Analytic relations between the elastic constants and the group velocity in an arbitrary direction of symmetry planes of media with orthorhombic or higher symmetry

Kwang Yul Kim
Department of Theoretical and Applied Mechanics, Thurston Hall, Cornell University, Ithaca, New York 14853
(Received 20 September 1993)

This paper presents various closed-form analytic formulas that relate the group velocity of elastic pulses propagating in an arbitrary direction of the symmetry planes of elastic media with orthorhombic or higher symmetry to their elastic constants. Simple equations relating the direction of a group velocity to that of the corresponding wave normal are derived for both quasilongitudinal and quasitransverse modes. A forward solution to obtaining the elastic constants from the group-velocity data on the symmetry planes by using these relations is illustrated with examples of transversely isotropic zinc and cubic silicon crystals. Both numerically simulated and experimental data are used to check the derived relations and to demonstrate their usefulness.

I. INTRODUCTION

The elastic constants of materials are conveniently obtained by measuring the phase velocities of elastic waves propagating in various directions of a medium. The relations between the elastic constants and the phase velocity in an arbitrary direction of the medium are found in the solution of the Christoffel equation.[1,2] For an elastic pulse propagating at a group velocity, no analytical equation is found in a closed-form in a general propagation direction of the medium. However, on the symmetry axes of media, the group and phase velocities coincide with each other and this yields some valuable analytic equations relating the group velocities with the elastic constants. While the measurements on the symmetry axes using both longitudinal (L) and transverse (T) modes are sufficient to obtain all three elastic constants of a cubic medium for either group or phase velocities, additional measurements are required in a nonsymmetry direction to determine all the elastic constants of media with hexagonal (transversely isotropic) or lower symmetry. This poses a difficulty with group-velocity data in the determination of elastic constants for the aforementioned reason.

There are other important reasons why we are concerned about the group-velocity measurement. Most acoustic emission (AE) sources found in nature such as crack generation (fracture), phase transformation, friction, dislocation motion, spark discharge, etc. are transient and the resulting elastic waves from these sources propagate at a group velocity. Many simulated AE sources recently used, both in laboratories and for nondestructive materials characterization and inspection, generate elastic pulses propagating at group velocities. Some examples of these simulated AE sources are piezoelectric elastic pulse excitation by a high-voltage electronic pulse generator, thermoelastic pulse generation by a high-power laser or x-ray pulse, and fracture of capillary or pencil-lead on the surface of a specimen and so on.

In order to relieve this difficulty associated with the group-velocity measurements we present in this paper the closed-form analytic relations between the group velocity of an elastic pulse of either quasilongitudinal (QL) or quasitransverse (QT) mode propagating in an arbitrary direction of the symmetry planes of media with orthorhombic or higher symmetry and the elastic constants of the propagating medium. On these symmetry planes one of the transverse waves is pure transverse (PT), and the analytic relations between the group velocity of the PT mode and the shear moduli of the medium are easily found.[1] These analytic group-velocity expressions on the symmetry planes together with those on the symmetry axes of the medium are in most cases more than sufficient to find all the elastic constants. This is not unduly restrictive in scope, because a great majority of materials found in nature belong to orthorhombic or higher-symmetry groups, and even in the phase-velocity measurements for the determination of elastic constants there exists overwhelming reliance on the data of symmetry axes and planes due to the associated simple analytic formulas. There are other great advantages: due to at least an associated mirror symmetry, the variation of the wave speed of some modes about the symmetry axes or planes is minimal and therefore the error associated with a misorientation of the sample in the determination of the elastic constants is also minimized; moreover, anisotropic samples such as single crystals and composites are easily grown along a symmetry axis or fabricated in this direction. The symmetry direction or the symmetry plane is easy to identify by microscopic observations, x-ray or electron diffraction analysis.

Even though these equations are slightly more complicated than the corresponding phase-velocity formulas, their solutions will be shown to be easily found with the aid of a hand calculator or computer algebra such as found in Ref. 3. Useful relations between the directions of a group velocity and the corresponding wave normal in the symmetry plane are derived. A forward solution to obtaining the elastic constants from the group-velocity data on these symmetry planes is illustrated with examples of transversely isotropic zinc and cubic silicon crystals, the QT modes of which have cusps around the symmetry axis. Both numerically simulated and experimen-

0163-1829/94/49(6)/3713(12)/$06.00

tal data are used to check the derived relations and to demonstrate their usefulness. It is shown that the solution is found not only for the QL mode but also for the QT mode within and without the cuspidal region.

II. THEORY

A. Outline of existing analytic formulas for orthorhombic symmetry

To give a general outline of analytic formulas relating the wave speed in a given direction with the elastic constants of the medium, we start with a medium with orthorhombic symmetry. We denote the three orthogonal principal axes of the medium by x_1, x_2, and x_3 directions. The orthorhombic medium is characterized by nine elastic constants: C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13} and C_{23}. The relation between the phase velocities and the elastic constants of the medium is found from the solution of the Christoffel equation[1,2]

$$\det|\Gamma_{ik}-\rho V^2\delta_{ik}|=0 \ , \tag{1}$$

where $\Gamma_{ik}\equiv C_{ijkl}n_j n_l$ is the Christoffel tensor, $\mathbf{n}$ the wave normal, ρ the density of the medium, V the phase velocity, and δ_{ik} the Kronecker delta. Defining the slowness $\mathbf{s}$ as

$$s\equiv\mathbf{n}/V \ , \tag{2}$$

one obtains from Eq. (1) the equation of the slowness surface

$$S=\det|C_{ijkl}s_j s_l-\rho\delta_{ik}|=0 \ . \tag{3}$$

Let ω denote the angular frequency. The group velocity $\mathbf{V}_g$ can be found from the phase velocity or slowness surface S by the following relations

$$\mathbf{V}_g\equiv\nabla_k\omega=\nabla_n V=\frac{\nabla_s S}{\mathbf{s}\cdot\nabla_s S} \ , \tag{4}$$

where $\mathbf{k}=(2\pi/\lambda)\mathbf{n}$ is in the direction of the wave normal $\mathbf{n}$ and λ is the wavelength. The Christoffel tensor Γ_{ik} of an orthorhombic medium is given by

$$\begin{aligned}
\Gamma_{11}&=n_1^2C_{11}+n_2^2C_{66}+n_3^2C_{55} \ ,\\
\Gamma_{22}&=n_1^2C_{66}+n_2^2C_{22}+n_3^2C_{44} \ ,\\
\Gamma_{33}&=n_1^2C_{55}+n_2^2C_{44}+n_3^2C_{33} \ ,\\
\Gamma_{23}&=n_2n_3(C_{23}+C_{44}) \ ,\\
\Gamma_{13}&=n_1n_3(C_{13}+C_{55}) \ ,\\
\Gamma_{12}&=n_1n_2(C_{12}+C_{66}) \ .
\end{aligned} \tag{5}$$

On the x_1, x_2, and x_3 principal axes of propagation the phase and group velocities coincide with each other, and both L and T waves on these axes are of pure mode. Substitution of Eq. (5) into Eq. (1) yields simple analytic equations that relate these wave speeds to the elastic constants of the medium. These relations are easily found in the literature[1,2] and will not be written here. Using these relations, the longitudinal moduli C_{11}, C_{22}, and C_{33} and the shear moduli C_{44}, C_{55}, and C_{66} can be obtained from measurement of the wave speeds of L and T modes propagating in the x_1, x_2, and x_3 directions, respectively.

The shear moduli C_{44}, C_{55}, and C_{66} and the mixed-index moduli C_{12}, C_{13}, and C_{23} can be obtained from measurements of the wave speeds traveling in an arbitrary direction in the symmetry planes, i.e., x_1x_2, x_1,x_3, and x_2x_3 planes. For waves traveling on these planes the basically identical relations between the elastic constants and their speed can be found by the proper rotation of indices. Therefore, we take a wave traveling, for example, in the x_1x_3 symmetry plane with its wave normal $\mathbf{n}$ and group velocity $\mathbf{V}_g$ oriented at angles θ and ζ, respectively, to the x_3 axis, as depicted in Fig. 1. Because of the reflection symmetry of the x_1x_3 plane across the x_1 axis for media of orthorhombic or higher symmetry, we restrict without loss of generality the range of both ζ and θ between $-90°$ and $90°$, that is, $-90°\le\zeta,\theta\le 90°$. Because of the mirror symmetry across this plane, the following identities hold

$$\Gamma_{12}=\Gamma_{23}=0 \ . \tag{6}$$

Using Eq. (6), Eq. (1) can be factored to yield

$$(\Gamma_{22}-\rho V^2)[(\Gamma_{11}-\rho V^2)(\Gamma_{33}-\rho V^2)-\Gamma_{13}^2)]=0 \ . \tag{7}$$

The use of the relations $n_1=\sin\theta$ and $n_3=\cos\theta$ in the first term on the right-hand side of Eq. (7) yields

$$\rho V^2=C_{66}\sin^2\theta+C_{44}\cos^2\theta \quad \text{(PT mode)} \ . \tag{8}$$

The wave mode associated with Eq. (8) is a PT that is polarized in the x_2 direction. Substituting Eq. (2) and the last part of Eq. (4) into Eq. (8) yields for the group velocity

$$\frac{1}{\rho V_g^2}=\frac{\sin^2\zeta}{C_{66}}+\frac{\cos^2\zeta}{C_{44}} \quad \text{(PT mode)} \ . \tag{9}$$

Equations (8) and (9) may be used to obtain both C_{66} and C_{44} by measuring the wave speeds in at least two different directions. By performing similar measurements in the x_1x_2 and x_2x_3 planes, all the shear moduli C_{44}, C_{55}, and C_{66} can be obtained.

