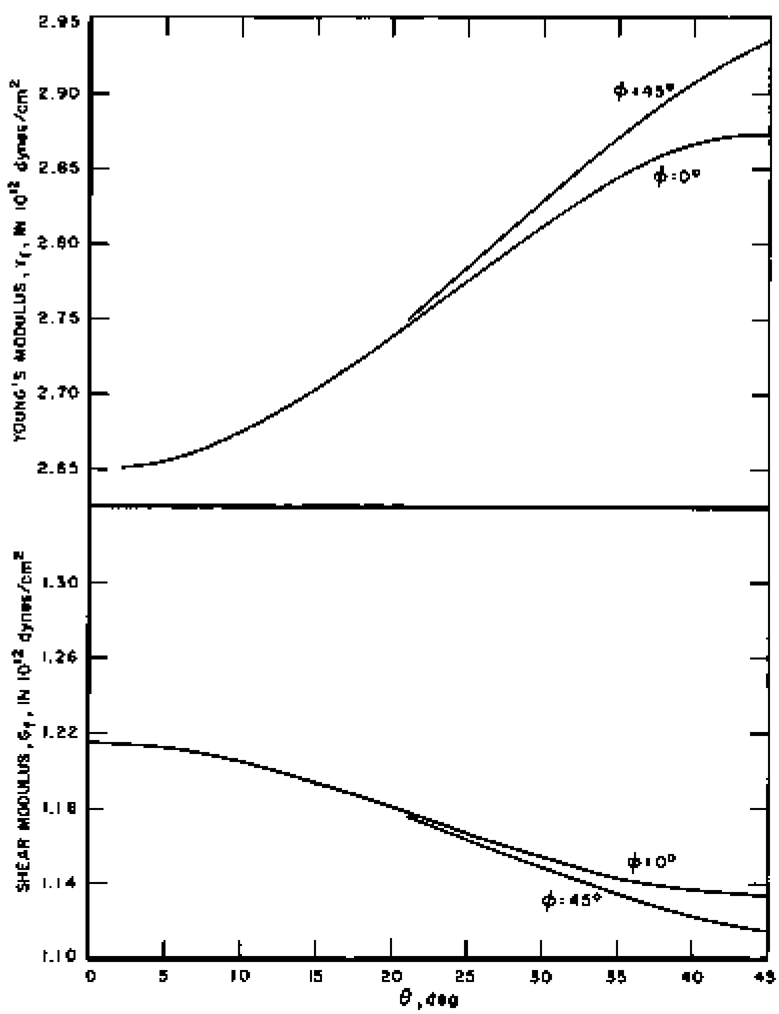


FIGURE 1. *Young's modulus, $Y_f$, and the shear modulus, $G_f$, as a function of orientation.*

The colatitude, θ, is the angle between the [001] direction and the direction of measurement. The azimuth, φ, is the angle between the [100] direction and the projection of the direction of measurement on the (001) plane. The subscript *f* indicates that the elastic moduli are for a free specimen which is under no constraint.

## 7. Summary

(1) Velocity measurements in a single direction in a cubic crystal provide enough information to determine the three elastic constants, $c_{ij}$, except for the [100] and [111] directions which are therefore excluded from consideration in this paper.

(2) For the [110] direction the computation of the elastic constants and their standard deviations is simple and is given in eqs (104) through (108).

(3) For all other directions the calculations are much more complex. The general procedure for the elastic constants (applicable also to the [110] direction) is given in eqs (2) through (54). The general procedure for the standard deviations (not applicable to the [110] direction) is given in eqs (59) through (102).

(4) The procedure for calculating the elastic compliances, $s_{ij}$, and their standard deviations is given in eqs (109) through (123). Throughout the statistical treatment the covariance terms are included and their importance is emphasized.

(5) The method is applied to $SrTiO_3$ and results in good agreement with previous workers are obtained.

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