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Orientation Dependence of Elastic Waves in Single Crystals*

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A description of the properties of plane elastic waves in single crystals is of interest both from a theoretical point of view and in the interpretation of high-frequency pulsed ultrasound experiments. The perturbed eigenvalue problem that arises when nearly *pure* transverse or compressional modes are propagated is considered, and the resulting phase velocities and displacement vectors tabulated for a number of cases of physical interest. A unified approach to the properties of pure modes is provided through a consideration of individual rotational symmetries of the crystals, and the energy flux associated with both pure and nearly pure modes is discussed.

1. INTRODUCTION

In recent years ultrasonics has become an important tool in the investigation of properties of solids. Perhaps the richest applications are realized in the study of single crystals where the presence of anisotropy, while of course increasing the complexity of measurement, provides a coordinate frame in which loss mechanisms will in general imbed themselves with a preferred orientation. By probing ultrasonically in different crystalline directions with the elastic modes available, one may examine the directional properties of these loss mechanisms. Phase velocity measurements of accuracy as high as one part in 10^5 are also of interest, both to correlate variations in elastic constants with specimen history and to observe dispersions associated with anelastic properties.

Using pulsed ultrasound reflection techniques in the megacycle range, a description of which has been given by Roderick and Truell,[1] it is advantageous to choose propagation directions in the crystal for which pure transverse and longitudinal modes can be obtained. The reasons are as follows. First, using x-cut and AC-cut quartz transducers, one may excite various modes individually instead of in proportions depending on the orientation of the propagation direction. Next, the computation of elastic constants from measured phase velocities is less involved. Further, the analysis required to explain observed losses is usually simplified because the crystal and hence many of the loss mechanisms will have a fairly high symmetry in the propagation coordinates. Finally, the direction of energy flux will almost always coincide with the propagation direction, so that pulses reflecting between two parallel crystal faces will not deteriorate due to impinging on side walls of the crystal.

In the pulsed reflection technique the propagation direction is normal to two plane-parallel mechanical surfaces of the crystal, and in actual practice it is impossible to cut these faces to exactly the desired orientation. Presumably extremely careful machining techniques can hold misorientation to a matter of several minutes of arc. In easily damaged specimens, however, which cannot be machined, misorientations incurred in a lapping procedure may easily be of the order of one or two degrees.

The main purpose of this paper is to develop a description of the perturbed quasi-pure modes which result due to these misorientations. Section 2 is devoted to setting up the solution of the perturbed secular equation in a general manner. In Sec. 3 the problem is broken down into various crystal systems, and the phase velocities and elastic displacement vectors are tabulated for the modes of interest. Section 4 presents a tabulation of the numerical parameters involved for cubic crystals, and in addition to giving an estimate of the order of magnitude of the effects being considered should serve as a useful working table for the experimenter. Finally in Sec. 5 the energy flux associated with both pure and quasi-pure elastic modes is discussed. The two cases of internal conical refraction are considered for the former, and for the latter some numerical calculations are made to indicate the degree of deviation of energy flux in certain cases.

The details of the perturbed eigenvalue problem leading to the phase velocity are presented perhaps more thoroughly than is justified by the straightforwardness of the calculation. The reasons for this are threefold. From the symmetry table of Sec. 3, for example, a unified picture of the properties of pure elastic modes is obtained. Thus one may at a glance pick out many of the directions along which pure elastic modes may propagate, check for degeneracy of the transverse modes, determine the displacement vectors and observe whether the energy flux deviates from the propagation direction, all in terms of the individual rotational (or reflectional) symmetries of the crystal. In addition, possession of the details of the perturbation problem enables one to more readily extend the calculations to obtain higher order terms in the perturbed phase velocities, treat cases not considered explicitly in this paper, and compute the components of stress and energy flux. Finally, a formalism which builds up results from individual symmetries of a crystal should be most convenient for considering the role of new loss mecha-

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nisms which invalidate only a fraction of the symmetry elements.

The problem of finding the directions in which pure elastic modes will propagate was considered by Sakadi in 1941,[2] and more recently by Borgnis,[3] for several crystal systems.

Gold has given a numerical tabulation of phase velocities as a function of orientation for certain cubic and hexagonal metals.[4] Musgrave has carried out detailed numerical calculations for certain cubic and hexagonal crystals, presenting his results in the form of polar plots of phase velocity surfaces and wave surfaces.[5] Approximation techniques for determining elastic constants from phase velocity measurements in an arbitrary direction in cubic and hexagonal crystals have been discussed by Arenberg,[6] and Neighbours and Smith.[7] Neighbours later discussed the application of this method to additional crystal symmetries.[8]

2. SOLUTION OF THE EIGENVALUE PROBLEM

In an anisotropic elastic medium there are in general several axes along which two pure transverse elastic modes and one pure longitudinal can propagate. A *pure mode axis* is defined to be any direction in a crystal with this property. For a review of the basic concepts of infinitesimal elasticity theory employed in the following discussion, see Sokolnikoff[9] or Love.[10]

The components ϵ_{ij} of the strain tensor, defined by

$$\epsilon_{ij}=\tfrac{1}{2}(u_{i,j}+u_{j,i}), \tag{2.1}$$

where u_i is the ith component of displacement, are related to the components σ_{ij} of the stress tensor by the generalized Hooke's law

$$\sigma_{ij}=F_{ijkl}\epsilon_{kl}, \tag{2.2}$$

where σ_{ij} is the jth component of stress on the plane of normal x_i. The σ_{ij} and ϵ_{ij} are symmetric, and if existence of an elastic potential is assumed, the F_{ijkl} obey the symmetry relations

$$F_{ijkl}=F_{klij}=F_{lkij}, \tag{2.3}$$

reducing the total number of independent elastic constants to 21.

The equations of motion in a medium with no body forces present are

$$\sigma_{ij,i}=\rho\ddot{u}_j, \tag{2.4}$$

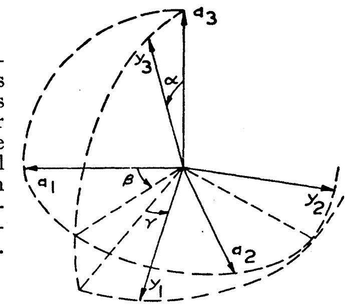

FIG. 1. The transforma- from the crystal coordinates $\{a_i\}$ to the coordinates $\{y_i\}$, utilizing the Euler angles. Two pure transverse and one pure longitudinal mode may be propagated in the y_3 direction, with respective elastic displacements in the y_i directions.

where ρ is the density of the medium. Making use of the preceding equations, Eq. (2.4) may be written in terms of the displacements as

$$F_{ijkl}u_{k,li}=\rho\ddot{u}_j, \tag{2.5}$$

providing the medium is homogeneous. If one now assumes a plane wave

$$u_j^{(m)}=A_j^{(m)}\exp\{i(\omega t-k_m x_3)\}, \tag{2.6}$$

propagating in the x_3 direction with propagation constant k_m and frequency ω, Eq. (2.5) become

$$(F_{3jk3}-\mu_m\delta_{jk})A_k^{(m)}=0, \tag{2.7}$$

where δ_{jk} is the Kronecker delta and the eigenvalues have been written as $\mu_m=\rho v_m^2$. $A_k^{(m)}$ is the kth component of the eigenvector associated with the eigenvalue μ_m. In order that Eq. (2.7) have a nontrivial solution, the eigenvalues must satisfy the secular equation

$$|F_{3jk3}-\mu_m\delta_{jk}|=0. \tag{2.8}$$

The propagation direction x_3 in the crystal is chosen normal to the mechanical surface of the crystal by the usual ultrasound propagation techniques. Hence the experimenter desiring to propagate pure modes in the crystal would prepare a surface normal to a pure mode axis. Due to limitations of orienting and machining equipment this cannot be done exactly. We suppose that a small error has been made, so that the angle between the x_3 axis and a pure mode axis is of the order of one or two degrees. The $\{x_i\}$ shall henceforth be referred to as the *misoriented coordinates*.

The F_{ijkl} are the elastic constants of the crystal referred to the misoriented coordinates. In order to find the solution of Eq. (2.8) one must first find the form of the F_{ijkl} and their relation to the known elastic constants c_{ijkl} described in the crystal coordinates $\{a_i\}$. It is convenient to do this by two coordinate transformations. The first transformation leading from the crystal coordinates to a second set of Cartesian coordinates $\{y_i\}$ is performed utilizing the Euler angles. The $\{y_i\}$ are chosen by the conditions that y_3 be the pure mode axis along which waves are to be propagated, and eigenvector $\mathbf{A}^{(i)}$ be along the y_i axis, for $i=1, 2, 3$. The second transformation leading from the $\{y_i\}$ to the misoriented coordinates $\{x_i\}$ is then performed, and

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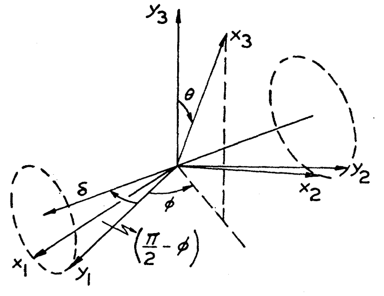

FIG. 2. The transformation from the pure mode coordinates $\{y_i\}$ to the misoriented coordinates $\{x_i\}$, accomplished by means of a single rotation through the angle θ about the axis $\boldsymbol{\delta}$.

the F_{ijkl} are obtained in terms of the c_{ijkl} by the usual tensor algorism.

For the first transformation the elastic constants D_{ijkl} described in the $\{y_i\}$ coordinates and the direction cosines are as follows:

$$\begin{aligned}
D_{ijkl}&=l_{ip}l_{jq}l_{kr}l_{ls}c_{pqrs},\\
l_{11}&=\cos\alpha\cos\beta\cos\gamma-\sin\beta\sin\gamma,\\
l_{12}&=\cos\alpha\sin\beta\cos\gamma+\cos\beta\sin\gamma,\\
l_{13}&=-\sin\alpha\cos\gamma,\\
l_{21}&=-\cos\alpha\cos\beta\sin\gamma-\sin\beta\cos\gamma,\\
l_{22}&=\cos\beta\cos\gamma-\cos\alpha\sin\beta\sin\gamma,\\
l_{23}&=\sin\alpha\sin\gamma,\\
l_{31}&=\sin\alpha\cos\beta,\\
l_{32}&=\sin\alpha\sin\beta,\\
l_{33}&=\cos\alpha.
\end{aligned}\tag{2.9}$$

It is evident from Eq. (2.9), and also Fig. 1, that the y_3 axis is determined by α and β alone. Hence, by proper choice of α and β, y_3 may be made a pure mode axis regardless of what value be chosen for γ. This is done as follows: rewriting Eq. (2.7) in the $\{y_i\}$ coordinates, it is seen that the pure longitudinal mode with displacement components $u_j=\delta_{j3}\exp\{i(\omega t-ky_3)\}$ may propagate providing $D_{3133}=D_{3233}=0$. Further, the symmetry of the array $\|D_{3ij3}\|$ guarantees that the eigenvectors are mutually orthogonal; hence the eigenvectors associated with the two other modes are both normal to the y_3 axis, and represent *pure* transverse modes.