Once the pure-index elastic moduli C_{11}, C_{22}, C_{33}, C_{44},

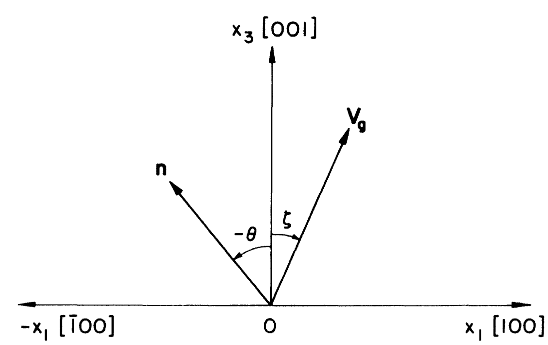

FIG. 1. A schematic for the directions of group velocity and wave normal in the x_1x_3 plane of an orthorhombic medium.

C_{55}, and C_{66} are determined by the method described above, the mixed-index elastic moduli C_{12}, C_{23}, and C_{13} can be obtained from the phase-velocity measurement of either quasilongitudinal (QT) or quasitransverse (QT) modes propagating in the x_1x_2, x_2x_3, and x_1x_3 planes, respectively. Again we take the case of a wave traveling in the x_1x_3 plane. We define for simplicity of notation the following identities

$$C_{11\pm} \equiv C_{11} \pm C_{55} , \tag{10}$$

$$C_{33\pm} \equiv C_{33} \pm C_{55} , \tag{11}$$

$$C_{13\pm} \equiv C_{13} \pm C_{55} . \tag{12}$$

The expression in the square bracket of the left-hand side of Eq. (7) yields for the phase velocity of the QL and QT modes

$$(\rho V^2)^2 - (\Gamma_{11} + \Gamma_{33})\rho V^2 + (\Gamma_{11}\Gamma_{33} - \Gamma_{13}^2) = 0 , \tag{13}$$

which can be solved for ρV^2. The solution for the QL and QT modes is

$$\begin{aligned} 2\rho V^2 = {} & C_{11+}\sin^2\theta + C_{33+}\cos^2\theta \\ & \pm[(C_{11-}\sin^2\theta - C_{33-}\cos^2\theta)^2 \\ & \quad + 4C_{13+}^2\sin^2\theta\cos^2\theta]^{1/2} , \end{aligned} \tag{14}$$

where the positive and negative signs in front of the square root of Eq. (14) correspond to the QL and QT modes, respectively. The above equation (14) relates the elastic constant C_{13} to the phase velocity of the QL or QT mode propagating in an arbitrary direction in the x_1x_3 symmetry plane. Similar equations can be found that relate C_{12} and C_{23} to the phase velocity of the QL or QT mode propagating in the x_1x_2 and x_2x_3 planes, respectively. Thus, for an orthorhombic medium, all nine elastic constants can be determined from the appropriate phase-velocity measurements. However, this is not the case with the group-velocity measurements, because the corresponding analytic expressions that relate the mixed-index elastic moduli to a group velocity are so far unknown to the author. The next subsection deals with the derivation of these analytic equations.

B. Analytic relation between group-velocity and mixed-index elastic constants

1. General formulations

The group velocities corresponding to the points in the x_1x_3 slowness plane can be calculated using the last part of Eq. (4). Because of the mirror symmetry across the plane, all the points in the x_1x_3 slowness plane will map themselves on the x_1x_3 symmetry plane in the group-velocity surface. However, except for a transversely isotropic medium, the converse is not in general true, as is well known in the theory of phonon focusing.[4,5] Because of the nonspherical, concave or convex shape of the QT-mode slowness surface of an anisotropic medium, some points that do not lie in the x_1x_3 section of the QT slowness surface may map themselves into the x_1x_3 group-velocity plane. The group-velocity sections that do not correspond to the x_1x_3 plane of the slowness surface are not of interest here and we deal with only those group-velocity sections that correspond to the x_1x_3 slowness plane.

We define here for simplicity of notation

$$A \equiv C_{11}C_{33} + C_{55}^2 - C_{13+}^2 , \tag{15}$$

$$B \equiv C_{11-}C_{33-} - 2C_{13+}^2 , \tag{16}$$

$$D \equiv [(C_{11-}\tan^2\theta - C_{33-})^2 + 4C_{13+}^2\tan^2\theta]^{1/2} > 0 , \tag{17}$$

$$P_1 \equiv 2C_{11}C_{55}\tan^2\theta + A - \rho s_3^{-2}C_{11+} , \tag{18}$$

$$P_3 \equiv A\tan^2\theta + 2C_{33}C_{55} - \rho s_3^{-2}C_{33+} , \tag{19}$$

$$Q \equiv C_{11+}\tan^2\theta + C_{33+} - 2\rho s_3^{-2} , \tag{20}$$

where the quantity ρs_3^{-2} can be obtained from Eq. (14) and expressed as

$$2\rho s_3^{-2} = C_{11+}\tan^2\theta + C_{33+} \pm D . \tag{21}$$

The positive and negative signs in front of D in Eq. (21) correspond to the QL and QT modes, respectively. D in Eq. (17) is by definition always greater than zero. B in Eq. (16) can be expressed in terms of D as

$$B = \frac{1}{2\tan^2\theta}(C_{11-}^2\tan^4\theta + C_{33-}^2 - D^2) . \tag{22}$$

Substitution of Eq. (21) into Eq. (20) yields the identity

$$Q = \mp D , \tag{23}$$

where the negative and positive signs correspond to the QL and QT modes, respectively.

The group velocity of the PT mode propagating at an angle ζ to the x_3 direction is already described in Eq. (9). The group velocity of both QL and QT modes can be found analytically from the equation of the slowness surface. For this purpose one derives from Eq. (13) the equation of the QL and QT sheets of the slowness surface,

$$\begin{aligned} S = {} & C_{11}C_{55}s_1^4 + C_{33}C_{55}s_3^4 + As_1^2s_3^2 \\ & - \rho(C_{11+}s_1^2 + C_{33+}s_3^2) + \rho^2 = 0 . \end{aligned} \tag{24}$$

The application of the last relation in Eq. (4) to Eq. (24) yields the group-velocity components given by

$$V_{g1} = \frac{s_1P_1}{\rho Q} , \tag{25}$$

$$V_{g3} = \frac{s_3P_3}{\rho Q} . \tag{26}$$

The direction of the group velocity or the energy flux, specified by the angle ζ, can be written as

$$\tan\zeta = \frac{V_{g1}}{V_{g3}} = \tan\theta\frac{P_1}{P_3} . \tag{27}$$

The magnitude of the group velocity is given by

$$\rho V_g^2=\rho(V_{g1}^2+V_{g3}^2)=\frac{s_1^2P_1^2+s_3^2P_3^2}{\rho Q^2}$$
$$=\frac{s_3^2}{\rho Q^2}(P_1^2\tan^2\theta+P_3^2) ,$$

which through Eq. (27) becomes

$$\rho V_g^2=\frac{P_3^2}{\rho s_3^{-2}Q^2\cos^2\zeta} . \tag{28}$$

To proceed further, first we pay attention to the separate case of the QL mode.

