GROUP VELOCITY FORMULAS OF ANISOTROPIC SOLIDS AND THEIR APPLICATIONS

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ABSTRACT

This paper presents various closed-form analytic formulas that relate elastic constants of elastically anisotropic solids with orthorhombic or higher symmetry to a group velocity of quasilongitudinal (QL) or quasitransverse (QT) mode propagating in an arbitrary direction of the symmetry planes of media. Simple equations relating the direction of a group velocity to that of the corresponding wave normal are also described for both QL and QT modes. Some useful applications of these relations are discussed: first, determination of group velocity surfaces and cuspidal features; second, determination of mixed-index elastic constants, given the pure-index elastic constants obtained in the symmetry and other directions; third, determination of all elastic constants of a cubic medium with longitudinal group velocities measured at least in three different directions. Examples are provided with transversely isotropic zinc and cubic silicon crystals and an orthotropic Poly Ether Ether Ketone (PEEK) composite plate. It is demonstrated that given the numerous group velocity data, one can efficiently determine the elastic constants by first converting them into phase velocity data and then applying a least squares optimization method to the phase velocity data.

I. INTRODUCTION

Complete determination of all the elastic constants of a specimen by the plane wave ultrasonic techniques usually requires two opposite faces of the specimen to be polished parallel to each other and oriented in various directions and rely on phase velocity measurements [1,2]. This is usually achieved by destructive sectioning of the specimen, which may be undesirable under certain circumstances. This difficulty may be circumvented by employing a point source and a point detector and measuring a group velocity in various directions.

Here we deal with only the group velocity data measured in symmetry planes, which yield analytically all the elastic constants by the formulas recently derived by Kim [3]. In an arbitrary direction of propagation there exist no closed-form analytic formulas that relate the group velocity to elastic constants of a medium and determination of elastic constants from group velocity data are in general carried out numerically [4]. He also derived the simple relationships between the directions of wave normal and group velocity in the corresponding symmetry planes for both quasilongitudinal (QL) and quasitransverse (QT) modes. The relationships are very useful for identifying the features of ray surfaces and in particular those of a cusp in a specific direction.

One major advantage of using the symmetry plane wave speeds is that the measurements errors are minimized with these data in comparison with those of other measurements in non-symmetry directions.

II. THEORETICAL BACKGROUNDS

Let us denote three principal axes of symmetry of an orthorhombic medium by x_1, x_2, and x_3 directions. Essentially identical relations between the elastic constants and sound wave speed can be found for waves traveling in the three symmetry planes, i.e., x_1x_2, x_2x_3, and x_1x_3, by the proper rotation of indices. Therefore, consider a wave traveling, for example, in the x_1x_3 plane with its wave normal **n** and group velocity $\mathbf{V}_g$ oriented at angles θ and ζ, respectively, to the x_3 axis. The positive sense of both θ and ζ is taken in a clockwise direction from the x_3 axis. 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 to $-90^\circ \le \zeta,\theta \le 90^\circ$. The elastic properties of an orthorhombic medium are characterized with nine elastic constants: C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23}.

The phase and group velocities coincide in the principal symmetry directions and the relations between the wave speeds in symmetry directions and elastic constants are described by many authors [5,6]. The pure index elastic constants are usually obtained from phase or group velocity data along the principal symmetry directions.

A. Phase velocity formulas for symmetry planes

The pure index shear elastic moduli can be also determined from the pure transverse (PT) modes propagating in an arbitrary direction of the symmetry planes. For example, the following relation holds for the phase velocity of PT mode polarized in the x_2 direction and traveling in the x_1x_3 plane:

$$\rho V_T^2 = C_{66}\sin^2\theta + C_{44}\cos^2\theta . \qquad \text{(PT mode)} \qquad (1)$$