Having chosen α and β so that D_{3133} and D_{3233} both vanish independent of γ, D_{3123} is computed, and γ is chosen so that $D_{3123}=0$. This step greatly simplifies the analysis. The eigenvectors now coincide in direction with the y_i axes. Actually, the form of the transformation is such that the rotation γ is unnecessary in most of the cases of higher symmetry, and the choice $\gamma=0$ automatically causes D_{3123} to vanish. In the y_i coordinates, the array $\|D_{3ij3}\|$ is diagonalized. At this point one may determine whether or not the problem is degenerate. A degeneracy corresponds physically to the velocities of the two pure transverse modes being equal, and is described mathematically by

$$D_{3113}=D_{3223}.\tag{2.10}$$

The second transformation to the mirioriented coordinates $\{x_i\}$ is now performed, and consists of a rotation in the negative sense through the angle θ about an axis δ lying in the (y_1y_2) plane, where δ has components $(\sin\phi,\ -\cos\phi,\ 0)$ in the $\{y_i\}$ coordinates. This is shown in Fig. 2. The elastic constants F_{ijkl} described in the $\{x_i\}$ coordinates, and the direction cosines of this transformation are as follows:

$$\begin{aligned}
F_{ijkl}&=n_{ip}n_{jq}n_{kr}n_{ls}D_{pqrs},\\
n_{11}&=\sin^2\phi+\cos^2\phi\cos\theta,\\
n_{22}&=\cos^2\phi+\sin^2\phi\cos\theta,\\
n_{33}&=\cos\theta,\\
n_{12}&=n_{21}=(\cos\theta-1)(\sin2\phi)/2,\\
n_{31}&=-n_{13}=\sin\theta\cos\phi,\\
n_{32}&=-n_{23}=\sin\theta\sin\phi.
\end{aligned}\tag{2.11}$$

The F_{3ij3} may be expanded in a power series in θ, obtaining

$$F_{3ij3}=f_{ij}{}^k\theta^k,\tag{2.12}$$

where "k" plays the role of an index on the $f_{ij}{}^k$, an exponent on θ, and the summation convention applies. The series (2.12) converge absolutely for all values of θ. Assuming a power series solution for the eigenvalues, one writes

$$\mu_m=a_m{}^k\theta^k,\tag{2.13}$$

where the above remarks on the index k apply.

Inserting Eqs. (2.12) and (2.13) in the secular equation, the result is

$$|(f_{ij}{}^k-a_m{}^k\delta_{ij})\theta^k|=0.\tag{2.14}$$

The compactness of the notation is rather deceptive. Equation (2.14) represents three equations, one for each of the three eigenvalues μ_m. The position of each term in the determinant is given by the indices (ij), and each term is summed separately over k. Observe further that $f_{ij}{}^k=f_{ji}{}^k$, and $f_{ij}{}^0=0$ for $i\neq j$.

The $a_m{}^k$ may now be determined in terms of the $f_{ij}{}^k$ by equating the coefficient of each power of θ in Eq. (2.14) to zero. As we are only interested in the results for θ small, we solve for the eigenvalues correct to quadratic terms in θ. In the degenerate case several coefficients vanish identically, and hence some results must be listed separately.

The nondegenerate case:

$$\begin{aligned}
&a_i{}^0=f_{ii}{}^0,\quad a_i{}^1=f_{ii}{}^1,\\
&a_i{}^2=f_{ii}{}^2+\sum_{j\neq i}\frac{(f_{ij}{}^1)^2}{f_{ii}{}^0-f_{jj}{}^0}.
\end{aligned}\tag{2.15}$$

The degenerate case:

The $a_m{}^i$ are the same as above, with the four exceptions

$$
\begin{aligned}
a_1^1 &= \tfrac{1}{2}(f_{11}^1+f_{22}^1)-\tfrac{1}{2}[(f_{11}^1-f_{22}^1)^2+4(f_{12}^1)^2]^{\frac{1}{2}},\\
a_2^1 &= \tfrac{1}{2}(f_{11}^1+f_{22}^1)+\tfrac{1}{2}[(f_{11}^1-f_{22}^1)^2+4(f_{12}^1)^2]^{\frac{1}{2}},\\
a_1^2 &= \tfrac{1}{2}(f_{11}^2+f_{22}^2)\\
&\quad +\tfrac{1}{2}[(f_{13}^1)^2+(f_{23}^1)^2]/(f_{11}^0-f_{33}^0)+\tfrac{1}{2}M^{\frac{1}{2}},\\
a_2^2 &= \tfrac{1}{2}(f_{11}^2+f_{22}^2)\\
&\quad +\tfrac{1}{2}[(f_{13}^1)^2+(f_{23}^1)^2]/(f_{11}^0-f_{33}^0)-\tfrac{1}{2}M^{\frac{1}{2}},
\end{aligned}
\tag{2.16}
$$

where

$$
\begin{aligned}
M \equiv (f_{22}^2-f_{11}^2)^2+4(f_{12}^2)^2+\frac{[(f_{13}^1)^2+(f_{23}^1)^2]^2}{(f_{33}^0-f_{11}^0)^2}\\
+\frac{2}{(f_{33}^0-f_{11}^0)}\{[(f_{13}^1)^2-(f_{23}^1)^2]\\
\times[f_{22}^2-f_{11}^2]-4f_{12}^2f_{13}^1f_{23}^1\},
\end{aligned}
$$

and a_1^2, a_2^2 have been derived on the basis that $f_{11}^1=f_{22}^1=f_{12}^1=0$. This does not involve any loss for our purposes, since if these terms do not vanish, the eigenvalues contain linear terms in θ, and we are no longer interested in the quadratic terms.

Having found the eigenvalues, the eigenvectors may be obtained from Eq. (2.7) in the form of power series expansions in θ. The normalization scheme is as follows: in the nondegenerate case, set $A_{(i)}^{(i)}=1$. In the degenerate case, take $A_3^{(3)}=1$, $A_1^{(1)}$ and $A_2^{(2)}$ as constants not involving θ, and

$$[A_1^{(i)}(\theta=0)]^2+[A_2^{(i)}(\theta=0)]^2=1 \quad \text{for } i=1,2.$$

Under this scheme, taking only the lowest order term in θ for each $A_i^{(j)}$, orthogonality and normality are both preserved to within order of θ^2. The results, correct to lowest order terms in θ, are as follows:

The nondegenerate case:

$$A_{(i)}^{(i)}=1,\quad A_i^{(j)}=\frac{f_{ij}^1\theta}{f_{(j)(j)}^0-f_{(i)(i)}^0},\quad i\neq j. \tag{2.17}$$

If $f_{12}^1=0$, then

$$
\begin{aligned}
A_2^{(1)} &= \frac{f_{13}^1f_{23}^1+(f_{11}^0-f_{33}^0)f_{12}^2}{(f_{33}^0-f_{11}^0)(f_{22}^0-f_{11}^0)}\theta^2,\\
A_1^{(2)} &= \frac{f_{13}^1f_{23}^1+(f_{22}^0-f_{33}^0)f_{12}^2}{(f_{33}^0-f_{22}^0)(f_{11}^0-f_{22}^0)}\theta^2.
\end{aligned}
$$

The degenerate case:

$$
\begin{aligned}
A_1^{(1)} &= A_2^{(2)}=[1+N^2]^{-\frac{1}{2}},\\
A_2^{(1)} &= -A_1^{(2)}=N[1+N^2]^{-\frac{1}{2}},\\
A_3^{(1)} &= \frac{f_{13}^1+Nf_{23}^1}{f_{11}^0-f_{33}^0}[1+N^2]^{-\frac{1}{2}}\theta,\\
A_3^{(2)} &= \frac{f_{23}^1-Nf_{13}^1}{f_{11}^0-f_{33}^0}[1+N^2]^{-\frac{1}{2}}\theta,\\
A_i^{(3)} &= \frac{f_{i3}^1\theta}{f_{33}^0-f_{11}^0},\quad i\neq 3\\
A_3^{(3)} &= 1,
\end{aligned}
\tag{2.18}
$$

where

$$
\begin{aligned}
N &\equiv \frac{2f_{12}^1}{f_{11}^1-f_{22}^1-[(f_{11}^1-f_{22}^1)^2+4(f_{12}^1)^2]^{\frac{1}{2}}} \quad \text{for } f_{12}^1\neq 0\\
&\equiv \frac{(f_{13}^1)^2-(f_{23}^1)^2+(f_{33}^0-f_{11}^0)(f_{22}^2-f_{11}^2+M^{\frac{1}{2}})}{2[f_{12}^2(f_{33}^0-f_{11}^0)-f_{13}^1f_{23}^1]}\\
&\qquad \text{for } f_{12}^1=f_{11}^1=f_{22}^1=0.
\end{aligned}
$$