2. QL mode

For the QL-mode propagation the upper sign in front of D is applied to Eqs. (21) and (23). The substitution of Eq. (21) into Eqs. (18) and (19) yields

$$P_1=\tfrac{1}{2}(B-C_{11-}^2\tan^2\theta-C_{11+}D) , \tag{29}$$

$$P_3=\tfrac{1}{2}(B\tan^2\theta-C_{33-}^2-C_{33+}D) . \tag{30}$$

Substitution of Eqs. (29) and (30) into Eq. (27) leads to the relationship between the directions of group velocity and wave normal, given by

$$\tan\zeta=\tan\theta\frac{B-C_{11-}^2\tan^2\theta-C_{11+}D}{B\tan^2\theta-C_{33-}^2-C_{33+}D} , \tag{31}$$

which through the use of Eq. (22) yields

$$\tan\zeta=\frac{D^2+2C_{11+}D\tan^2\theta+C_{11-}^2\tan^4\theta-C_{33-}^2}{\tan\theta(D^2+2C_{33+}D-C_{11-}^2\tan^4\theta+C_{33-}^2)} . \tag{32}$$

We rewrite Eq. (31) in the form

$$C_{11-}^2\tan^3\theta+\tan\zeta(B\tan^2\theta-C_{33-}^2)$$
$$-B\tan\theta+(C_{11+}\tan\theta-C_{33+}\tan\zeta)D=0 . \tag{33}$$

Equation (31) or (33) can be used to find the wave normal corresponding to a given group direction lying in the same symmetry plane, and vice versa. Equation (32) is quadratic in D, the solution of which as a function of $\tan\theta$ is written as

$$D(\tan\theta)=\frac{1}{1-\tan\zeta\tan\theta}\{\tan\theta(C_{33+}\tan\zeta-C_{11+}\tan\theta)$$
$$\pm[\tan^2\theta(C_{33+}\tan\zeta-C_{11+}\tan\theta)^2-(1-\tan^2\zeta\tan^2\theta)(C_{11-}^2\tan^4\theta-C_{33-}^2)]^{1/2}\} . \tag{34}$$

In the above equation we choose the region of $\tan\theta$ where D is real and positive. Substituting Eqs. (21), (23), and (30) into Eq. (28), we find finally the relation for the group velocity,

$$\rho V_g^2=\frac{(C_{11-}^2\tan^4\theta-C_{33-}^2-2C_{33+}D-D^2)^2}{8\cos^2\zeta D^2(C_{11+}\tan^2\theta+C_{33+}+D)} . \tag{35}$$

The above equation, when D is substituted by the expression on the right-hand side of Eq. (34), yields the group velocity as a function of $\tan\theta$. Usually, experimentally or by other means as described in Sec. II A, the magnitude of group velocity V_g, its direction ζ, C_{11+}, C_{11-}, C_{33+}, and C_{33-} are known. Equation (35) can be solved to find $\tan\theta$, which makes D in Eq. (34) real and positive. Once the value of this $\tan\theta$ is found, one can obtain the values of D, B, C_{13+} and finally C_{13}, using Eqs. (34), (22), (16), and (12), respectively. On the other hand, given the known values of all elastic constants of a medium, Eq. (31) or (33) combined with Eq. (35) predicts the value of a QL group velocity in any direction in the symmetry plane.

3. QT mode

In the propagation of the QT mode, Eqs. (21) and (23) are both determined with the lower sign in front of D. The application of very similar procedures to those taken in the QL mode yields

$$P_1=\tfrac{1}{2}(B-C_{11-}^2\tan^2\theta+C_{11+}D) , \tag{36}$$

$$P_3=\tfrac{1}{2}(B\tan^2\theta-C_{33-}^2+C_{33+}D) , \tag{37}$$

$$\tan\zeta=\tan\theta\frac{B-C_{11-}^2\tan^2\theta+C_{11+}D}{B\tan^2\theta-C_{33-}^2+C_{33+}D} , \tag{38}$$

$$C_{11-}^2\tan^3\theta+\tan\zeta(B\tan^2\theta-C_{33-}^2)-B\tan\theta-(C_{11+}\tan\theta-C_{33+}\tan\zeta)D=0 , \tag{39}$$

$$D(\tan\theta)=\frac{1}{1-\tan\zeta\tan\theta}$$
$$\times\{\tan\theta(C_{11+}\tan\theta-C_{33+}\tan\zeta)$$
$$\pm[\tan^2\theta(C_{11+}\tan\theta-C_{33+}\tan\zeta)^2-(1-\tan^2\zeta\tan^2\theta)(C_{11-}^2\tan^4\theta-C_{33-}^2)]^{1/2}\} , \tag{40}$$

$$\rho V_g^2=\frac{(C_{11-}^2\tan^4\theta-C_{33-}^2+2C_{33+}D-D^2)^2}{8\cos^2\zeta D^2(C_{11+}\tan^2\theta+C_{33+}-D)} . \tag{41}$$

Equation (39) gives a relation between the directions of a QT-mode group velocity and the corresponding wave normal lying in the symmetry plane. Equations (39) and (41) can be used to calculate a group velocity in an arbitrary direction on the symmetry plane, once all the values of the elastic constants are known. In the case that C_{13} is unknown, again among the roots of $\tan\theta$ of Eq. (41) we take only those that satisfy the condition $D>0$. Then D is found by Eq. (40). Finally, the value of C_{13} can be determined in a way similar to the case of the QL mode.

4. *Propagation of QL and QT modes in other symmetry planes*

a. Propagation in the x_2x_3 plane. We consider a traveling wave with group velocity $\mathbf{V}_g$ and wave normal $\mathbf{n}$ at angles ζ and θ to the x_3 axis, respectively. In this case replace the subscript index number 1 in the notations of the elastic constant C_{ij}, wave normal n_i, and slowness s_i by the subscript index 2, and C_{55} by C_{44}, in all the appropriate equations following after Eq. (9). With these replacements made, Eqs. (33)–(35) for the QL mode and Eqs. (39)–(41) for the QT mode can be applied to find the root $\tan\theta$ and the corresponding value of D. Once the value of D is known, the mixed-index elastic constant C_{23} can be obtained by using the relations corresponding to Eqs. (22), (16), and (12) for each mode.

b. Propagation in the x_1x_2 plane. Consider an elastic pulse propagating with $\mathbf{V}_g$ and $\mathbf{n}$ at angles ζ and θ to the x_1 axis, respectively. Replace first C_{55} by C_{66} and substitute the subscript index 3 by 1 and the subscript index 1 by 2 in the notations of the elastic constant C_{ij}, wave normal n_i, and slowness s_i in all the appropriate equations following after Eq. (9). With these replacements made, the elastic constant C_{12} can be obtained in a similar way as described for the QL and QT mode propagations in the x_2x_3 or x_1x_3 plane.

C. Extension to other higher-symmetry groups

1. *Tetragonal and cubic symmetry groups*

The tetragonal symmetry groups are divided into two groups: one group containing the class of 4, $\bar{4}$, $4/m$ symmetry that has $C_{16}=-C_{26}\neq 0$, and the other group containing the remaining higher-symmetry classes for which $C_{16}=-C_{26}=0$. The nonzero elastic constant C_{16} of the former class of tetragonal media can be eliminated by a rotation about the x_3 axis through an angle ϕ given by[6]

$$\tan 4\phi = 4C_{16}/(C_{11}-C_{12}-2C_{66}) , \tag{42}$$

where the denominator $\Delta = C_{11}-C_{12}-2C_{66}$ indicates a deviation from transverse isotropy. Equation (42) yields two solutions of ϕ, which are 45° apart. One may choose either value of ϕ to set new coordinate axes, which render C_{16} zero. Thus, with an appropriate choice of axes, every class of the tetragonal groups has the same form of elastic-constant matrix.

Nine different elastic constants of an orthorhombic medium are reduced to six in the tetragonal group by the identities

$$C_{11}=C_{22};\quad C_{13}=C_{23};\quad C_{44}=C_{55} \tag{43}$$

and to three in the cubic symmetry group by the relations

$$C_{11}=C_{22}=C_{33};\quad C_{12}=C_{23}=C_{13};\quad C_{44}=C_{55}=C_{66} . \tag{44}$$

a. Propagation in the x_1x_2, x_2x_3, or x_1x_3 symmetry plane. There is no distinction between the x_1x_3 and x_2x_3 planes for the tetragonal medium and no distinction between all three x_1x_2, x_2x_3, and x_1x_3 planes for a cubic medium. The relations that hold for the symmetry planes of an orthorhombic medium extend to the corresponding symmetry planes with the substitution of Eqs. (43) and (44) for tetragonal and cubic symmetry, respectively.