Once the pure index elastic moduli C_{11}, C_{22}, C_{33}, C_{44}, 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 quasi-longitudinal (QL) or quasi-transverse (QT) mode propagating in the x_1x_2, x_2x_3, and x_1x_3 planes, respectively. Again, we consider a wave traveling in the x_1x_3 plane. Let's define for simplicity of notation the following identities:

$$C_{11\pm} \equiv C_{11} \pm C_{55}; \quad C_{33\pm} \equiv C_{33} \pm C_{55}; \quad C_{13\pm} \equiv C_{13} \pm C_{55} \qquad (2)$$

The relations for the QL and QT modes are given by

$$2\rho V_{QL,QT}^2 = C_{11+}\sin^2\theta + C_{33+}\cos^2\theta \pm \left[\left(C_{11-}\sin^2\theta - C_{33-}\cos^2\theta\right)^2 + 4C_{13+}^2\sin^2\theta\cos^2\theta\right]^{1/2}, \qquad (3)$$

where the positive and negative signs in front of the square root of Eq. (3) correspond to the QL and QT modes, respectively. The Eq. (3) relates the elastic constant C_{13} to the phase velocity of QL or QT mode propagating in an arbitrary direction in the x_1x_3 symmetry plane. Suppose that for a wave normal specified by an angle θ, both QL and QT phase velocities, V_{QL} and V_{QT}, are known for the same angle θ. Then, Eq. (3) can be utilized to lead to the following simple relations:

$$\rho\left(V_{QL}^2 + V_{QT}^2\right) = C_{33+} + (C_{11+} - C_{33+})\sin^2\theta, \qquad (4)$$

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$$\rho^2\left(V_{QL}^2 - V_{QT}^2\right)^2$$
$$= C_{33-}^2 - 2\,(B + C_{33-}^2)\,\sin^2\theta + (C_{11-}^2 + 2B + C_{33-}^2)\,\sin^4\theta, \tag{5}$$

where the quantity B is defined as

$$B \equiv C_{11-}C_{33-} - 2C_{13+}^2. \tag{6}$$

B. Group velocity formulas for symmetry planes

A simple formula that relates group velocity with ζ is found for the PT waves with shear horizontal (SH) polarization [3,5] and is written as

$$\frac{1}{\rho V_g^2} = \frac{\sin^2\zeta}{C_{66}} + \frac{\cos^2\zeta}{C_{44}}. \qquad \text{(PT mode)} \tag{7}$$

Eq. (7) indicates that two shear elastic moduli C_{44} and C_{66} can be obtained by measuring the group velocities of PT modes propagating at least in two different directions. By performing similar experiments in the x_1x_2 and x_2x_3 symmetry planes all shear elastic moduli C_{44}, C_{55}, and C_{66} can be determined.

Let's define for simplicity of notation

$$p \equiv \tan\theta, \qquad q \equiv \tan\zeta, \tag{8}$$

$$D \equiv \left[\left(C_{11-}p^2 - C_{33-}\right)^2 + 4C_{13+}^2 p^2\right]^{1/2} > 0. \tag{9}$$

Then it can be shown that B in Eq. (6) and the above D are related by

$$B = \frac{1}{2p^2}\left(C_{11-}^2 p^4 + C_{33-}^2 - D^2\right). \tag{10}$$

Kim [3] derived the following Eqs. (11)-(13):

$$C_{11-}^2 p^3 + q\left(Bp^2 - C_{33-}^2\right) - Bp \pm \left(C_{11+}p - C_{33+}q\right)D = 0. \tag{11}$$

Eq. (11) can be used to find the wave normal corresponding to a given group velocity direction lying in the same symmetry plane, and vice versa. D in Eq. (9) can be expressed as

$$D(p) = \frac{1}{1-pq}\left\{\begin{array}{l} p\left(\pm C_{33+}q \mp C_{11+}p\right) \\ \pm\left[p^2\left(C_{33+}q - C_{11+}p\right)^2 - \left(1 - p^2q^2\right)\left(C_{11-}^2p^4 - C_{33-}^2\right)\right]^{1/2}\end{array}\right\}. \tag{12}$$