The required f_{ij}^k may be obtained in terms of the D_{pqrs} from Eqs. (2.11) and (2.12). Before doing this, however, it is convenient to shift to the more usual index notation by writing

$$D_{ijkl}=D_{pq}, \tag{2.19}$$

where $p=i$ if $i=j$; $p=m+3$ if $i\neq j$, with $i\neq m\neq j$. Now Eqs. (2.11) yield, using the fact that $D_{34}=D_{35}=D_{45}=0$,

$$
\begin{aligned}
f_{11}^0 &= D_{55}\\
f_{22}^0 &= D_{44},\\
f_{33}^0 &= D_{33},\\
f_{11}^1 &= 2D_{15}\cos\phi+2D_{56}\sin\phi,\\
f_{22}^1 &= 2D_{46}\cos\phi+2D_{24}\sin\phi,\\
f_{33}^1 &= 0,\\
f_{12}^1 &= (D_{14}+D_{56})\cos\phi+(D_{25}+D_{46})\sin\phi,\\
f_{13}^1 &= (2D_{55}-D_{33}+D_{13})\cos\phi+D_{36}\sin\phi,\\
f_{23}^1 &= (2D_{44}-D_{33}+D_{23})\sin\phi+D_{36}\cos\phi,\\
f_{11}^2 &= (D_{11}+D_{33}-2D_{13}-4D_{55})\cos^2\phi,\\
&\quad +(D_{66}-D_{55})\sin^2\phi+(D_{16}-D_{36})\sin 2\phi,\\
f_{22}^2 &= (D_{22}+D_{33}-2D_{23}-4D_{44})\sin^2\phi\\
&\quad +(D_{66}-D_{44})\cos^2\phi+(D_{26}-D_{36})\sin 2\phi,\\
f_{33}^2 &= 2(2D_{44}+D_{23}-D_{33})\sin^2\phi\\
&\quad +2(2D_{55}+D_{13}-D_{33})\cos^2\phi+2D_{36}\sin 2\phi,\\
f_{12}^2 &= (D_{16}-D_{36})\cos^2\phi+(D_{26}-D_{36})\sin^2\phi\\
&\quad +(2D_{33}+2D_{66}+2D_{12}-2D_{13}-2D_{23}\\
&\qquad -3D_{44}-3D_{55})\tfrac{1}{4}\sin 2\phi.
\end{aligned}
\tag{2.20}
$$

In order to avoid any confusion, it should be mentioned that in the reduced index notation, the stress-strain law becomes

$$\sigma_i=D_{ij}\epsilon_j,\quad i=1,\cdots,6, \tag{2.21}$$

where the σ_i and ϵ_j are defined by $\sigma_1=\sigma_{11}$, $\sigma_2=\sigma_{22}$, $\sigma_3=\sigma_{33}$, $\sigma_4=\sigma_{23}$, $\sigma_5=\sigma_{31}$, $\sigma_6=\sigma_{12}$; $\epsilon_1=\epsilon_{11}$, $\epsilon_2=\epsilon_{22}$, $\epsilon_3=\epsilon_{33}$, $\epsilon_4=2\epsilon_{23}$, $\epsilon_5=2\epsilon_{31}$, and $\epsilon_6=2\epsilon_{12}$. Observe that the reduced index strains ϵ_i are no longer components of a tensor, and hence it is impractical to use the form (2.21) of the stress-strain law, or for that matter any equation containing the reduced index strains, in a computation which involves transformation of coordinates. No difficulty is encountered in manipulating the D_{ij} alone, however, provided one keeps in mind that they are the

TABLE I. The forms of the elastic constant arrays for various rotational or reflectional symmetries of the coordinate axes. S_{ij} indicates that the ith axis has j-fold rotational symmetry or, if $j=2$, is either a twofold symmetry axis or is normal to a plane of reflection symmetry.

$$S_{12}: \begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 0 \\ 12 & 22 & 23 & 24 & 0 & 0 \\ 13 & 23 & 33 & 34 & 0 & 0 \\ 14 & 24 & 34 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 55 & 56 \\ 0 & 0 & 0 & 0 & 56 & 66 \end{bmatrix} \quad S_{22}: \begin{bmatrix} 11 & 12 & 13 & 0 & 15 & 0 \\ 12 & 22 & 23 & 0 & 25 & 0 \\ 13 & 23 & 33 & 0 & 35 & 0 \\ 0 & 0 & 0 & 44 & 0 & 46 \\ 15 & 25 & 35 & 0 & 55 & 0 \\ 0 & 0 & 0 & 46 & 0 & 66 \end{bmatrix} \quad S_{32}: \begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 16 \\ 12 & 22 & 23 & 0 & 0 & 26 \\ 13 & 23 & 33 & 0 & 0 & 36 \\ 0 & 0 & 0 & 44 & 45 & 0 \\ 0 & 0 & 0 & 45 & 55 & 0 \\ 16 & 26 & 36 & 0 & 0 & 66 \end{bmatrix}$$

$$S_{13}: \begin{bmatrix} 11 & 12 & 12 & 0 & 0 & 0 \\ 12 & 22 & 23 & 0 & 25 & 26 \\ 12 & 23 & 22 & 0 & -25 & -26 \\ 0 & 0 & 0 & \frac{1}{2}(22-23) & -26 & 25 \\ 0 & 25 & -25 & -26 & 55 & 0 \\ 0 & 26 & -26 & 25 & 0 & 55 \end{bmatrix} \quad S_{23}: \begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 16 \\ 12 & 22 & 12 & 0 & 0 & 0 \\ 13 & 12 & 11 & -14 & 0 & -16 \\ 14 & 0 & -14 & 44 & -16 & 0 \\ 0 & 0 & 0 & -16 & \frac{1}{2}(11-13) & 14 \\ 16 & 0 & -16 & 0 & 14 & 44 \end{bmatrix} \quad S_{33}: \begin{bmatrix} 11 & 12 & 13 & 14 & -25 & 0 \\ 12 & 11 & 13 & -14 & 25 & 0 \\ 13 & 13 & 33 & 0 & 0 & 0 \\ 14 & -14 & 0 & 44 & 0 & 25 \\ -25 & 25 & 0 & 0 & 44 & 14 \\ 0 & 0 & 0 & 25 & 14 & \frac{1}{2}(11-12) \end{bmatrix}$$

$$S_{14}: \begin{bmatrix} 11 & 12 & 12 & 0 & 0 & 0 \\ 12 & 22 & 23 & 24 & 0 & 0 \\ 12 & 23 & 22 & -24 & 0 & 0 \\ 0 & 24 & -24 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 55 & 0 \\ 0 & 0 & 0 & 0 & 0 & 55 \end{bmatrix} \quad S_{24}: \begin{bmatrix} 11 & 12 & 13 & 0 & 15 & 0 \\ 12 & 22 & 12 & 0 & 0 & 0 \\ 13 & 12 & 11 & 0 & -15 & 0 \\ 0 & 0 & 0 & 44 & 0 & 0 \\ 15 & 0 & -15 & 0 & 55 & 0 \\ 0 & 0 & 0 & 0 & 0 & 44 \end{bmatrix} \quad S_{34}: \begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 16 \\ 12 & 11 & 13 & 0 & 0 & -16 \\ 13 & 13 & 33 & 0 & 0 & 0 \\ 0 & 0 & 0 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 44 & 0 \\ 16 & -16 & 0 & 0 & 0 & 66 \end{bmatrix}$$

$$S_{16}: \begin{bmatrix} 11 & 12 & 12 & 0 & 0 & 0 \\ 12 & 22 & 23 & 0 & 0 & 0 \\ 12 & 23 & 22 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(22-23) & 0 & 0 \\ 0 & 0 & 0 & 0 & 55 & 0 \\ 0 & 0 & 0 & 0 & 0 & 55 \end{bmatrix} \quad S_{26}: \begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 0 \\ 12 & 22 & 12 & 0 & 0 & 0 \\ 13 & 12 & 11 & 0 & 0 & 0 \\ 0 & 0 & 0 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(11-13) & 0 \\ 0 & 0 & 0 & 0 & 0 & 44 \end{bmatrix} \quad S_{36}: \begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 0 \\ 12 & 11 & 13 & 0 & 0 & 0 \\ 13 & 13 & 33 & 0 & 0 & 0 \\ 0 & 0 & 0 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 44 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(11-12) \end{bmatrix}$$

components of a fourth-order tensor in a shorthand notation.

The general solution for the eigenvalues and eigenvectors in terms of the D_{ij} is now complete, and expressed by Eqs. (2.13), (2.15), (2.16), (2.17), (2.18), and (2.20). It is interesting to note from the sixth of Eqs. (2.20) that the longitudinal velocities never contain a linear term in θ.

The general solution could now be written down in terms of the usual elastic constants c_{ij} of the medium by invoking Eqs. (2.9). As this would involve a large number of terms, it is more expedient to break the analysis down into the various crystal systems at this point.

3. EXPLICIT SOLUTION FOR SEVERAL CRYSTAL SYSTEMS

The eigenvalues and eigenvectors will now be tabulated for the cubic, tetragonal, hexagonal and trigonal crystal systems. For a description of these systems see, for example, Kittel.[11] Instead of computing the D_{ij} entirely from Eqs. (2.9), one may eliminate much of the computation by invoking the symmetry properties of the various systems involved. To this end a symmetry table (Table I) is constructed, based on concepts first set forth by Voigt[12] and later summarized by Zener.[13] Table I gives the *form of the elastic constants* referred to any Cartesian coordinate system in which one of the axes possesses rotational symmetry or a normal reflection plane, and is read as follows: S_{ij} indicates that the ith axis has j-fold rotational symmetry or, if $j=2$, is either a twofold symmetry axis or is normal to a plane of reflection symmetry. Notice that the usual crystal notations will not suffice here, as we are referring to symmetries about specific axes. Each array is obtained by requiring that it be invariant under the appropriate coordinate transformation. Those elastic constants which must vanish are indicated by a zero, and of the remainder any interrelations are indicated by appropriate repetition of indices. The usefulness of the table lies in the fact that various arrays may be simply *superposed.* The zeros and interrelations of each of the component arrays all appear in the superposed one.

Inspection of Table I immediately gives two interesting results:

(1) For x_3 to be a pure mode axis, it is sufficient that it be an axis of twofold or higher rotational symmetry, or normal to a reflection plane, or normal to an axis of sixfold symmetry.

(2) For x_3 to be a degenerate pure mode axis, it is sufficient that it be an axis of threefold or higher rotational symmetry.

The use of the symmetry table in the computation of the D_{ij} is indicated by the following example. Consider propagation near the pure mode axis [101] in a cubic crystal. $\alpha=\pi/4$, $\beta=\gamma=0$ in Fig. 1, with the result that the y_1 and y_3 axes are twofold, and the y_2 axis fourfold. The superposition of symmetry elements S_{12}, S_{32}, and

[11] C. Kittel, *Introduction to Solid State Physics* (John Wiley and Sons, Inc., New York, 1956), second edition, p. 24.

[12] W. Voigt, *Lehrbuch der Kristallphysik* (B. G. Teubner, Leipzig, 1910), p. 583.

[13] C. Zener, *Elasticity and Anelasticity of Metals* (University of Chicago Press, Chicago, 1948), p. 14.