Because a great majority of crystals in nature belong to the cubic group, we explicitly write down here the formulas for cubic symmetry. The directions of the group velocity and wave normal, ζ and θ, are measured from any cubic axes. There are only three distinct elastic constants, C_{11}, C_{12}, and C_{44}, as indicated in Eq. (44) for cubic symmetry. We define

$$\begin{aligned} &C_{11+}\equiv C_{11}+C_{44} ,\quad C_{11-}\equiv C_{11}-C_{44} ,\\ &C_{12+}\equiv C_{12}+C_{44} , \end{aligned} \tag{45}$$

$$D\equiv[C_{11-}^2(1-\tan^2\theta)^2+4C_{12+}^2\tan^2\theta]^{1/2} , \tag{46}$$

$$\begin{aligned} B&\equiv C_{11-}^2-2C_{12+}^2\\ &=[C_{11-}^2(1+\tan^4\theta)-D^2]/(2\tan^2\theta) . \end{aligned} \tag{47}$$

Then, for QL modes propagating in the cubic faces, we obtain

$$C_{11-}^2\tan^3\theta+\tan\zeta(B\tan^2\theta-C_{11-}^2)-B\tan\theta+C_{11+}(\tan\theta-\tan\zeta)D=0 , \tag{48}$$

$$\begin{aligned} D(\tan\theta)=&\frac{1}{1-\tan\zeta\tan\theta}\\ &\times\{C_{11+}\tan\theta(\tan\zeta-\tan\theta)\pm[C_{11+}^2\tan^2\theta(\tan\zeta-\tan\theta)^2-C_{11-}^2(1-\tan^2\zeta\tan^2\theta)(\tan^4\theta-1)]^{1/2}\} , \end{aligned} \tag{49}$$

$$\rho V_g^2=\frac{(C_{11-}^2\tan^4\theta-C_{11-}^2-2C_{11+}D-D^2)^2}{8\cos^2\zeta\, D^2(C_{11+}\tan^2\theta+C_{11+}+D)} . \tag{50}$$

Similarly for the QT modes propagating in the cubic faces, we find

$$C_{11-}^2\tan^3\theta+\tan\zeta(B\tan^2\theta-C_{11-}^2)-B\tan\theta-C_{11+}(\tan\theta-\tan\zeta)D=0 , \tag{51}$$

$$D(\tan\theta)=\frac{1}{1-\tan\zeta\tan\theta}\{C_{11+}\tan\theta(\tan\theta-\tan\zeta)\pm[C_{11+}^2\tan^2\theta(\tan\theta-\tan\zeta)^2-C_{11-}^2(1-\tan^2\zeta\tan^2\theta)(\tan^4\theta-1)]^{1/2}\}\ , \tag{52}$$

$$\rho V_g^2=\frac{(C_{11-}^2\tan^4\theta-C_{11-}^2+2C_{11+}D-D^2)^2}{8\cos^2\zeta D^2(C_{11+}\tan^2\theta+C_{11+}-D)}\ . \tag{53}$$

In the above Eqs. (48)–(53) we choose the range of $\tan\theta$ that makes D real and positive.

b. Propagation in the (n_1,n_1,n_3)*-type diagonal plane.* Consider the elastic wave propagating in this diagonal symmetry plane with group velocity $\mathbf{V}_g$ and wave normal $\mathbf{n}$ at angles ζ and θ to the x_3 axis, respectively. Then, $n_3=\cos\theta$ and we define n_d, the base-diagonal component of the wave normal, as

$$n_d^2\equiv n_1^2+n_2^2=2n_1^2=\sin^2\theta\ . \tag{54}$$

The corresponding slowness components s_d and s_3, and the relation between them are, respectively,

$$s_d=\sin\theta/V\ ,\quad s_3=\cos\theta/V\ ,$$

and

$$s_d/s_3=\tan\theta\ . \tag{55}$$

We begin with the tetragonal symmetry. The Christoffel equation in this case can be factorized as

$$(\Gamma_{11}-\Gamma_{12}-\rho V^2)\times[(\Gamma_{33}-\rho V^2)(\Gamma_{11}+\Gamma_{12}-\rho V^2)-2\Gamma_{13}^2]=0\ . \tag{56}$$

The first factor on the right-hand side of the above equation yields the relation

$$\rho V^2=n_d^2(C_{11}-C_{12})/2+n_3^2C_{44} \tag{57}$$

for the PT wave polarized in the $[\overline{n}_1,n_1,0]$ direction normal to the propagation direction. The corresponding group-velocity section in the $V_{g1}=V_{g2}$ plane is given by

$$\frac{\sin^2\zeta}{(C_{11}-C_{12})/2}+\frac{\cos^2\zeta}{C_{44}}=\frac{1}{\rho V_g^2}\ , \tag{58}$$

which can be used to determine the elastic constants $(C_{11}-C_{12})/2$ and C_{44} by measuring the group velocities of the PT waves propagating in at least two different directions. The terms in the square bracket of Eq. (56) result for QL and QT modes in the relation for phase velocity

$$(\rho V^2)^2-(\Gamma_{11}+\Gamma_{33}+\Gamma_{12})\rho V^2+\Gamma_{33}(\Gamma_{11}+\Gamma_{12})-2\Gamma_{13}^2=0\ . \tag{59}$$

To simplify notations, we introduce the quantities defined by

$$K\equiv\tfrac{1}{2}(C_{11}+C_{12}+2C_{66})\ , \tag{60}$$

$$K_\pm\equiv K\pm C_{44}\ , \tag{61}$$

$$C_{33\pm}\equiv C_{33}\pm C_{44}\ , \tag{62}$$

$$C_{13\pm}\equiv C_{13}\pm C_{44}\ , \tag{63}$$

$$A\equiv KC_{33}+C_{44}^2-C_{13+}^2\ , \tag{64}$$

$$B\equiv K_-C_{33-}-2C_{13+}^2\ , \tag{65}$$

$$D\equiv[(K_-\tan^2\theta-C_{33-})^2+4C_{13+}^2\tan^2\theta]^{1/2}=(K_-^2\tan^4\theta-2B\tan^2\theta+C_{33-}^2)^{1/2}\ . \tag{66}$$

Using these new notations, the solution for ρV^2 in Eq. (59) is written as

$$2\rho V^2=K_+\sin^2\theta+C_{33+}\cos^2\theta\pm[(K_-\sin^2\theta-C_{33-}\cos^2\theta)^2+4C_{13+}^2\sin^2\theta\cos^2\theta]^{1/2}\ , \tag{67}$$

from which one finds

$$2\rho s_3^{-2}=K_+\tan^2\theta+C_{33+}\pm D\ . \tag{68}$$

In Eqs. (67) and (68) the positive and negative signs in the $\pm$ symbol correspond to the QL and QT modes, respectively. B in Eq. (65) is written in terms of D and $\tan\theta$ as

$$B=\frac{1}{2\tan^2\theta}(K_-^2\tan^4\theta+C_{33-}^2-D^2)\ . \tag{69}$$

The equation of the slowness surfaces for the QL and QT modes is found from Eq. (59) as

$$S=KC_{44}s_d^4+C_{33}C_{44}s_3^4+As_d^2s_3^2-\rho(K_+s_d^2+C_{33+}s_3^2)+\rho^2=0\ . \tag{70}$$

Comparing Eqs. (60)–(70) with the corresponding expressions in Sec. II B, one finds that exactly the same relations between V_g, $\tan\zeta$, $\tan\theta$, and elastic moduli as those found in Eqs. (33)–(35) and Eqs. (39)–(41) can be obtained for the QL and QT modes, respectively, by simply replacing C_{11} by K, C_{55} by C_{44}, $C_{11\pm}$ by $K_\pm$, and s_1 by s_d. We list here final results for the QL and QT modes.

For the QL mode they are

$$K_-^2\tan^3\theta+\tan\zeta(B\tan^2\theta-C_{33-}^2)-B\tan\theta+(K_+\tan\theta-C_{33+}\tan\zeta)D=0\ , \tag{71}$$

$$D(\tan\theta)=\frac{1}{1-\tan\zeta\tan\theta}\times\{\tan\theta(C_{33+}\tan\zeta-K_+\tan\theta)\pm[\tan^2\theta(C_{33+}\tan\zeta-K_+\tan\theta)^2-(1-\tan^2\zeta\tan^2\theta)(K_-^2\tan^4\theta-C_{33-}^2)]^{1/2}\}\ , \tag{72}$$

$$\rho V_g^2 = \frac{(K_-^2 \tan^4\theta - C_{33-}^2 - 2C_{33+}D - D^2)^2}{8\cos^2\zeta D^2(K_+ \tan^2\theta + C_{33+} + D)} \ . \tag{73}$$

We choose the root of $\tan\theta$ in Eq. (73) that satisfies $D > 0$ and find the corresponding value of D. Hence, obtaining the value of the elastic constant C_{13} is straightforward.