In the above equation we choose the region of $p = \tan\theta$ where D is real and positive. Finally the relation for group velocity is given by

$$\rho V_g^2 = \frac{\left(1+q^2\right)\left(C_{11-}^2p^4 - C_{33-}^2 \mp 2C_{33+}D - D^2\right)^2}{8D^2\left(C_{11+}p^2 + C_{33+} \pm D\right)}. \tag{13}$$

The upper and lower signs either in $\pm$ or in $\mp$ in Eqs. (11)-(13) apply to the QL and QT modes, respectively, except in the $\pm$ sign in front of the square bracket for square root in Eq. (12), which applies to both QL and QT modes.

Eq. (13) expresses the group velocity as a function of $p = \tan\theta$, when D is substituted by the expression on the right hand side of Eq. (12). Usually, experimentally or by other means as described in this section, the magnitude of group velocity V_g, its direction ζ, C_{11+}, C_{11-}, C_{33+}, and C_{33-}, are known. Then, Eq. (13) can be solved to find $p = \tan\theta$, which makes D in Eq. (12) real and positive. Once the value of this $p = \tan\theta$ is found, one can obtain the values of D, B, C_{13+}, and finally C_{13}, using Eqs. (12), (10), (6), and (2), respectively. On the other hand, given the known values of all elastic constants of a medium, Eq. (11) combined with Eq. (13) predicts the value of QL or QT group velocity in any direction in the symmetry plane.

Other elastic constants such as C_{23} and C_{12} can be obtained by the proper rotation of indices in Eqs. (11)-(13). Note that the formulas for various pure modes in the x_3 and x_1 symmetry directions are obtained by setting $\theta = \zeta = 0°$ and $\theta = \zeta = 90°$, respectively, in Eqs. (1), (3)-(5), (7), and (11)-(13). The equations for pure L and T modes along the face-diagonal direction of a cubic medium are also contained in Eqs. (11)-(13) as a special case of $\zeta = 45°$. For extension of Eqs. (11)-(13) to higher symmetry groups and more detail, readers refer to Ref. 3.

Let's consider elastic pulses of both QL and QT modes traveling in the $\{n_1,n_1,0\}$-type diagonal symmetry planes of tetragonal and cubic symmetry media. The directions of wave normal **n** and group velocity are specified by angles θ and ζ to the x_3-axis, respectively. It is shown in Ref. 3 that exactly the same relations between V_g, $\tan\zeta$, $\tan\theta$, and elastic moduli as those found in Eqs. (11)-(13), can be obtained, respectively, by simply replacing C_{11} by K, C_{55} by C_{44}, $C_{11\pm}$ by $K_\pm$. The quantities K, $K_\pm$, and $C_{11\pm}$ are now defined as

$$K \equiv (C_{11} + C_{12} + 2C_{66})/2, \quad K_\pm \equiv K \pm C_{44}, \quad C_{11\pm} \equiv C_{11} \pm C_{44}. \tag{14}$$

A group velocity formula for a PT wave traveling in the $\{n_1,n_1,0\}$-type diagonal plane and polarized normal to the plane is found by replacing C_{66} by $(C_{11} - C_{12})/2$ in Eq. (7).

C. Conversion between phase and group velocities

The normal surface is the pedal surface of the ray surface and conversely the ray surface is the envelope of planes drawn at right angles to the phase velocity **V** on the normal surface [5,6]. The phase and group velocities propagating in the symmetry planes, which have been discussed in Sections IIA and IIB, are related by

$$\mathbf{V} = \mathbf{V}_g\cdot\mathbf{n}; \qquad V = V_g\cos\varphi = V_g\cos(\zeta - \theta), \tag{15}$$

where φ denotes an angle between the directions of a wave normal and the corresponding group velocity and is given by

$$\tan\varphi = \frac{1}{V}\frac{dV}{d\theta} = \frac{1}{V_g}\frac{dV_g}{d\zeta}. \tag{16}$$