S_{24} in Table I gives for the array of D_{ij}'s the form

$$\begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 0 \\ 12 & 22 & 12 & 0 & 0 & 0 \\ 13 & 12 & 11 & 0 & 0 & 0 \\ 0 & 0 & 0 & 44 & 0 & 0 \\ 0 & 0 & 0 & 0 & 55 & 0 \\ 0 & 0 & 0 & 0 & 0 & 44 \end{bmatrix}; \tag{3.1}$$

hence one needs to compute only D_{11}, D_{12}, D_{13}, D_{22}, D_{44}, and D_{55} from Eqs. (2.9).

Using Table I, we may immediately write down the elastic constants in the crystal coordinates $\{a_i\}$ for any crystal system. This is done in Table II for the four systems of interest here, with the symmetry elements S_{ij} listed for each system.

As velocities rather than elastic moduli are measured experimentally, it is more appropriate to give results in terms of fractional changes in velocity, defined by

$$\Delta v_i/v_i = \Delta\mu_i/2\mu_i = (\mu_i - a_i^0)/2\mu_i. \tag{3.2}$$

The resulting velocities, fractional changes in velocity, and eigenvectors are given below, correct to lowest order terms in the *polar misorientation angle* θ.

Table II. The form of the crystalline elastic constants c_{ij} for cubic, hexagonal, tetragonal, and trigonal symmetry. The symmetry elements S_{ij} are indicated in each case.

Cubic: S_{14}, S_{24}, S_{34}	$\begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix}$
Hexagonal: S_{36}	$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}$
Tetragonal: S_{12}, S_{22}, S_{34}	$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix}$
Trigonal: S_{33}	$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & -c_{25} & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & c_{25} & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & c_{25} \\ -c_{25} & c_{25} & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & c_{25} & c_{14} & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}$

Cubic System

Define

$$K_1 = c_{11} - c_{12} - 2c_{44},$$
$$K_2 = K_1/(c_{44} - c_{11}) + 2,$$
$$K_3 = K_1/(c_{12} + c_{44}) + \tfrac{3}{2},$$
$$K_4 = K_1/2(c_{11} + c_{12}) + \tfrac{3}{2}.$$

Propagation direction $\approx[001]$: S_{14}, S_{24}, S_{34}; $\alpha=\beta=\gamma=0$

$$v_1 = v_2 = (c_{44}/\rho)^{\frac{1}{2}}; \quad v_3 = (c_{11}/\rho)^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1} = \frac{K_1\theta^2}{4c_{44}}\{K_2 + [K_2^2 - \sin^2 2\phi(2K_2-1)]^{\frac{1}{2}}\},$$

$$\frac{\Delta v_2}{v_2} = \frac{K_1\theta^2}{4c_{44}}\{K_2 - [K_2^2 - \sin^2 2\phi(2K_2-1)]^{\frac{1}{2}}\},$$

$$\frac{\Delta v_3}{v_3} = \frac{-K_1K_2}{2c_{11}}\theta^2,$$

$$N = \frac{K_2(\cos^2\phi - \sin^2\phi) - [K_2^2 - \sin^2 2\phi(2K_2-1)]^{\frac{1}{2}}}{2\sin\phi\cos\phi(1-K_2)},$$

$$A_1{}^{(1)} = A_2{}^{(2)} = [1+N^2]^{-\frac{1}{2}},$$
$$A_2{}^{(1)} = -A_1{}^{(2)} = N[1+N^2]^{-\frac{1}{2}},$$
$$A_3{}^{(1)} = (2-K_2)[1+N^2]^{-\frac{1}{2}}(\cos\phi + N\sin\phi)\theta,$$
$$A_3{}^{(2)} = (2-K_2)[1+N^2]^{-\frac{1}{2}}(\sin\phi - N\cos\phi)\theta,$$
$$A_1{}^{(3)} = \theta\cos\phi(K_2-2),$$
$$A_2{}^{(3)} = \theta\sin\phi(K_2-2),$$
$$A_3{}^{(3)} = 1.$$

Propagation direction $\approx[101]$: S_{12}, S_{24}, S_{32}; $\alpha=\pi/4$, $\beta=\gamma=0$

$$v_1 = [(c_{11}-c_{12})/2\rho]^{\frac{1}{2}}; \quad v_2 = (c_{44}/\rho)^{\frac{1}{2}};$$
$$v_3 = [(c_{11}+c_{12}+2c_{44})/2\rho]^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1} = \frac{-K_1\theta^2}{2(c_{11}-c_{12})}[2K_3\cos^2\phi + 1],$$

$$\frac{\Delta v_2}{v_2} = \frac{K_1(3-K_4)}{2c_{44}}\theta^2\sin^2\phi,$$

$$\frac{\Delta v_3}{v_3} = \frac{K_1\theta^2[(2K_3+1)\cos^2\phi + (2K_4-5)\sin^2\phi]}{2(c_{11}+c_{12}+2c_{44})},$$

$$A_{(i)}{}^{(i)} = 1,$$
$$A_2{}^{(1)} = \theta^2\cos\phi\sin\phi(K_3-3),$$
$$A_1{}^{(2)} = \theta^2\sin 2\phi(15/4 - 2K_4),$$
$$A_3{}^{(1)} = -A_1{}^{(3)} = \theta\cos\phi(3-2K_3)/2,$$
$$A_3{}^{(2)} = -A_2{}^{(3)} = \theta\sin\phi(2K_4-3).$$

Propagation direction $\approx[111]$: S_{22}, S_{33}; $\alpha=\tan^{-1}\sqrt{2}$, $\beta=\pi/4$, $\gamma=0$

$$v_1 = v_2 = [(c_{11}-c_{12}+c_{44})/3\rho]^{\frac{1}{2}};$$
$$v_3 = [(c_{11}+2c_{12}+4c_{44})/3\rho]^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1} = \frac{-K_1\theta}{2(c_{11}-c_{12}+c_{44})}, \quad \frac{\Delta v_2}{v_2} = \frac{+K_1\theta}{2(c_{11}-c_{12}+c_{44})},$$

$$\frac{\Delta v_3}{v_3} = \frac{K_1[2K_3+3]\theta^2}{3(c_{11}+2c_{12}+4c_{44})},$$

$A_1^{(1)}=A_2^{(2)}=\cos(\phi/2)$,

$A_2^{(1)}=-A_1^{(2)}=-\sin(\varphi/2)$,

$A_3^{(1)}=\frac{1}{3}[2K_3-3]\theta\cos(\phi/2)[4\sin^2(\phi/2)-1]$,

$A_3^{(2)}=\frac{1}{3}[2K_3-3]\theta\sin(\phi/2)[1-4\cos^2(\phi/2)]$,

$A_1^{(3)}=\frac{1}{3}[2K_3-3]\theta\cos\phi$,

$A_2^{(3)}=\frac{1}{3}[2K_3-3]\theta\sin\phi$,

$A_3^{(3)}=1$.

Hexagonal System

Propagation direction $\approx$*[0001]*: S_{12}, S_{22}, S_{36}; $\alpha=\beta=\gamma=0$

$$v_1=v_2=(c_{44}/\rho)^{\frac{1}{2}};\quad v_3=(c_{33}/\rho)^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1}=\frac{\theta^2}{2c_{44}}\left[c_{11}-\frac{c_{13}^2+c_{44}(c_{33}+2c_{13})}{c_{33}-c_{44}}\right],$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta^2}{4c_{44}}[c_{11}-c_{12}-2c_{44}],$$

$$\frac{\Delta v_3}{v_3}=\theta^2\frac{(2c_{44}+c_{13}-c_{33})(c_{33}+c_{13})}{2c_{33}(c_{33}-c_{44})},$$

$A_1^{(1)}=A_2^{(2)}=\cos\phi$,

$A_2^{(1)}=-A_1^{(2)}=\sin\phi$,

$A_3^{(1)}=\theta(2c_{44}-c_{33}+c_{13})/(c_{44}-c_{33})$,

$A_3^{(2)}=O(\theta^2)$,

$A_1^{(3)}=\theta\cos\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44})$,

$A_2^{(3)}=\theta\sin\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44})$,

$A_3^{(3)}=1$.

Propagation direction nearly in base plane: S_{16}; $\alpha=\pi/2$, β *arbitrary*, $\gamma=0$

$$v_1=(c_{44}/\rho)^{\frac{1}{2}};\quad v_2=[(c_{11}-c_{12})/2\rho]^{\frac{1}{2}};\quad v_3=(c_{11}/\rho)^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1}=\frac{\theta^2\cos^2\phi}{2c_{44}}\left[c_{33}+\frac{c_{13}^2+(c_{11}+2c_{13})c_{44}}{c_{44}-c_{11}}\right],$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta^2\cos^2\phi}{2(c_{11}-c_{12})}[2c_{44}+c_{12}-c_{11}],$$

$$\frac{\Delta v_3}{v_3}=\frac{\theta^2\cos^2\phi}{2c_{11}}\frac{(c_{11}+c_{13})(2c_{44}+c_{13}-c_{11})}{c_{11}-c_{44}},$$

$A_{(i)}^{(i)}=1$,

$A_2^{(1)}=-A_1^{(2)}=-\frac{1}{4}\theta^2\sin2\phi$,

$A_3^{(1)}=-A_1^{(3)}=\theta\cos\phi[c_{11}-c_{13}-2c_{44}]/(c_{11}-c_{44})$,

$A_3^{(2)}=O(\theta^?)$,

$A_2^{(3)}=O(\theta^2)$.