For the QT mode we obtain

$$K_-^2 \tan^3\theta + \tan\zeta(B \tan^2\theta - C_{33-}^2) - B \tan\theta - (K_+ \tan\theta - C_{33+} \tan\zeta)D = 0 \ , \tag{74}$$

$$D(\tan\theta) = \frac{1}{1 - \tan\zeta \tan\theta}\{\tan\theta(K_+ \tan\theta - C_{33+} \tan\zeta) \pm [\tan^2\theta(K_+ \tan\theta - C_{33+} \tan\zeta)^2 - (1 - \tan^2\zeta \tan^2\theta)(K_-^2 \tan^4\theta - C_{33-}^2)]^{1/2}\} \ , \tag{75}$$

$$\rho V_g^2 = \frac{(K_-^2 \tan^4\theta - C_{33-}^2 + 2C_{33+}D - D^2)^2}{8\cos^2\zeta D^2(K_+ \tan^2\theta + C_{33+} - D)} \ . \tag{76}$$

The value of C_{13} can be found from the above equations in the straightforward method already mentioned.

For a cubic medium, there is no distinction between three diagonal-type (n_1, n_1, n_3), (n_1, n_2, n_2), and (n_1, n_2, n_1) planes. We replace C_{66} by C_{44} in Eq. (60) for K, C_{33} by C_{11}, C_{13} by C_{12}, C_{13+} by C_{12+}, C_{33+} by C_{11+}, and C_{33-} by C_{11-}. With these replacements made, Eqs. (71)–(73) apply to the QL mode and Eqs. (74)–(76) hold for the QT mode in a cubic medium.

2. *Hexagonal or transversely isotropic groups*

A hexagonal or transversely isotropic medium is characterized by five nonzero elastic constants

$$C_{11} = C_{22}; \quad C_{33}; \quad C_{12}; \quad C_{13} = C_{23}; \quad C_{44} = C_{55} \ . \tag{77}$$

The following relation holds for a transverse isotropic medium:

$$C_{66} = \tfrac{1}{2}(C_{11} - C_{12}) \ . \tag{78}$$

For a hexagonal or transversely isotropic medium, only the wave normals of both QL and QT modes lying in the symmetry planes map themselves into the corresponding symmetry planes of group-velocity surfaces, and vice versa. Hence, the formulas developed in orthorhombic and tetragonal media apply unambiguously to a transversely isotropic medium with Eqs. (77) and (78) used for appropriate elastic constants.

a. Propagation in the [0001] zonal plane. Consider an elastic pulse propagating with group velocity $\mathbf{V}_g$ and wave normal $\mathbf{n}$ at angles ζ and θ respectively to the symmetry axis [0001], in a zonal plane parallel to this symmetry axis. In this case, using the relations (77) and (78), one finds that there is no distinction between the propagations in the x_1x_3, x_2x_3, and (n_1, n_1, n_3) type of diagonal planes. Replacing C_{55} by C_{44} in the defining equations (10)–(12), we see that Eqs. (33)–(35) and Eqs. (39)–(41) respectively hold for the QL and QT modes propagating in the zonal plane.

b. Propagation in the basal plane. Consider an elastic pulse traveling with group velocity $\mathbf{V}_g$ and wave normal $\mathbf{n}$ at angles ζ and θ respectively to the [100] axis in the x_1x_2 basal plane. The same analytic expressions for the QL and QT mode propagations in the x_1x_2 plane of an orthorhombic medium are extended to the basal plane of a transversely isotropic medium, using Eqs. (77) and (78).

III. APPLICATIONS ILLUSTRATED WITH DATA OF ZINC AND SILICON

In Sec. II, various formulas relating the group velocity $\mathbf{V}_g$ to the wave normal $\mathbf{n}$ and the elastic constants of media are described. In this section we illustrate some important applications with hexagonal zinc and cubic silicon crystals. In summary, basically two sets of formulas, Eqs. (33)–(35) for the QL mode and Eqs. (39)–(41) for the QT mode, provide these relations with appropriate replacements in elastic constants for various anisotropic media.

A. Determination of group velocity surfaces and cuspidal features

In this subsection we discuss the construction of the group-velocity sheet of a zonal section of a transversely isotropic zinc crystal. The extension of the method described here to the determination of group velocities corresponding to the wave normals lying in the symmetry planes in other anisotropic media is straightforward from the descriptions given in the Sec. II. Kim and Sachse[7] obtained the five elastic constants of zinc from the group-velocity data measured in two principal symmetry directions. They are $C_{11} = 163.75$, $C_{12} = 36.278$, $C_{13} = 52.476$, $C_{33} = 62.928$, and $C_{44} = 38.677$ GPa. For transversely isotropic zinc Eq. (78) holds. The density of zinc ρ used is 7134 kg/m^3. The (010) zonal section of the slowness surfaces of zinc, generated using this data and Eqs. (14), (8), and (2), are plotted in Fig. 2(a), where the [001] axis is a direction of rotational symmetry. Because of transverse isotropy about the [001] axis, any zonal section is identical to the (010) section. From these slowness surfaces, the corresponding group-velocity surfaces are constructed using the last part of Eq. (4), and they are shown in Fig. 2(b), which also shows the phase-velocity section for reference. Note that Eq. (4) indicates that the direction of group velocity or energy flux at any point of the slowness surface is parallel to the surface normal at

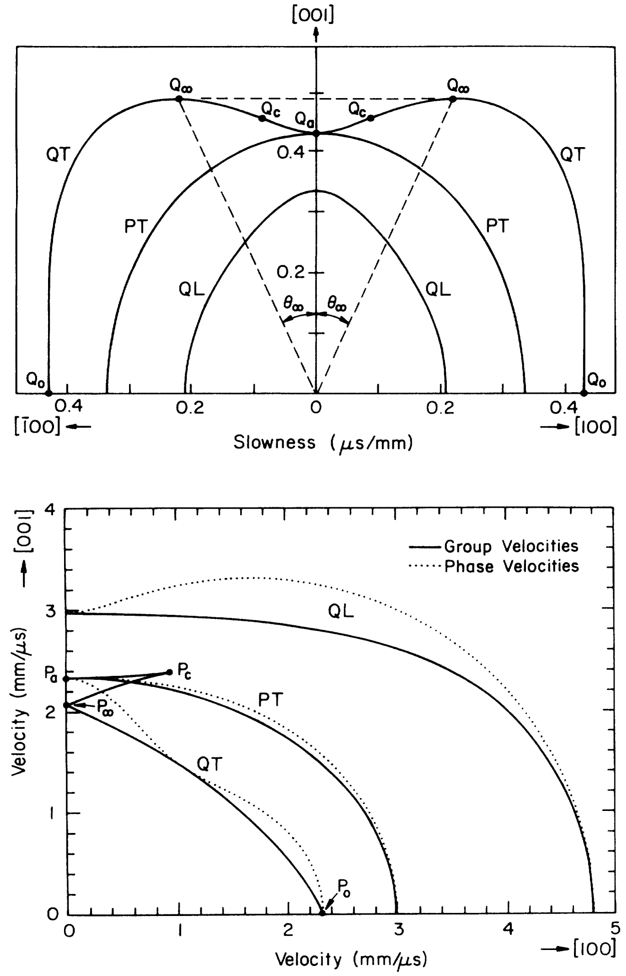

FIG. 2. (a) (010) section of the slowness surface in zinc. (b) (010) section of the group- and phase-velocity surfaces in zinc.

that point. Usually, an isotropic distribution of wave normals in every direction is assigned and the group velocity corresponding to each wave normal is calculated, according to Eq. (4).

As shown in Fig. 2(a), the QL and PT slowness sheets of zinc are everywhere convex and therefore their corresponding group-velocity sheets are not folded in any direction. Near the point Q_a on the [001] symmetry axis, the QT sheet of the slowness surface is concave, with both principal curvatures being negative. At Q_c the principal curvature in the zonal section changes sign, and between here and the point Q_∞ the surface is saddle shaped. At Q_∞ the principal curvature transverse to the zonal section changes sign and the energy fluxes at the points lying on the circle generated by rotating the line from the origin to Q_∞ about the [001] axis are all parallel to this symmetry direction. In Fig. 2(b) the points P_a and P_∞ on the symmetry axis, P_c on the cuspidal edge, and the point P_0 on the basal plane correspond to the points Q_a, Q_∞, Q_c, and Q_0 in Fig. 2(b), respectively. There is a region on either side of the basal plane near Q_0 where the in-plane curvature is again negative, leading to the folding of the group-velocity surface in a tiny region surrounding the point P_0. This cusp is not apparent in Fig. 2(b) because of its miniature shape. For simplicity of nomenclature, let us call the ray branches of the QT mode between P_a and P_c, P_c and P_∞, and P_∞ and P_0 by their acronyms, FQT (faster QT) mode, IQT (intermediate QT) mode, and SQT (slower QT) mode, respectively.