Given many group velocity data measured along various directions in the symmetry plane, a statistical optimization approach based on a curve-fitting to be described next may be more convenient in obtaining elastic constants than the method described in Section IIB. We follow the approaches of Kim et al. [7] Since we primarily deal with measured group velocity data, we pay our attention to the conversion from the group velocity to the corresponding phase velocity data. Combining Eq. (15) with Eq. (16), one obtains

$$V = \frac{V_g^2}{\sqrt{V_g^2 + \left(dV_g/d\zeta\right)^2}}. \tag{17}$$

The dependence of group velocity on a directional angle ζ for a PT mode is given by Eq. (7). The conversion of PT mode group velocities into phase velocities offers no advantage for determination of shear elastic moduli, as can be seen in Eqs. (1) and (7). We choose conveniently to fit the group velocity data of both QL and QT modes in a polynomial form as

$$V_g = \sum_{n=0}^{N} c_n\zeta^n, \tag{18}$$

where all the coefficients c_n can be determined by a linear least squares method and the constant c_o represents the group velocity of QL or QT mode along the principal axis for which $\zeta = 0$. With these coefficients thus determined, one calculates the phase velocities $V(\theta)$ corresponding to the group velocity data $V_g(\zeta)$, according to Eqs. (16)-(18). In case that either QL or QT phase velocity $V(\theta)$ can be determined, we fit either of them into

Eq. (3) by a nonlinear least squares method to obtain relevant elastic constants. On the other hand, when both QL and QT phase velocities can be calculated for the same angle θ, it is much easier to fit both of them into Eqs. (4) and (5) using a much simpler linear least squares technique for determination of relevant elastic constants. For plate-shaped composite materials and crystals aligned, e.g., in the x_3 direction normal to the plate, C_{33} and C_{44} can be easily obtained by measuring L and T wave speeds propagating normal to the plate. Then, one invokes Eq. (4) to find C_{11+}, C_{11}, and C_{11-}. Finally, from Eq. (5) one obtains B, C_{13+} and C_{13}.

III. GROUP VELOCITY SURFACES, CUSPIDAL FEATURES and ELASTIC CONSTANTS OF ZINC

Using a (0001)-oriented zinc disk of 75 mm diameter, 25. 8 mm thickness, and its density equal to 7134 kg/m^3, Kim and Sachse [8] obtained the five elastic constants of zinc from the group-velocity data measured in two principal symmetry directions. They are

$$C_{11} = 163.75,\ C_{12} = 36.278,\ C_{13} = 52.476,$$
$$C_{33} = 62.928,\ \text{and}\ C_{44} = 38.677\ \text{GPa}. \tag{19}$$

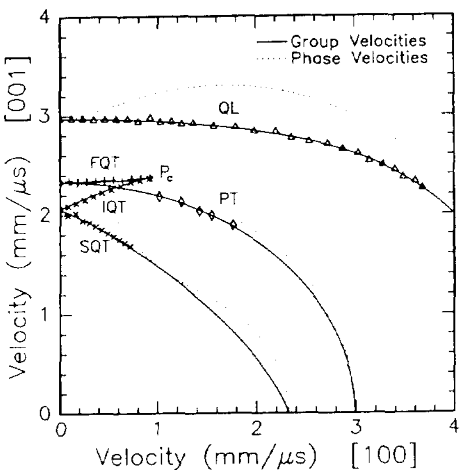

Fig. 1. (010) section of group and phase velocity surfaces in zinc, where the measured group velocity data are juxtaposed.