Tetragonal System

Propagation direction $\approx$*[001]*: S_{12}, S_{22}, S_{32}; $\alpha=\beta=\gamma=0$

$$v_1=v_2=(c_{44}/\rho)^{\frac{1}{2}};\quad v_3=(c_{33}/\rho)^{\frac{1}{2}},$$

$$\begin{aligned}M=&\cos^2 2\phi(c_{11}+c_{33}-c_{66}-2c_{13}-3c_{44})\\&\times\left\{c_{11}+c_{33}-c_{66}-2c_{13}-3c_{44}-\frac{2(2c_{44}-c_{33}+c_{13})^2}{c_{33}-c_{44}}\right\}\\&+\sin^2 2\phi(c_{33}+c_{66}+c_{12}-2c_{13}-3c_{44})\\&\times\left\{c_{33}+c_{66}+c_{12}-2c_{13}-3c_{44}-\frac{2(2c_{44}-c_{33}+c_{13})^2}{c_{33}-c_{44}}\right\}\\&+(2c_{44}-c_{33}+c_{13})^4/(c_{33}-c_{44})^2,\end{aligned}$$

$$\frac{\Delta v_1}{v_1}=\frac{\theta^2}{4c_{44}}\left\{c_{11}-c_{44}+c_{66}+\frac{c_{13}^2+(c_{33}-2c_{13})c_{44}}{c_{33}-c_{44}}+M^{\frac{1}{2}}\right\},$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta^2}{4c_{44}}\left\{c_{11}-c_{44}+c_{66}+\frac{c_{13}^2+(c_{33}-2c_{13})c_{44}}{c_{33}-c_{44}}-M^{\frac{1}{2}}\right\},$$

$$\frac{\Delta v_3}{v_3}=\frac{\theta^2}{2c_{33}}\frac{(c_{13}+c_{33})(2c_{44}+c_{13}-c_{33})}{c_{33}-c_{44}},$$

$$N=\tan\varphi[1+(c_{11}-c_{12})\cos2\phi/D],$$

where

$$\begin{aligned}D\equiv&(c_{11}-c_{12}-c_{66})\sin^2\phi+c_{66}\cos^2\phi\\&+[2c_{44}-c_{33}+c_{13}]^2/2(c_{33}-c_{44})\\&-\tfrac{1}{2}(c_{11}+c_{33}+c_{66}-2c_{13}-7c_{44})-\tfrac{1}{2}M^{\frac{1}{2}},\end{aligned}$$

$A_1^{(1)}=A_2^{(2)}=[1+N^2]^{-\frac{1}{2}}$,

$A_2^{(1)}=-A_1^{(2)}=N[1+N^2]^{-\frac{1}{2}}$,

$$A_3^{(1)}=(\cos\phi+N\sin\phi)[1+N^2]^{-\frac{1}{2}}\times[(2c_{44}-c_{33}+c_{13})/(c_{44}-c_{33})]\theta,$$

$$A_3^{(2)}=(\sin\phi-N\cos\phi)[1+N^2]^{-\frac{1}{2}}\times[(2c_{44}-c_{33}+c_{13})/(c_{44}-c_{33})]\theta,$$

$A_1^{(3)}=\theta\cos\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44})$,

$A_2^{(3)}=\theta\sin\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44})$,

$A_3^{(3)}=1$.

Propagation direction $\approx$*[100]*: S_{14}, S_{22}, S_{32}; $\alpha=\pi/2$, $\beta=\gamma=0$

$$v_1=(c_{44}/\rho)^{\frac{1}{2}};\quad v_2=(c_{66}/\rho)^{\frac{1}{2}};\quad v_3=(c_{11}/\rho)^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1}=\frac{\theta^2\cos^2\phi}{2c_{44}}\left\{c_{33}+\frac{c_{13}^2+(c_{11}+2c_{13})c_{44}}{c_{44}-c_{11}}\right\},$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta^2}{2c_{66}}\left\{c_{44}-c_{66}+\sin^2\phi\left[c_{11}-c_{44}+\frac{(c_{12}+c_{66})^2}{c_{66}-c_{11}}\right]\right\},$$

$$\frac{\Delta v_3}{v_3}=\frac{\theta^2}{2c_{11}}\left\{\sin^2\phi\frac{(2c_{66}+c_{12}-c_{11})(c_{11}+c_{12})}{c_{11}-c_{66}}+\cos^2\phi\frac{(2c_{44}+c_{13}-c_{11})(c_{11}+c_{13})}{c_{11}-c_{44}}\right\},$$

$A_{(i)}^{(i)}=1,$

$$A_2^{(1)}=\frac{\theta^2\sin2\phi[c_{44}(5c_{66}-c_{11}+2c_{12}-3c_{44})+2c_{13}(2c_{66}-c_{11}+c_{12})-c_{11}c_{66}]}{4(c_{11}-c_{44})(c_{66}-c_{44})},$$

$$A_1^{(2)}=\frac{\theta^2\sin2\phi[c_{44}(7c_{66}-3c_{11}+2c_{12})+2c_{13}(c_{12}-c_{11}+2c_{66})+c_{66}(c_{11}-c_{12}-3c_{66})]}{4(c_{11}-c_{66})(c_{44}-c_{66})},$$

$$A_3^{(1)}=-A_1^{(3)}=\theta\cos\phi(2c_{44}-c_{11}+c_{13})/(c_{44}-c_{11}),$$

$$A_3^{(2)}=-A_2^{(3)}=\theta\sin\phi(2c_{66}-c_{11}+c_{12})/(c_{66}-c_{11}).$$

Propagation direction $\approx[110]$: S_{14}, S_{22}, S_{32}; $\alpha=\pi/2$, $\beta=\pi/4$, $\gamma=0$

$$v_1=(c_{44}/\rho)^{\frac{1}{2}};\quad v_2=[(c_{11}-c_{12})/2\rho]^{\frac{1}{2}};$$
$$v_3=[(c_{11}+c_{12}+2c_{66})/2\rho]^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1}=\frac{\theta^2\cos^2\phi}{2c_{44}}\left\{c_{33}-c_{44}+\frac{2(c_{13}+c_{44})^2}{2c_{44}-c_{11}-c_{12}-2c_{66}}\right\},$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta^2}{2(c_{11}-c_{12})}\left\{\cos^2\phi(2c_{44}+c_{12}-c_{11})+2\sin^2\phi\frac{(2c_{66}+c_{12}-c_{11})(4c_{66}+3c_{12}-c_{11})}{c_{12}+c_{66}}\right\}$$

$$\frac{\Delta v_3}{v_3}=\frac{\theta^2}{2(c_{11}+c_{12}+2c_{66})}\left\{2\sin^2\phi\frac{(c_{11}-c_{12}-2c_{66})(c_{11}+c_{12})}{c_{12}+c_{66}}-\cos^2\phi\frac{(c_{11}+c_{12}+2c_{13}+2c_{66})\times(c_{11}+c_{12}-2c_{13}-4c_{44}+2c_{66})}{c_{11}+c_{12}-2c_{44}+2c_{66}}\right\},$$

$A_{(i)}^{(i)}=1,$

$$A_2^{(1)}=\frac{\theta^2\sin\phi\cos\phi}{2(c_{11}+c_{12}+2c_{66}-2c_{44})(c_{11}-c_{12}-2c_{44})}\times[c_{11}(8c_{13}+14c_{44}-c_{11})-2c_{66}(c_{11}+8c_{13}+4c_{44})+c_{12}(c_{12}+2c_{66}-6c_{44}-8c_{13})-8c_{44}^2],$$

$$A_1^{(2)}=\frac{\theta^2\sin\phi\cos\phi}{2(c_{12}+c_{66})(2c_{44}-c_{11}+c_{12})}\times[c_{11}(4c_{13}+8c_{44}-2c_{11}+3c_{12}+3c_{66})-c_{12}(c_{12}+4c_{13}+4c_{44}-3c_{66})-4c_{66}(2c_{13}+3c_{44})],$$

$$A_3^{(1)}=-A_1^{(3)}=\theta\cos\phi\frac{(c_{11}+c_{12}+2c_{66}-4c_{44}-2c_{13})}{c_{11}+c_{12}+2c_{66}-2c_{44}},$$

$$A_3^{(2)}=-A_2^{(3)}=\theta\sin\phi(c_{12}+2c_{66}-c_{11})/(c_{12}+c_{66}).$$

Trigonal System

Propagation direction $\approx[001]$: S_{33}; $\alpha=\beta=\gamma=0$

$$v_1=v_2=(c_{44}/\rho)^{\frac{1}{2}};\quad v_3=(c_{33}/\rho)^{\frac{1}{2}},$$

$$\frac{\Delta v_1}{v_1}=-\frac{\theta[c_{14}^2+c_{25}^2]^{\frac{1}{2}}}{c_{44}},$$

$$\frac{\Delta v_2}{v_2}=\frac{\theta[c_{14}^2+c_{25}^2]^{\frac{1}{2}}}{c_{44}},$$

$$\frac{\Delta v_3}{v_3}=\theta^2\frac{(2c_{44}+c_{13}-c_{33})(c_{13}+c_{33})}{2c_{33}(c_{33}-c_{44})},$$

$$N=\frac{c_{25}\cos\phi-c_{14}\sin\phi-[c_{14}^2+c_{25}^2]^{\frac{1}{2}}}{c_{14}\cos\phi+c_{25}\sin\phi},$$

$$A_1^{(1)}=A_2^{(2)}=[1+N^2]^{-\frac{1}{2}},$$
$$A_2^{(1)}=-A_1^{(2)}=N[1+N^2]^{-\frac{1}{2}},$$
$$A_3^{(1)}=\theta(\cos\phi+N\sin\phi)[1+N^2]^{-\frac{1}{2}}\times(2c_{44}-c_{33}+c_{13})/(c_{44}-c_{33}),$$
$$A_3^{(2)}=\theta(\sin\phi-N\cos\phi)[1+N^2]^{-\frac{1}{2}}\times(2c_{44}-c_{33}+c_{13})/(c_{44}-c_{33}),$$
$$A_1^{(3)}=\theta\cos\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44}),$$
$$A_2^{(3)}=\theta\sin\phi(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44}),$$
$$A_3^{(3)}=1.$$

4. NUMERICAL RESULTS FOR SEVERAL CUBIC CRYSTALS

It is appropriate to interrupt the theoretical discussion at this point to give some numerical results for fractional velocity changes, in order that the reader gain insight to the order of magnitude of effects being discussed.

The anisotropy factor A for cubic crystals is defined by[14]

$$A=2c_{44}/(c_{11}-c_{12}). \tag{4.1}$$

A crystal becomes elastically isotropic when $A=1$, so that pure transverse and longitudinal modes with fixed velocities will propagate in any direction. This is borne out in the preceding tabulation, as all fractional changes in velocity for cubic crystals are proportional to $K_1\equiv c_{11}-c_{12}-2c_{44}$, and the condition for isotropy may be written as

$$K_1=0. \tag{4.2}$$

The elastic constants for several cubic crystals are listed in Table III. Zener[15] has compiled a large share of the constants given. From the elastic constants the K_i, as defined in Sec. 3, are computed and tabulated, and from the K_i fractional velocity changes for any propagation direction may be obtained easily. Specifi-

[14] Reference 11, p. 95.
[15] Reference 13, p. 17.