The group-velocity surfaces plotted in Fig. 2(b) can be easily generated by using the formulas derived in Sec. II. The easiest of them is certainly the PT group-velocity surface generated by using Eq. (9). The group-velocity direction ζ in terms of the wave-normal direction θ is explicitly given by Eqs. (31) and (38) for the QL and QT modes, respectively. To calculate the wave-normal direction θ of either QL or QT mode corresponding to a group-velocity direction ζ, let us write for notational simplicity

$$r \equiv \tan\zeta \quad \text{and} \quad x \equiv \tan\theta \; . \tag{79}$$

The Eqs. (33) and (39) can now be expressed as

$$y \equiv C_{11-}^2 x^3 + Brx^2 - Bx - C_{33-}^2 r \pm (C_{11+}x - C_{33+}r)\sqrt{C_{11-}^2 x^4 - 2Bx^2 + C_{33-}^2} \; , \tag{80}$$

$$y = 0 \; , \tag{81}$$

where the $\pm$ in front of the parenthesis correspond to the QL and QT modes, respectively, and the square-root quantity is identical to D defined by Eq. (17). The leading terms in Eq. (80) for large values of $|x|$ and a given finite r are

$$\begin{aligned} y &\sim 2C_{11}(C_{11} - C_{44})x^3 \; , \quad \text{(QL mode)} \\ y &\sim -2C_{44}(C_{11} - C_{44})x^3 \quad \text{(QT mode)} \; . \end{aligned} \tag{82}$$

Equation (82) ensures that Eq. (81) has at least one real root of x corresponding to a given ζ for both QT and QL modes. Equations (80) and (81) for the QL mode are found to have only one real root of x for all values of r in zinc. Duff[8] has shown that the QL slowness surface of all media is everywhere convex, which implies that Eq. (80) has in fact only one real root and two complex conjugate roots for all values of r. However, for the QT mode, Eq. (81) may possess more than one real root up to the maximum of three for some range of group-velocity direction ζ, which is called a cuspidal region. As shown in Fig. 2(b) for ζ lying between P_a (or P_∞) and P_c, Eq. (81) for the QT mode has three distinctive real roots with two real roots in the direction of the cuspidal edge P_c, in which one root is of multiplicity degree 2. Outside the cuspidal region the QT equation has only one real root. Once these real roots are found for a given group-velocity direction specified by $r = \tan\zeta$, D is obtained through Eq. (17) and the corresponding group-velocity values are determined by using Eqs. (35) and (41) respectively for the QL and QT modes. The group-velocity curves generated in this way are of course virtually identical to those in Fig. 2(b).

Equations (80) and (81) are particularly suitable for calculating the directions of the inflection points Q_c and Q_∞ of the slowness surface and cuspidal edge P_c of the group-velocity surface to an arbitrary precision, which are not easily obtainable with the conventional method described in the first paragraph above in this subsection. Using the computer algebra found, for example, in the Plot and FindRoot routines of Ref. 3, we solve with the QT mode equations (80) and (81) for the nonzero-group-velocity direction r that gives a real root of multiplicity degree 2. The solution yields $r=\tan\zeta=\tan 21.53553436°$ for the direction of the cuspidal edge P_c in Fig. 2(b) and $x=\tan\theta=\tan(-9.3036671°)$ for the direction of inflection point Q_c in Fig. 2(a). The corresponding QT-mode group velocity is calculated to be 2.55646 mm/μs. The direction of the point Q_∞ in Fig. 2(a) is on substituting $r=0$ found to be $x=\tan\theta=\tan(\pm 24.5244°)$, which yields the group velocity of the QT mode equal to 2.05998 mm/μs. For the group-velocity direction $r=\tan\zeta=\tan 10°$, roughly midway in the cuspidal region, the solution of the QT-mode equations yields three real values of $x=\tan(-2.30438°)$, $\tan(-20.01006°)$, and $\tan 28.1366°$, which respectively give the group velocities $V_g=2.37253$ mm/μs (FQT mode), 2.25501 mm/μs (IQT mode), and 1.92376 mm/μs (SQT mode). Likewise, the solution of the QL-mode equations yields one real root $x=\tan 1.68993°$, which results in a group velocity equal to 3.00805 mm/μs (QL mode). Outside the cuspidal region, at say $r=\tan 45°=1$, Eqs. (80) and (81) yield only one real root for both QL and QT modes, which are respectively $x=\tan 15.1942°$ and $x=\tan 38.9054°$. The corresponding group velocities are calculated to be 3.81945 mm/μs and 1.80133 mm/μs.

There exists a tiny cusp around the [100] direction, which is not visible in the resolution of Fig. 2(b) but is apparent on a greatly magnified scale. Musgrave[1] and later McCurdy[9] discussed the conditions for the existence of a cusp around the symmetry axes of a transversely isotropic medium. The cuspidal condition around the [100] axis is

$$(C_{13}+C_{44})^2 > C_{33}(C_{11}-C_{44}) , \tag{83}$$

which is satisfied for zinc. A similar condition with the interchange of indices 1 and 3 in Eq. (83) holds for the existence of a folding QT sheet around the [001] axis, which zinc also meets. Equations (80) and (81) for the QT mode are also very useful for plotting this cusp to an arbitrary precision. For this purpose it is more convenient to measure the directions of wave normal and group velocity, $x=\tan\theta$ and $r=\tan\zeta$, from the [100] direction. We interchange the indices 1 and 3 in Eq. (80), which is then expressed in the form

$$y \equiv C_{33-}^2 x^3 + Brx^2 - Bx - C_{11-}^2 r \pm (C_{33+}x - C_{11+}r)\sqrt{C_{33-}^2 x^4 - 2Bx^2 + C_{11-}^2} . \tag{84}$$

The quantities B, C_{13}, and C_{13+} are invariant under the operation of this particular index interchange. Equations (84), (81), (17), and (41) are used to calculate detailed features of the cusp around the basal plane. They are shown in Fig. 3, which is very similar to the greatly magnified cusp found in Ref. 10.

For media other than those of transverse isotropy, Eqs. (80) and (81) also apply to determine their QL-mode group-velocity surfaces in the symmetry plane. The QL

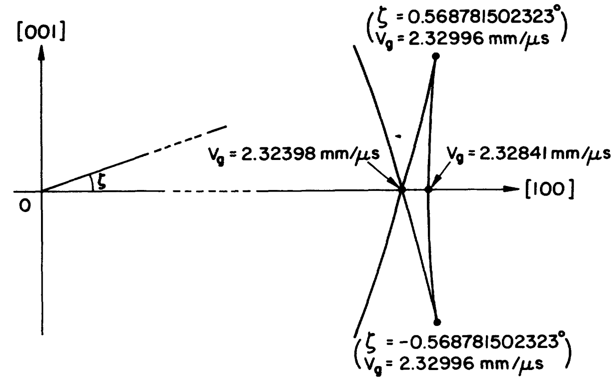

FIG. 3. A magnified view of a cusp about the [100] axis in zinc.

ray surfaces are not folded, because their corresponding QL slowness surfaces are shown to be everywhere convex.[8] This is not generally true for the QT modes of nonhexagonal media. All the points on the symmetry plane of both QL and QT slowness surfaces map onto the corresponding symmetry plane of group-velocity surfaces. However, the converse is not true for the QT modes. Depending on the direction, the QT slowness surface is concave, convex, or transitional between them. Some points of zero Gaussian curvature lying outside the symmetry planes of the slowness surface may have their caustics mapping across the mirror-symmetry plane and others map onto a cusp on the symmetry plane of the corresponding group-velocity surfaces, where Eqs. (80) and (81) no longer hold. In the cuspidal region the group velocity is multivalued for a given direction of $r=\tan\zeta$ and there is at least one branch of the QT-mode group velocity that corresponds to the wave normals in the corresponding symmetry plane of the slowness surface. Equations (80) and (81) for the QT mode then apply to determine the group velocities and cusps, which are strictly due to the wave normals of the corresponding symmetry plane of the slowness surface. These equations also apply to the region outside the cusps in the symmetry plane of an actual group-velocity surface, since the group velocity therein is single valued and one surely finds the corresponding wave normal in the symmetry plane of the slowness surface. Here, we exclude the fictitious group-velocity directions in which no energy flux flows, as in the case of internal conical refraction about the [111] direction of some crystals.[1,2] Equations (80) and (81) may be unambiguously applied to the QL and QT modes in the symmetry planes of media that are weakly deviating from transverse isotropy.[11]

A detailed treatment of Eqs. (80) and (81) for transversely isotropic and other media and their applications will be treated elsewhere.