Using these data, Eqs. (1) and (7) for the PT mode, and Eqs. (3), (11) and (13) for the QL and QT modes, the (010) sections of group and phase velocity surfaces in zinc are plotted in Figure 1, where the measured group velocity data detailed in Ref. 9 are juxtaposed for comparison. Note that the group velocity section in Fig. 1 is virtually identical to that obtained by a Monte-Carlo calculation. For a given direction inside a cuspidal region, there are five group velocities: one QL, one PT, and three QT modes which are fast QT (FQT), intermediate speed QT (IQT) and slow QT (SQT) modes. Using Eqs. (11) and (13) for QT mode, one find the group velocity direction and magnitude of the cuspidal edge P$_c$ in Fig. 1 to be $\zeta = 21.5355°$ and $V_g = 2.55646$ mm/μs, respectively. The direction of the corresponding wave normal is calculated to be $\theta = -9.303667°$. Similarly, the direction of the wave normal corresponding to the conical point along the [001] symmetry direction in Fig. 1, where the IQT and SQT branches cross, is found to be $\theta = \pm 24.5244°$ and the group velocity of the conical point is 2.05998 mm/μs. There exists a tiny cusp around the [100] direction, which is not visible in the resolution of Fig. 1 but is apparent on a great magnified scale. The accurate calculation of this tiny cuspidal features is very difficult to obtain numerically but easy to carry out using Eqs. (11) and (13). For example, the direction of cuspidal edge measured from the [100] axis and its group velocity are calculated to be $\zeta = \pm 0.5687815°$ and $V_g = 2.32996$ mm/μs.

The elastic constants of zinc can be determined using the measured group velocity data shown in Fig. 1. The measured pure index elastic constants of zinc, C_{11}, C_{33}, and C_{44}, are identical to those in Eq. (19). Using QL $V_g = 3.910$ mm/μs at $\zeta = 47.34°$ in Fig. 1 and Eqs. (12) and (13), one obtains $C_{13} = 52.52$ GPa. Similarly, the IQT $V_g = 2.293$ mm/μs and SQT V_g =1.899 mm/μs both at $\zeta = 11.01°$ in Fig. 1 yield C_{13} equal to 51.30 GPa and 53.30 GPa. These are in good agreement to the C_{13} value listed in Eq. (19). Using the PT group velocities at $\zeta = 0°$ and 37.89°, Eq. (7), and the relation $C_{66} = (C_{11} - C_{12})/2$ yields $C_{44} = 38.68$ GPa and $C_{12} = 36.30$ GPa in excellent agreement with those in Eq. (19).

An alternative approach is to use statistical optimization to determine the elastic constants. For this purpose first fit QL, FQT, and IQT-SQT group velocity data into Eq. (18) by setting $N = 4$ and determine their coefficients c_n by a linear least squares method. The IQT and SQT branches are in fact one smoothly joining branch when their reflected images are extended across the symmetry axis [001]. The coefficients c_o of the QL and FQT branches yield respectively

$$\rho\left(c_o^2\right)_{QL} = C_{33} \qquad \text{and} \qquad \rho\left(c_o^2\right)_{FQT} = C_{44}. \tag{20}$$

Then, one obtains $C_{33\pm}$ and the phase velocities $V(\theta)$ of QL and QT modes using Eqs. (15)-(17). Next, the quantities on the left hand side of Eqs. (4) and (5) versus $\sin^2\theta$ are calculated and they are fitted into these equations by the linear least squares method to determine C_{11+}, C_{13+}, C_{11}, and C_{13}. Using the C_{44} found above and $C_{66} = (C_{11} - C_{12})/2$, C_{12} is obtained from the PT group velocity data by the linear least squares fit into Eq. (7). All five elastic constants of zinc thus determined by the statistical linear optimization technique are $C_{11} = 164.08$, $C_{12} = 37.33$, $C_{13} = 52.24$, $C_{33} = 62.63$, and $C_{44} = 38.82$ GPa in excellent agreement with those in Eq. (19). Though computationally demanding, one may as well use a nonlinear least squares method, trying to minimize the number of elastic constants to be optimized. Using the C_{44} and C_{33} as determined right above and the nonlinear least squares method, the converted QL $V(\theta)$ data are fitted into Eq. (3) of the QL mode to obtain $C_{11} = 163.66$ GPa and $C_{13} = 52.43$ GPa, which are again in excellent agreement with those in Eq. (19).