TABLE III. A tabulation of the c_{ij} and K_i for several cubic crystals. K_1 and the c_{ij} are in units of 10^{12} dyne cm^{-2}. The last three columns give the ratios of the maximum fractional difference velocities to the square of the polar misorientation angle θ for the three quasi-pure modes which may be propagated nearly along the [001] direction.

Crystal	c_{11}	c_{12}	c_{44}	K_1	K_2	K_3	K_4	$\frac{1}{\theta^2}\left(\frac{\Delta v_1}{v_1}\right)_{\max}$	$\frac{1}{\theta^2}\left(\frac{\Delta v_2}{v_2}\right)_{\max}$	$\frac{1}{\theta^2}\left(\frac{\Delta v_3}{v_3}\right)$
Ag[a]	1.20	0.897	0.436	−0.56	2.73	1.08	1.37	−1.7	−0.32	+0.63
Al[a]	1.08	0.622	0.284	−0.11	2.14	1.38	1.18	−0.41	−0.097	+0.11
Au[a]	1.86	1.57	0.420	−0.55	2.38	1.22	1.420	−1.5	−0.32	+0.35
α-brass[a]	1.47	1.11	0.72	−1.08	3.44	0.910	1.291	−2.58	−0.375	+1.26
β-brass[b]	1.279	1.091	0.822	−1.456	5.18	0.739	1.193	−4.58	−0.443	+2.95
C (diamond)[c]	9.2	3.9	4.3	−3.3	2.67	1.10	1.38	−1.0	−0.19	+0.48
Cu[a]	1.70	1.23	0.753	−1.03	3.08	0.979	1.324	−2.12	−0.342	+0.933
Cu_3Au[d]	2.25	1.73	0.663	−0.80	3.35	1.17	1.40	−2.0	−0.30	+0.60
Fe(α)[a]	2.37	1.41	1.16	−1.36	3.12	0.971	1.320	−1.83	−0.293	+0.895
Ge[e]	1.30	0.49	0.67	−0.53	2.84	1.05	1.36	−1.12	−0.197	+0.579
K[f]	0.0459	0.0372	0.0263	−0.0439	4.24	0.808	1.236	−3.54	−0.417	+2.03
KBr[g]	0.35	0.058	0.050	+0.20	1.34	3.3	1.75	+2.6	+1.0	−0.38
KCl[g]	0.40	0.062	0.062	+0.22	1.36	3.3	1.74	+2.4	+0.88	−0.37
Na[h]	0.0555	0.0425	0.0491	−0.0852	15.3	0.569	1.065	−13.3	−0.434	+10.7
NaCl[g]	0.49	0.124	0.126	+0.12	1.68	1.98	1.60	+0.80	+0.23	−0.17
Pb[i]	0.483	0.409	0.144	−0.214	2.63	1.113	1.380	−1.95	−0.372	+0.583
Si[j]	1.67	0.65	0.79	−0.56	2.63	1.11	1.38	−0.93	−0.17	+0.44
W[a]	5.01	1.98	1.51	−0.01	1.997	1.497	1.499	−0.006	−0.001	+0.002

[a] E. Schmid and W. Boas, *Kristallplastizität* (Verlag Julius Springer, Berlin, 1935), pp. 21, 200.
[b] D. Lazarus, Phys. Rev. **74**, 1726 (1948).
[c] S. Bhagavantam and J. Bhimasenachar, Nature **154**, 546 (1944).
[d] S. Siegel, Phys. Rev. **57**, 537 (1940).
[e] Bond, Mason, McSkimin, Olsen, and Teal, Phys. Rev. **78**, 176 (1950).
[f] O. Bender, Ann. Physik **34**, 359 (1939).
[g] J. K. Galt, Phys. Rev. **73**, 1460 (1948).
[h] S. L. Quimby and S. Sigel, Phys. Rev. **54**, 293 (1938).
[i] E. Goens and J. Weerts, Physik. Z. **37**, 321 (1936).
[j] McSkimin, Bond, Buehler, and Teal, Phys. Rev. **83**, 1080 (1951).

cally for propagation nearly in the [001] direction, one has

$$\frac{\Delta v_1}{v_1}=\frac{K_1\theta^2}{4c_{44}}\{K_2+[K_2^2-\sin^2 2\phi(2K_2-1)]^{\frac{1}{2}}\} \quad (4.3)$$

from Sec. 3. For convenience in tabulating, we remove the dependence on the *azimuthal misorientation angle* ϕ by choosing ϕ such that $\Delta v_1/v_1$ is maximum. Since $K_2>0.5$ for all the crystals considered in Table III, this maximum occurs when $\phi=0$. This choice is made with an eye to presenting a table of some use to the experimenter interested in measuring velocities. Lacking explicit knowledge of the misorientation angles from x-ray measurements, he may have an order-of-magnitude estimate of the *polar misorientation angle* θ from the technique employed to orient the specimen faces, whereas ϕ can be quite arbitrary. Using the estimated value of θ, he may obtain the maximum resulting fractional velocity change from Table III, and if this is not sufficiently large to influence his measurements, no correction is necessary.

Setting $\phi=0$ and dividing through by θ^2 gives

$$\frac{1}{\theta^2}\left(\frac{\Delta v_1}{v_1}\right)_{\max}=\frac{K_1K_2}{2c_{44}}. \quad (4.4)$$

In like manner one obtains

$$\frac{1}{\theta^2}\left(\frac{\Delta v_2}{v_2}\right)_{\max}=\frac{K_1}{4c_{44}} \quad (4.5)$$

for the other quasi-transverse mode. As the quasi-longitudinal mode is independent of ϕ, one has

$$\frac{1}{\theta^2}\frac{\Delta v_3}{v_3}=\frac{-K_1K_2}{2c_{11}}. \quad (4.6)$$

The three fractional velocity changes, defined in this manner, are tabulated in Table III. From the table we get for silicon, for example,

$$(\Delta v_1/v_1)_{\max}=-0.93\theta^2. \quad (4.7)$$

For a polar misorientation angle $\theta=1°=0.0174$ rad, one obtains

$$(\Delta v_1/v_1)_{\max}=-2.8\times10^{-4}, \quad (4.8)$$

which is significant in a velocity measurement of 0.01% desired accuracy. The choice confronting the experimenter is obvious. He must either orient the specimen precisely enough that his measurements are not influenced by fractional velocity changes, or determine the degree of misorientation by x-ray or other methods and correct his measurements accordingly.

5. ENERGY FLUX

The energy flux vectors associated with plane elastic modes are of considerable interest both theoretically and experimentally. Those cases in which internal conical refraction arises present an intriguing problem in the nearly virgin field of diffraction effects in anisotropic media. The incidence of a plane wave on a stress-free surface gives rise to a rather peculiar law of reflection. With regard to pulsed ultrasound experiments, when the specimen cross section is not appreciably larger than the cross section of the excited region or when for some reason it becomes necessary to excited the specimen near an edge, deviation of energy from the propagation direction may cause the wave to impinge on side walls, giving rise to mode conversion and deteriorating the echo train. It is hoped that the discussion to follow will serve the dual purpose of pointing out such difficulties, at the same time stimulating further experimental investigation of the energy flux itself.

The derivation of the energy flux associated with an arbitrary excitation is discussed by Love.[16] Briefly, the x_i component of the energy flux vector is given by the scalar product $-\mathbf{T}^{(i)}\cdot(\partial\mathbf{u}/\partial t)$ of the stress vector $\mathbf{T}^{(i)}$ on the surface normal to the x_i direction, having components $T_j^{(i)}=\sigma_{ij}$, with the particle velocity $\partial\mathbf{u}/\partial t$. The minus sign arises from the convention used in defining the stress tensor. Averaging over one period, one then obtains for the ith component of the energy flux vector $\mathbf{P}^{(j)}$ associated with mode j

$$P_i^{(j)}=\frac{(p\omega)^2}{2v_j}F_{imn3}A_m^{(j)}A_n^{(j)}. \tag{5.1}$$

Here p is the amplitude of elastic displacement, $A^{(j)}$ the unit displacement vector, and v_j the phase velocity. The displacement $u^{(j)}$ is as given in Eq. (2.6) but now multiplied by p. Note that the term *propagation direction* has become somewhat ambiguous. We shall use it to refer to the normal to surfaces of equal phase.

Consider first the perfectly oriented case; that is, x_3 is a pure mode axis and $F_{ijkl}\equiv D_{ijkl}$. One finds from Eq. (5.1) that the energy flux associated with a pure longitudinal mode may never deviate from the propagation direction—that is, the energy flux vector is parallel to the x_3 axis. The same result holds for a pure transverse mode, provided the D_{ij} have the form

$$\begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 16\\ 12 & 22 & 23 & 0 & 0 & 26\\ 13 & 23 & 33 & 0 & 0 & 36\\ 0 & 0 & 0 & 44 & 45 & 0\\ 0 & 0 & 0 & 45 & 55 & 0\\ 16 & 26 & 36 & 0 & 0 & 66 \end{bmatrix}. \tag{5.2}$$

Inspection of the symmetry table of Sec. 3 reveals that this form is met if the propagation direction is a twofold, fourfold, or sixfold symmetry axis, or normal to a plane of reflection symmetry. If the propagation direction is not included in these four categories, then one may expect in general a *deviation* of energy flux from the propagation direction.