B. Determination of elastic constants with mixed indices

It is well known that pure-index elastic constants of orthorhombic or higher-symmetry media, C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, and C_{66}, can be accurately obtained from the phase- or group-velocity data of pure longitudinal and pure transverse waves propagating in the direction of the symmetry axes of the media.[12,13] The mixed-index elastic constants, C_{12}, C_{23}, and C_{13}, are usually determined by transmitting either QL or QT waves along an arbitrary direction in the symmetry plane and measuring their phase velocities and then by using Eq. (14) for, say, C_{13}. This requires preparation of a sample with two opposite faces parallel to each other in a nonsymmetry direction to quite an accurate degree to minimize error in the phase-velocity measurement. The accurate alignment of the sample to a nonsymmetry direction is considerably more difficult than its similar alignment to a symmetry direction. Moreover, sometimes there arises a situation in which faceting of samples in a nonsymmetry direction is not desired, as often found in the case of composite materials fabricated along the fiber direction. These difficulties can be easily overcome by measuring the group velocity of either the QL or the QT mode in an arbitrary direction of the symmetry plane and using Eqs. (34) and (35) for the QL mode and Eqs. (40) and (41) for the QT mode to calculate a mixed-index elastic constant. This can be easily achieved by using pointlike sources such as capillary fracture and irradiation of a focused laser beam on the surface of a sample and by employing pointlike detectors such as small-diameter piezoelectric and capacitive transducers.[14] We illustrate here with the determination of C_{13} in zinc with the numerically simulated data shown above and the determination of C_{12} in silicon with experimental data.

Above in Sec. III A, the group velocities of the QL and QT modes of zinc in the directions of 10° and 45° on the zonal plane are calculated. Suppose now that for zinc the pure-index elastic moduli, C_{11}, C_{33}, and C_{44}, have been accurately measured and their values are the same as those listed in Sec. III A. Suppose also that we have measured the group velocities of both QL and QT modes in these two directions, which are exactly the same as those calculated in Sec. III A; namely, $V_g=3.00805$ mm/μs (QL mode), 2.37253 mm/μs (FQT mode), 2.25501 mm/μs (IQT mode), 1.92376 mm/μs (SQT mode), for the 10° direction; $V_g=3.81945$ mm/μs (QL mode), 1.80133 mm/μs (QT mode), for the 45° direction that is outside the cuspidal region. Given these values, can the elastic constant C_{13} be calculated, resulting in the same value 52.476 GPa as listed in Sec. III A? The answer is definitely yes, and we illustrate with the cases of the QL mode in the 45° direction and QL and IQT modes in the 10° direction.

We deal first with the QL mode propagating with $V_g=3.81945$ mm/μs in the 45° direction. Substitution of D in Eq. (34) with the negative square root into Eq. (35) yields no real solution for $x=\tan\theta$. However, simultaneous equations for x and D of Eq. (34) with the positive square root and Eq. (35) produce the solution $x=\tan\theta=\tan 15.1941°=0.271583$ and $D=51.7413$ GPa, which through the use of Eqs. (22), (16), and (12) finally yields $C_{13}=52.4766$ GPa in excellent agreement with the value of C_{13} listed (52.476 GPa) in Sec. III A. Similarly, for the QL mode propagating with $V_g=3.00805$ mm/μs in the 10° direction inside the cuspidal region, D with the positive square root in Eq. (34) and Eq. (35) yield two real values of $x=0.521046$ and 0.0295008. They respectively provide D with the values of -7.28858 GPa (thus discarded) and $D=24.734$ GPa, which yields $C_{13}=52.4804$ GPa. Again, it is found that D with a negative square root has no real solution for x. For the IQT mode propagating with $V_g=2.25501$ mm/μs in the 10° direction, D with a negative square root in Eq. (40) and Eq. (41) possess no real solution for x. D with a positive square root and Eq. (41) yield two solutions: $x=0.337463$, $D=45.6684$ GPa, $C_{13}=27.3427$ GPa; $x=-0.364172$, $D=66.8319$ GPa, $C_{13}=52.4766$ GPa. The former C_{13} value is certainly wrong, judging from comparison with other C_{13} values obtained with the QL group-velocity values. Both values of C_{13} satisfy the constraints required for the positivity of the strain energy of a hexagonal crystal. They are expressed as[15]

$$(C_{11}+C_{12})C_{33}>2C_{13}^2 \quad \text{and} \quad C_{11}C_{33}>C_{13}^2 \ . \tag{85}$$

The FQT and SQT group-velocity values in the 10° direction also lead to one correct and the other wrong C_{13} value, both of which satisfy the conditions of Eq. (85). For the SQT group velocity in the 45° direction, D with a positive square root in Eq. (40) yields $C_{13}=100.645$ GPa, while D with a negative square root in Eq. (40) gives the correct value of $C_{13}=52.4763$ GPa. The former value is discarded, because it fails to satisfy the latter condition of Eq. (85).

For determination of C_{13} from the experimentally measured group velocities, it is certainly recommended that one chooses the group velocities of the QL mode, the arrival of which can be unambiguously determined at the point from which the signal first jumps above the noise level for virtually all materials. The materials in which the transverse group velocity exceeds the longitudinal group velocity are extremely rare and even in such materials it occurs in a narrow range of directions. Examples include a tetragonal tellurium dioxide crystal[2] and the wood of orthorhombic spruce.[1] Except for the displacement signal detected by a capacitive transducer with a known type of source, e.g., a capillary fracture whose time function resembles a Heaviside step,[16] the unambiguous identification of QT-mode arrival is generally quite difficult in the signal generated by a pointlike broadband source and detected by a piezoelectric transducer, partly because of the lingering QL mode and in some directions head waves superimposed on the QT mode and partly because of the ringing of the detecting transducer. There is another reason why the QL group velocity is preferred. As mentioned before, Eqs. (33)–(35) or their equivalents for the QL mode of various symmetry groups are safely applied to determine uniquely the elastic constant C_{13}. However, as shown in Fig. 4, which shows the complicated (010) section of silicon group-velocity surfaces, some of the QT-mode wave normals lying in nonsymmetry planes may map themselves as one or more cusps in the symmetry plane of the group-velocity surfaces. In this circumstance, Eqs. (39)–(41) and their equivalents are no longer valid for these cusps, and in the cuspidal region one has to choose judiciously the arrivals of those QT modes which originate from the QT wave normals in the

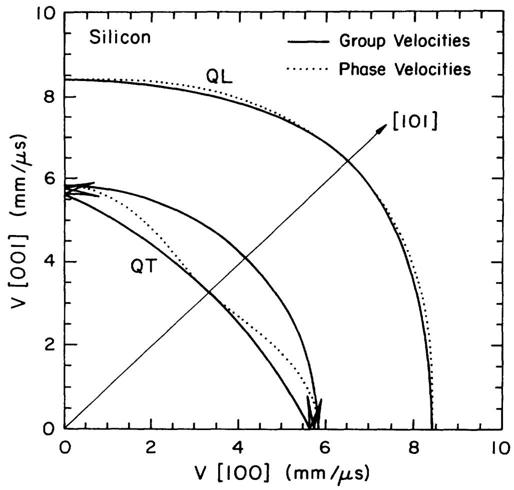

FIG. 4. (010) section of the group- and phase-velocity surfaces in silicon.

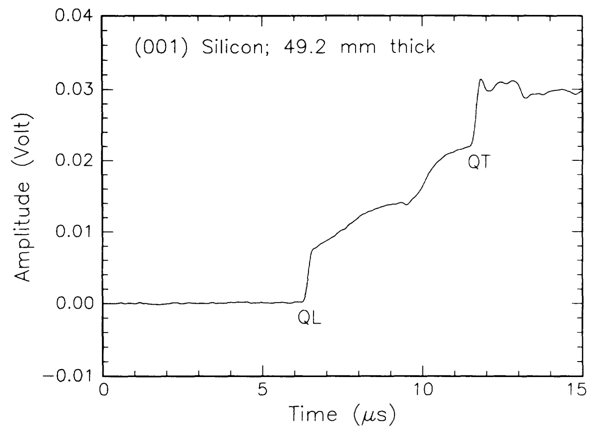

FIG. 5. A displacement signal detected by the capacitive transducer at a distance of 25 mm from the epicenter in the [100] direction on the top surface of a 49.2-mm-thick (001) silicon disk with a capillary fracture source on the bottom side.

corresponding symmetry plane. This is of course not an easy task. Otherwise, one has to completely avoid a cuspidal region, the direction of which is not known *a priori* in the absence of prior knowledge of the C_{12}, C_{13}, or C_{23} value.