Kim and Sachse [8] derived an analytic equation that relates $C_{13+} = C_{13} + C_{44}$ to the coefficient $c_o = 2.051$ mm/μs obtained from the fitting of the IQT and SQT group velocity data and it is expressed as

$$(C_{13} + C_{44})^2 = C_{11}C_{33} + C_{44}^2 - \rho c_o^2(C_{11} + C_{44}) + 2\left[C_{11}C_{44}(C_{33} - \rho c_o^2)(C_{44} - \rho c_o^2)\right]^{1/2}, \tag{21}$$

which yields $C_{13} = 52.82$ GPa in good agreement with that in Eq. (19). A relation similar to Eq. (21) is obtained for the corresponding conical point of the $\{n_1, n_1, 0\}$-type diagonal plane of cubic and tetragonal media by replacing C_{11} by K, C_{55} by C_{44}, $C_{11\pm}$ by $K_\pm$, the quantities defined in Eq. (14).

IV. ELASTIC CONSTANTS OF CUBIC SILICON AND ORTHOTROPIC PEEK

For cubic silicon a (001)-oriented single crystal disk of 100 mm diameter and 49.15 mm thick was used to measure group velocities in various directions of the symmetry planes. $C_{11} = \rho\left(V_g^2\right)_{PL} = 165.7$ GPa and $C_{44} = \rho\left(V_g^2\right)_{PT} = 79.56$ GPa are obtained from the PL and PT group velocity data measured in the [001] direction and using $\rho = 2332$ kg/m^3. The PL and PT group velocities in the <110> direction ($\zeta = 45°$), which are related to C_{12} by $\rho\left(V_g^2\right)_{PL} = (C_{11} + C_{12} + 2C_{44})/2$ and $\rho\left(V_g^2\right)_{PT} = (C_{11} - C_{12})/2$, yield $C_{12} = 63.90$ GPa.

The QL group velocity 8.830 mm/μs is determined from the QL mode arrival in Figure. 2 in the direction of $\zeta = 26.94°$ in the (010) plane. Using $C_{11} = 165.7$ GPa and $C_{44} = 79.56$ GPa as above, and Eqs. (12) and (13) for a cubic medium, one obtains $C_{12} = 64.404$ GPa in good agreement with the C_{12} obtained above. Using the arrival of the QT mode in Fig. 2 leads to a similar result. It is also possible to determine all three elastic constants of silicon from the L mode group velocity data measured at least in three different directions in the symmetry plane as the L mode arrival is unambiguously and accurately identified as a point at which the signal first jumps out of noise level. Using the above PL group velocity data in the

[001] and <110> directions, that of the QL mode in Fig. 2, and Eqs. (12) and (13), yields C_{12} = 50.54 GPa and C_{44} = 86.24 GPa, which are in substantial error. It is shown in Ref. 3 that very precise measurements of wave speeds with error less than 0.01 % are required to obtain the elastic constants with error less than a few %.

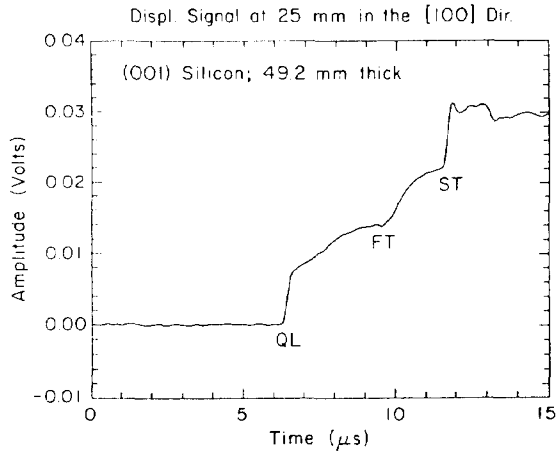

Fig. 2. Displacement signal detected at ζ = 26.94° on the (010) plane in a silicon disk specimen