Specifically for propagation along an axis of threefold symmetry, this deviation manifests itself in the form of internal conical refraction. A propagation axis of threefold symmetry is encountered twice in the explicit solutions considered in Sec. 3: first, the [111] direction of a cubic crystal, and second the [001] direction of a trigonal crystal. As a threefold symmetry propagation direction is degenerate, there are no preferred directions of particle vibration for a pure transverse mode and one may take

$$A_1^{(1)}=\cos\psi,\quad A_2^{(1)}=\sin\psi,\quad A_3^{(1)}=0, \tag{5.3}$$

as the components of the eigenvector $\mathbf{A}^{(1)}$ associated with eigenvalue μ_1. Inserting $\mathbf{A}^{(1)}$ in Eq. (5.1) gives

$$P_i^{(1)}=[(p\omega)^2/2v_1][D_{i113}\cos^2\psi + (D_{i123}+D_{i213})\sin\psi\cos\psi+D_{i223}\sin^2\psi]. \tag{5.4}$$

To obtain the D_{ij} for propagation in the [111] direction of a cubic crystal, one performs the coordinate transformation with $\alpha=\tan^{-1}\sqrt{2}$, $\beta=\pi/4$, $\gamma=0$. Observing that the x_2 and x_3 axes ($x_i\equiv y_i$) are, respectively, twofold and threefold, by superposition of elements S_{22} and S_{33} of the symmetry table one obtains for the form of the D_{ij} the array

$$\begin{bmatrix} 11 & 12 & 13 & 0 & -25 & 0\\ 12 & 11 & 13 & 0 & 25 & 0\\ 13 & 13 & 33 & 0 & 0 & 0\\ 0 & 0 & 0 & 44 & 0 & 25\\ -25 & 25 & 0 & 0 & 44 & 0\\ 0 & 0 & 0 & 25 & 0 & \frac{1}{2}(11-12) \end{bmatrix}. \tag{5.5}$$

From Eq. (2.9) one may obtain

$$D_{44}=\tfrac{1}{3}(K_1+3c_{44}),\quad D_{25}=(\sqrt{2}/6)K_1, \tag{5.6}$$

where $K_1\equiv c_{11}-c_{12}-2_{44}$ as defined in Sec. 3. Making use of these results, Eq. (5.4) gives for the components of energy flux

$$\begin{aligned} P_1^{(1)}&=-\frac{2(p\omega)^2K_1}{12v_1}\cos 2\psi,\\ P_2^{(1)}&=+\frac{2(p\omega)^2K_1}{12v_1}\sin 2\psi,\\ P_3^{(1)}&=+\frac{(p\omega)^2(K_1+3c_{44})}{6v_1}. \end{aligned} \tag{5.7}$$

Thus as the plane of particle vibration is rotated about the [111] direction through the angle π, the energy flux vector rotates about the [111] direction *in the opposite sense* through the angle 2π, generating a cone of possible directions for energy flow, as illustrated in Fig. 3. From Eqs. (5.7) one sees that the semiangle of this cone of refraction is given by $\tan^{-1}|K_1/\sqrt{2}(K_1+3c_{44})|$. Similar results have also been given by deKlerk and Musgrave, omitting calculation of the sense of rotation.[17] Using the values of Table III the semiangle is given for

[16] Reference 10, p. 177.

[17] J. deKlerk and M. J. P. Musgrave, Proc. Phys. Soc. (London) **B68**, 81 (1955).

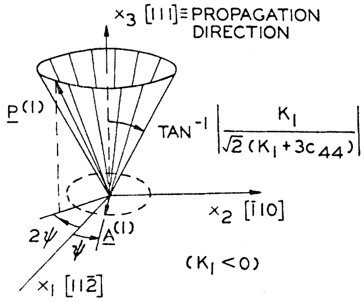

FIG. 3. The geometry of the cone of internal refraction for propagation of a pure transverse mode in the [111] direction in a cubic crystal. The energy flux vector $\mathbf{P}^{(1)}$ associated with polarization $\mathbf{A}^{(1)}$ of the elastic displacement is shown.

several cubic materials as follows: Al, 6 deg; Cu, 31; Ge, 14; KCl, 21; NaCl, 10; Si, 12.

In the same manner, one obtains for propagation in the [001] direction of a trigonal crystal

$$P_1^{(1)}=-\frac{(p\omega)^2(c_{14}^2+c_{25}^2)^{\frac{1}{2}}}{2v_1}\cos(2\psi+B),$$

$$P_2^{(1)}=\frac{(p\omega)^2(c_{14}^2+c_{25}^2)^{\frac{1}{2}}}{2v_1}\sin(2\psi+B),\tag{5.8}$$

$$P_3^{(1)}=\frac{(p\omega)^2c_{44}}{2v_1},$$

where $\tan B=c_{14}/c_{25}$. In this case, shown in Fig. 4, the semiangle of the cone of refraction is given by $\tan^{-1}[c_{25}^2+c_{14}^2]^{\frac{1}{2}}/c_{44}$.

The diffraction effects arising due to the finite size of the source merit brief mention. At first glance one might guess that excitation is nearly confined to a cylindrical region with axis along the direction of energy flux, energy gradually spreading out of this region in much the same manner as it does with a sound source radiating into a semi-infinite perfect fluid.[18] Such a picture is probably qualitatively correct for the perturbed quasi-pure modes discussed below.

In the internal conical refraction cases, however, degeneracy of the pure transverse modes introduces questions of superposition. Assume (in order to sketch a proof by contradiction) that a circular source generating a pure transverse mode gives rise to a single beam of sound energy with axis along the energy flux direction appropriate to the elastic displacements involved. The necessary threefold symmetry under rotation of the displacement direction is met, as may be seen from a study of Fig. 3. Now imagine a second circular source placed at the same location as the first, but with a different direction of the associated (transverse) elastic displacements. Superposition of the sources yields an equivalent source generating, by assumption, a single beam of excitation, whereas superposition of the *effects* of the two sources gives two beams of excitation, clearly an impossible situation.

This dilemma could be avoided if one adopted instead the assumption that a source capable of producing transverse waves with a given displacement direction actually excites a conical region in the medium, various azimuths having *directions* of transverse particle displacement in accord with the geometry of Fig. 3 for the case of propagation in the [111] direction in a cubic crystal. These remarks of course only apply to points sufficiently far removed from the source that their direction cosines relative to all points on the source vary little.

If the superposition principle is to be satisfied, the *magnitude* of transverse particle displacement at various azimuths must be obtained from the displacement vector associated with the source by an operation which commutes with the operation of (vector) addition of the displacements associated with two sources. One suitable operation is that of *projecting* the displacement vector associated with the source on the line of particle motion appropriate to each azimuth. Since the sum of the projections of two vectors in a given direction equals the projection of the vector sum, the same resultant excitation is obtained regardless of whether sources or effects are superposed. The dependence of transverse amplitude on azimuth has the form $|\cos(\phi/2)|$, with ϕ measured from the azimuth at which displacements are parallel to the displacement vector associated with the source. Threefold rotational symmetry is also preserved. When the displacement vector associated with the source is rotated through $2\pi/3$ about the [111] direction, the azimuth of maximum response ($\phi=0$) rotates through $-4\pi/3$, so that an identical geometry is obtained.

This scheme is illustrated in Fig. 5. In Fig. 5(a) the source, shown at the center, is beneath the page, with propagation up out of the page in the [111] direction. The remaining two crystallographic axes are indicated. We are interested in the magnitude of transverse displacements on the large circle representing the intersection of the cone of refraction with the plane of the figure. The lines of particle displacement at four azimuths of the circle, determined from Fig. 3, are shown

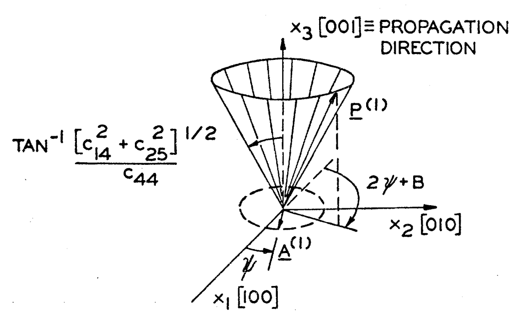

FIG. 4. The geometry of internal conical refraction occurring when a pure transverse mode is propagated along the threefold symmetry axis [001] of a trigonal crystal. The angle B is given by $\tan B=c_{14}/c_{25}$.

[18] Seki, Granato, and Truell, J. Acoust. Soc. Am. **28**, 230 (1956).

dashed. In Fig. 5(b) the displacements (solid arrows) associated with a source polarized in the [11$\bar{2}$] direction are obtained by projecting the displacement vector of the source on the lines of particle motion. The magnitude of displacement at each azimuth is given schematically by the radial distance between the two outermost circles. In Fig. 5(c) the same situation is indicated for a source polarized in the [$\bar{1}$10] direction. Finally, in Fig. 5(d) the displacements associated with the source resulting from superposition of sources Figs. 5(b) and 5(c) are obtained in the same manner. But these displacements are the same as one obtains by superposing those of the preceding two figures, as can be seen at a glance—therefore, superposition holds.

Thus, apart from the detailed diffraction computations required, the general features of the wave motion in cases of internal conical refraction appear to be rather well defined by the three considerations of symmetry, superposition, and geometrical relation between energy flux and direction of particle displacement. Further analysis and experimental work on this topic is warranted. The same approach also appears applicable to the analogous problem in optics, discussed in some detail by Wooster,[19] but has not been considered to the author's knowledge.

Consider next the misoriented case. One would expect the energy flux vector to be perturbed in direction to the order of the polar misorientation angle θ, and this is actually what occurs. As a first example, consider propagation of a quasi-longitudinal mode nearly along the [001] direction of a cubic crystal. From Sec. 3, one has for the components of the perturbed eigenvector

$$\begin{aligned} A_1^{(3)} &= (K_2-2)\theta\cos\phi, \\ A_2^{(3)} &= (K_2-2)\theta\sin\phi, \\ A_3^{(3)} &= 1. \end{aligned} \tag{5.9}$$

Keeping only terms of zeroth and first order in θ *due to contributions of the $A_i^{(3)}$ only*, Eq. (5.1) becomes

$$P_i^{(3)} = \frac{(p\omega)^2}{2v_3}\left[(F_{i133}+F_{i313})A_1^{(3)} + (F_{i233}+F_{i323})A_2^{(3)} + F_{i333}\right]. \tag{5.10}$$

Keeping only terms of zeroth and first order in θ in Eqs. (5.10), one obtains

$$P_i^{(3)} = \frac{(p\omega)^2}{2v_3}\left[(c_{i133}+c_{i313})A_1^{(3)} + (c_{i233}+c_{i323})A_2^{(3)} + \delta_{i3}c_{33} + f_{i3}{}^1\theta\right]. \tag{5.11}$$

Inserting the c_{ij} from Table II and the $f_{i3}{}^1$ from Eqs.

[19] W. A. Wooster, *Crystal Physics* (Cambridge University Press, Cambridge, 1938), p. 148.