Finally, we illustrate a determination of the elastic constant C_{12} of silicon using Eqs. (49) and (50) for a cubic medium and a QL-mode group velocity measured in the direction lying in the (010) plane. The values of elastic constants $C_{11}=165.7$ GPa and $C_{44}=79.56$ GPa are obtained from the pure L and pure T group-velocity data measured in the [001] direction and the density of 2332 kg/m^3. Another independent measurement of pure L and pure T modes propagating in the [110] direction yields $C_{12}=63.90$ GPa. Using these values of elastic constants, the Monte Carlo–generated (010) section of group-velocity surfaces is plotted in Fig. 4, which also shows the phase velocities for reference. It displays very complex folded features of the QT-mode group-velocity sheets, the enlarged view of which (not shown here) manifests one cusp arising due to the wave normals lying in the (010) plane and the other three foldings due to the wave normals oriented in the nonsymmetry planes.[17] The QL group velocity 8.830 mm/μs is determined from the QL-mode arrival indicated in the signal shown in Fig. 5, which is detected by a miniature capacitive transducer located at a distance of 25 mm ($\zeta=29.9365°$) from the epicenter in the [100] direction on the top surface of a 49.2-mm-thick disk of (001) silicon. Broadband ultrasonic waves are generated by a capillary fracture source located at the origin on the bottom face. Use of D with a positive square root in Eq. (49) and Eq. (50), together with $C_{11}=165.7$ GPa, $C_{44}=79.56$ GPa, $V_g=8.830$ mm/μs, and $\rho=2332$ kg/m^3, yields only one real value of $C_{12}=64.604$ GPa in good agreement with the $C_{12}=63.90$ GPa listed above. D with a negative square root in Eq. (49) and Eq. (50) have no real root for $x=\tan\theta$. Substitution of $C_{12}=63.90$ GPa in Eqs. (48) and (50) predicts a QL group velocity equal to 8.82720 mm/μs in the direction of the detector. Note that an error as small as 0.032% in group-velocity measurement results in an error as large as 0.79% in the elastic constant C_{12}. Use of the QT-mode arrival in Fig. 5 with Eqs. (52) and (53) leads to similar results.

C. Determination of all elastic constants of a cubic medium with longitudinal group velocity data

The question arises: is it possible to determine all three elastic constants of a cubic medium with only the QL-mode group-velocity data measured in at least three different directions lying in the symmetry plane? The answer is in principle yes, judging from Eqs. (48)–(50) and (71)–(73), which do not preclude this possibility. In this subsection we demonstrate briefly how this works out with the (001)-oriented silicon sample used in Fig. 5. The method described here can be applied to the (110)-oriented sample with an appropriate replacement of elastic constants as described in Sec. II. Kim *et al.*,[17] without relying on the group-velocity formulas derived here, provide some approximate methods of determining all elastic constants of a cubic medium using the group-velocity data of both modes measured in an arbitrary direction on the symmetry plane of silicon disks of various orientations. The method provided here, using analytical formulas developed in the previous section, is exact.

A broadband source, which can be excited either by a capillary fracture or by a focused laser pulse, is located on the top surface of the sample. We choose either the (001) top surface or the bottom part of the (010) plane to detect the generated waves. To simplify and thus minimize errors, we choose $\langle 100\rangle$ and $\langle 110\rangle$ directions. The third direction chosen is that of the detector used ($\zeta=26.9365°$) in Fig. 5. Equations (48) and (50) yield simple formulas, $\rho V_g^2=C_{11}$ and $\rho V_g^2=(C_{11}+C_{12}+2C_{44})/2$, for the $\langle 100\rangle$ and $\langle 101\rangle$ directions, respectively. Let us suppose that the measurement of the QL group velocities in these two directions gives $C_{11}=165.7$ GPa and $C_c \equiv (C_{12}+2C_{44})=223.02$ GPa and a similar measurement in the third direction yields $V_g=8.8272$ mm/μs, with all these values as predicted using the three elastic constants provided in Sec. III B ($C_{11}=165.7$ GPa, $C_{12}=63.9$ GPa, and $C_{44}=79.56$ GPa). Use of $C_{11}=165.7$ GPa, $C_c=223.02$ GPa, $V_g=8.8272$ mm/μs for the third direction in Eqs. (48) and (50) yields the two correct values of elastic constants $C_{12}=63.9$ GPa and $C_{44}=79.56$ GPa, exactly identical to the values used in Sec. III B. However, using the actual measured value for the third direction, $V_g=8.830$ mm/μs, with the same values of C_{11} and C_c, provides us with $C_{12}=50.54$ GPa and $C_{44}=86.24$ GPa, which are in substantial error. Similarly, using for the third direction $V_g=8.828$ mm/μs, which deviates less than 0.01% from the predicted value, one obtains $C_{12}=60.02$ GPa and $C_{44}=81.50$ GPa, which deviate a few percent from the supposedly correct values. The implication here with these numerical experiments is that the determination of three elastic constants from the measured longitudinal-wave group-velocity data alone requires precise measurements of them with accuracy better than 0.01%. This is partly attributed to the fact that directional variations of the QL group velocity in the $\{100\}$ plane of silicon are relatively small, as evident in Fig. 4.

A detailed description on the determination of elastic constants from group-velocity data measured in cubic and hexagonal crystals, and transversely isotropic and orthotropic fiber-reinforced composite materials, using the formulas derived in Sec. II, will be published elsewhere.

IV. CONCLUSIONS

We have derived closed-form analytic equations that relate the group velocities of both QL and QT modes propagating in an arbitrary direction of the symmetry planes of a medium with orthorhombic and higher symmetry to the elastic constants of the medium. Analytic formulas relating the directions of the group velocity and the corresponding wave normal in the symmetry plane are also presented for both modes. Applications of these relations to the determination of group-velocity surfaces in a transversely isotropic medium, and a forward solution for obtaining the mixed-index elastic constants, are illustrated with examples of hexagonal zinc and cubic silicon.

ACKNOWLEDGMENTS

The author deeply appreciates the financial support of the Office of Naval Research. The author is grateful to Professor Arthur G. Every at the University of the Witwatersrand in South Africa for fruitful discussions and valuable comments, to Rok Sribar for checking some of the numerical calculations with zinc, and to Professor Wolfgang Sachse for his interest in this work. The author also thanks B. F. Addis for providing a zinc crystal of fine quality.

[1]M. J. P. Musgrave, *Crystal Acoustics* (Holden-Day, San Francisco, 1970).

[2]B. A. Auld, *Acoustic Fields and Waves in Solids,* 2nd ed. (Krieger, Malabar, FL, 1990), Vols. 1 and 2.

[3]S. Wolfram, *Mathematica,* 2nd ed. (Addison-Wesley, Redwood City, CA, 1991).

[4]See for a review G. A. Northrop and J. P. Wolfe, in *Nonequilibrium Phonon Dynamics,* edited by W. E. Bron (Plenum, New York, 1985), p. 165.

[5]A. G. Every, Phys. Rev. B **34**, 2852 (1986).

[6]F. I. Fedorov, *Theory of Elastic Waves in Crystals* (Plenum, New York, 1968).

[7]K. Y. Kim and W. Sachse, Phys. Rev. B **47**, 10 993 (1993).

[8]G. F. D. Duff, Philos. Trans. R. Soc. London, Ser. A **252**, 31 (1960).

[9]A. K. McCurdy, Phys. Rev. B **9**, 466 (1974).

[10]R. G. Payton, *Elastic Wave Propagation in Transversely Isotropic Media* (Martinus Nijhoff, The Hague, 1983).

[11]A. G. Every, Phys. Rev. B **37**, 9964 (1988).

[12]H. J. McSkimin, in *Physical Acoustics,* edited by W. P. Mason (Academic, New York, 1964), Vol. 1, Part A.

[13]E. P. Papadakis, in *Physical Acoustics,* edited by W. P. Mason and R. N. Thurston (Academic, New York, 1976), Vol. 12.

[14]K. Y. Kim, L. Niu, B. Castagnede, and W. Sachse, Rev. Sci. Instrum. **60**, 2785 (1989).

[15]G. A. Alers and J. R. Neighbors, J. Appl. Phys. **28**, 1514 (1957).

[16]F. R. Breckenridge, C. E. Tschiegg, and M. Greenspan, J. Acoust. Soc. Am. **57**, 626 (1975).

[17]K. Y. Kim, W. Sachse, and A. G. Every, J. Acoust. Soc. Am. **93**, 1393 (1993).