A small dimple found around 9.5 μs in Fig. 2 is caused by the arrival of nearly SH polarized fast transverse (FT) modes which travel at a group velocity indistinguishably close to $(C_{44}/\rho)^{1/2}$. Note that using the arrivals of QL, FT, and QT modes in one directional signal of Fig. 2, it is possible to determine all three elastic constants of cubic silicon. It is shown by Kim et al. [10] that all three elastic constants of silicon can be easily and accurately determined from one broadband signal propagating in the <100> direction.

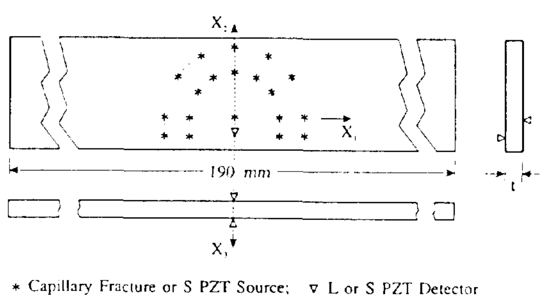

Fig. 3. Geometric configurations of a PEEK specimen, its principal axes with the detector and scanning sources

A geometric configuration of a fiber-reinforced PEEK thin plate specimen with detector and scanning source is shown in Figure. 3. The composite specimen has 30 % weight fraction of the carbon fibers, the density of 1500 kg/m³, thickness t =3.26 mm, and three principal symmetry directions along the x_1, x_2, and x_3 directions. Various combinations of a glass capillary, L and shear (S) mode PZT source and detector are used to determine the elastic constants. First, C_{33} = 10.65 GPa is obtained from the PL group velocity in the x_3-thickness direction. The surface skimming pseudo L mode group velocities in the x_1 and x_2 directions on the surface yield respectively C_{11} = 28.52 GPa and C_{22} = 15.21 GPa. Next, using the PT group velocities measured with S PZT source and S PZT detector in various directions of the x_1x_3 and x_2x_3 symmetry planes and Eq. (7), one obtains C_{44} = 2.23 GPa and C_{55} = 2.41 GPa, and C_{66} = 5.71 GPa. A detailed description of obtaining PT group velocities is given elsewhere [7,11,12]. Using Eqs. (12) and (13), C_{12} = 7.70 GPa is calculated from the surface skimming pseudo L group velocities in various directions on the x_1x_2 surface. Finally, C_{13} = 6.00 GPa and C_{23} = 7.65 GPa are obtained from the QL group velocities along various directions in the x_1x_3 and x_2x_3 planes.

The calculated Young's modulus in the x_1 direction , obtained using the above elastic constants, is 24.0 GPa, which compares well with the Young's modulus obtained by the static tension test performed in the same direction.

The measurement of the elastic constants of glass and carbon fiber reinforced PEEK specimens is described in detail by Kim et al. [12].

V. CONCLUSIONS

We have demonstrated various novel techniques by which the elastic constants of anisotropic solids are analytically determined from the group velocity data measured along arbitrary directions in the symmetry planes. The usefulness of this analytical technique was illustrated with the specimens of transversely isotropic zinc, cubic silicon, and orthotropic PEEK. The first technique is a direct method which calculates the elastic constant from the group velocity data . The other technique is an indirect approach adapted to numerous group velocity data. It first converts the group velocity data into phase velocity data, and then uses least squares methods to obtain the elastic constants. It is also shown that a simple relationship derived between the directions of wave normal and group velocity in the corresponding symmetry planes is very useful for investigation of the features of the normal and group velocity surfaces within and without a cuspidal region.

ACKNOWLEDGMENT

We deeply appreciate the financial support of the Office of Navel Research and the use of the facilities of the Materials Science Center of Cornell University, which is funded by the National Science Foundation.

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