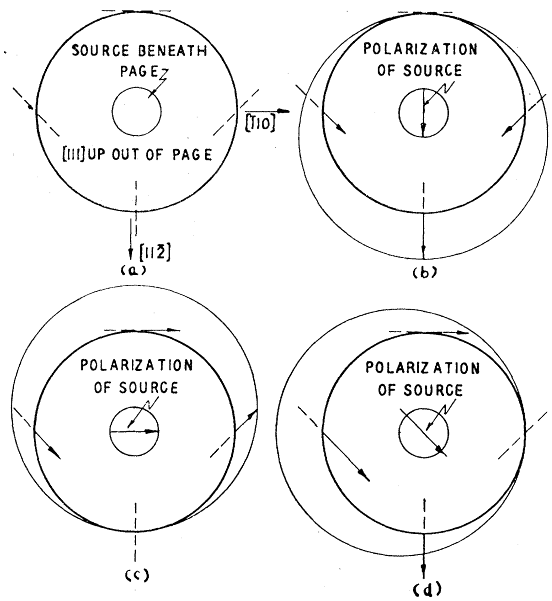

FIG. 5. The geometry of the projection rule for determining the amplitude of transverse particle displacements at various azimuths on the cone of internal refraction. Propagation is up out of the page in the [111] direction. In (a) the directions of particle motion appropriate to four azimuths on a cone with vertex at the center of the source (beneath the page) are shown as dashed lines. In (b) and (c) solid arrows indicate the displacements corresponding to sources polarized in the [11$\bar{2}$] and [$\bar{1}$10] directions, respectively. In (d) the situation is illustrated for a source consisting of the superposition of the previous two. The displacements here may be obtained either by projection or by superposition of the displacements of the two preceding cases, thus verifying that the projection rule satisfies the principle of superposition.

(2.20), one gets finally

$$\begin{aligned} P_1^{(3)} &= \frac{(p\omega)^2(c_{11}+c_{12})(K_2-2)}{2v_3}\theta\cos\phi, \\ P_2^{(3)} &= \frac{(p\omega)^2(c_{11}+c_{12})(K_2-2)}{2v_3}\theta\sin\phi, \\ P_3^{(3)} &= \frac{(p\omega)^2c_{11}}{2v_3}. \end{aligned} \tag{5.12}$$

Defining d_A and d_P as the angles between the eigenvector $\mathbf{A}^{(3)}$ or the energy flux vector $\mathbf{P}^{(3)}$, respectively, and the x_3 axis, one obtains correct to lowest order in θ from Eqs. (5.9) and (5.12)

$$d_A = (K_2-2)\theta, \quad d_P = [(c_{11}+c_{12})(K_2-2)/c_{11}]\theta. \tag{5.13}$$

From the values of Table III one obtains numerical results as follows: Ge, $d_A = 0.84\theta$, $d_P = 1.16\theta$; Cu, $d_A = 1.08\theta$, $d_P = 1.86\theta$. These results are illustrated in Figs. 6 and 7, with θ exaggerated for clarity.

As a second example, consider propagation of a quasi-longitudinal mode nearly along the hexagonal axis of a hexagonal crystal. From Sec. 3, the components of the

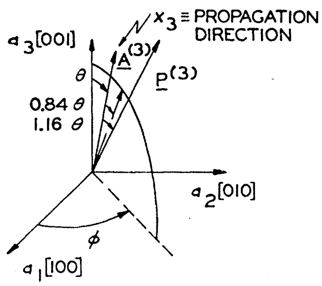

FIG. 6. The displacement $\mathbf{A}^{(3)}$ and energy flux $\mathbf{P}^{(3)}$ associated with a nearly pure longitudinal wave propagating nearly along the [001] direction in germanium.

perturbed eigenvector are given by

$$A_1^{(3)}=L\theta\cos\phi,\quad A_2^{(3)}=L\theta\sin\phi,\quad A_3^{(3)}=1,\tag{5.14}$$

where

$$L\equiv(2c_{44}-c_{33}+c_{13})/(c_{33}-c_{44}).$$

Following the same procedure as above, one obtains correct to lowest order terms in θ

$$P_1^{(3)}=\frac{(p\omega)^2}{2v_3}(c_{13}+c_{33})L\theta\cos\phi,$$

$$P_2^{(3)}=\frac{(p\omega)^2}{2v_3}(c_{13}+c_{33})L\theta\sin\phi,\tag{5.15}$$

$$P_3^{(3)}=\frac{(p\omega)^2}{2v_3}c_{33}.$$

The deviation angles for this case are given by

$$d_A=L\theta,\quad d_P=[(c_{13}+c_{33})/c_{33}]L\theta.\tag{5.16}$$

Using Musgrave's[5] values of the elastic constants for zinc, $c_{11}=1.430$, $c_{12}=0.170$, $c_{13}=0.330$, $c_{33}=0.500$, $c_{44}=0.400\times10^{12}$ dynes/cm^2, one obtains for the deviation angles

$$d_A=6.3\theta,\quad d_P=10.4\theta.\tag{5.17}$$

These results are shown in Fig. 8.

The situation occurring when a plane wave is reflected from a stress-free surface (the back face of a specimen in pulsed ultrasound experiments) is also of interest. It is easily established that an arbitrary infinite plane wave incident normally on a stress-free plane is reflected

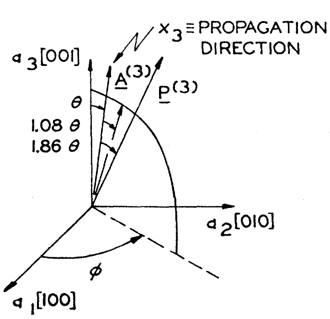

FIG. 7. The displacement $\mathbf{A}^{(3)}$ and energy flux $\mathbf{P}^{(3)}$ of a quasi-longitudinal mode propagating nearly along the [001] direction in copper.

intact, with no mode conversion taking place. This may be verified by substituting the appropriate expressions for elastic displacements in the stress-strain law.

With a finite source the role of the energy flux enters in. As mentioned above, we assume here that the excitation is reasonably well confined to a cylindrical region with axis along the direction of energy flux. Upon striking a stress-free plane surface with angle of *beam incidence* equal to the deviation angle of the energy flux (and with surfaces of equal phase parallel to the reflecting surface) the original mode is reflected. Substituting the appropriately modified expressions for the displacements in the scalar product form of the energy flux vector which precedes Eq. (5.1), the modified energy flux vector is seen to be simply reversed in direction. Thus, regardless of the angle of incidence, the beam is seen to be *reflected back on itself*.

Concerning the influence of energy flux on measurement of ultrasound losses, some comments seem appropriate. First, no major difficulties should arise due to *deviations* of the energy flux from the propagation direction. Because of the peculiar law of reflection for such beams, the signal neglecting diffraction effects

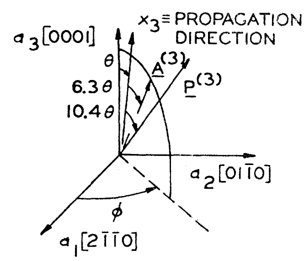

FIG. 8. The displacement $\mathbf{A}^{(3)}$ and energy flux $\mathbf{P}^{(3)}$ of a quasi-longitudinal mode propagating nearly along the hexagonal axis [0001] in zinc. The deviation of energy flux from the propagation direction x_3 is an order of magnitude larger than the polar misorientation angle θ.

should return exactly to the source, where it is observed, with no shift in position. Such deviations may, however, cause the beam to impinge on side walls in specimens of limited cross section, giving rise to mode conversion and general deterioration of the pattern.

The propagation of a quasi-longitudinal mode nearly along the hexagonal axis of a zinc crystal gives a severe example of this, as from the second of Eqs. (5.17) one sees that a misorientation of the order of one degree gives rise to an energy flux deviation of the order of ten degrees. However, if the misorientation angles are known, one may compensate for this deviation by relocating the source. Figure 9(a) shows in cross section a slightly misoriented zinc specimen with quartz transducer cemented on the top surface. The ultrasound beam thus generated impinges on one of the vertical walls of the specimen, resulting in mode conversion losses. In Fig. 9(b) the transducer has been placed so that the beam does not contact any side walls, thus eliminating side-wall interference.

Finally, the combination of diffraction and refraction appears capable of giving rise to severe beam spread in some crystallographic directions. Thus for propagation of a quasi-transverse mode in the neighborhood of a conically refracting direction, for example, one infers from the previous discussion of conical refraction and from continuity arguments that the beam cross section would be crescent-shaped and rapidly increasing with distance.

The speculative nature of much of the above discussion is apparent. It is hoped, however, that such speculations will prove a stimulus to experimental investigation of some of the points in question, thus leading in the end to a more complete picture of the entire situation.

6. SUMMARY

Starting with the equations of motion, the perturbed phase velocities and displacement vectors associated with nearly pure transverse and longitudinal elastic modes have been computed and tabulated for a large number of cases of physical interest. The tabulations are given directly in terms of the conventional crystal elastic constants and the misorientation angles of the

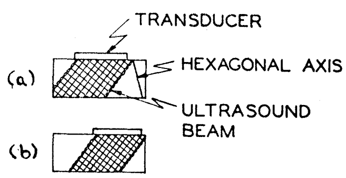

FIG. 9. A cross section of a misoriented zinc specimen, showing the beam geometry for propagation of a quasi-compressional mode nearly along the [0001] (hexagonal) axis. In (a) the quartz transducer is centered on the top face of the specimen, and due to deviation of energy flux the ultrasound beam impinges on a side wall of the specimen, giving rise to mode conversion losses. In (b) the transducer has been moved to one side, thus eliminating this difficulty. Observe that on striking the bottom face, the beam is reflected back in the original direction of incidence.

specimen surface, thus facilitating the corrections necessary to obtain accurate values of the constants from measured phase velocities.

Using the displacements, the components of strain may then be computed from the defining equations. The stresses may next be computed from the generalized Hooke's law, and the components of energy flux computed in the manner described in Sec. 5. In both the latter computations the expansion coefficients f_{ij}^{k} of the misoriented elastic constants, given in Sec. 2, will be indispensable.

A unified approach to the properties of pure elastic modes is provided through the consideration of individual symmetries as discussed in Sec. 3. Such an approach appears convenient for application to situations where lattice defects destroy a part of the crystal symmetry.

There are other immediate applications to the field of ultrasonic measurements in solids. A small misorientation from a degenerate propagation direction splits the transverse phase velocities apart slightly, the vector nature of the two modes resulting giving rise to easily observable interference effects. Such observations have been reported previously by Teutonico and the author,[20] and may prove useful as a technique for fine orientation of specimens.

Finally, the behavior of the energy flux associated with various pure and nearly pure modes was discussed. The influence of energy flux deviations on loss measurements was considered, and some speculations were given on the probable behavior of diffracted waves when conical refraction is present.

ACKNOWLEDGMENTS

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[20] P. C. Waterman and L. J. Teutonico, J. Appl. Phys. **28**, 266 (1957).