Determination of the elastic constants of anisotropic solids from acoustic-wave group-velocity measurements

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A method is proposed for determining the elastic constants of an anisotropic solid from acoustic-wave group velocities measured in off-symmetry directions in a specimen. The method corresponds to a two-stage optimization procedure in which the elastic constants are varied so as to obtain a least-squares fit of measured to calculated group velocities. At each iterative step a numerical minimization process is employed to find the wave normals and velocities of waves having the required ray directions. The method is demonstrated with synthetic data generated for a number of cubic crystals, and to experimental data obtained on single crystals of silicon using the ultrasonic *point-source–point-receiver* technique. When provided with longitudinal- and transverse-mode velocity data, the method is able to accurately recover all three independent elastic constants. When only longitudinal mode data is provided, C_{11} and the combination $C_{12}+2C_{44}$ can be accurately recovered, but not C_{12} and C_{44} individually.

I. INTRODUCTION

Most determinations of elastic constants of anisotropic solids are based on acoustic-wave-speed measurements.[1–3] Usually in these investigations it is the phase velocity rather than group velocity that is measured. The reasons for this are partly experimental and partly have to do with the methods that are available for data inversion. Some techniques, such as neutron scattering[4] and Brillouin scattering,[5,6] provide direct access to the dispersion relation of a medium, and hence to the phase velocities in various directions. Other techniques such as the pulse-superposition and pulse-echo–overlap techniques,[7] while nominally concerned with the transmission of wave packets, also yield values of the phase velocities rather than the group velocities, when applied to nondispersive media. The reason for this is that the experimental arrangement is usually such that one measures only the component of the group velocity in the direction of the wave normal and this equals the phase velocity. As regards the inverse problem, the methods for recovering elastic constants from phase-velocity data are fairly straightforward and well established, but the same is not true for group velocities. The recovery process from phase velocities is particularly simple for data pertaining to high-symmetry directions, where the formulas relating velocities to elastic constants are very simple and easily inverted.[8] On occasion, the need arises to take account of phase velocities in off-symmetry directions. It often happens in this situation that there are more velocity measurements than independent elastic constants to be determined, and an optimization method is used to obtain a least-squares fit.[9,10]

Group velocities also carry information about the elastic constants and, in principle, this information should be recoverable. There are a number of areas in which group velocities are measured and where a method for extracting elastic constants from such measurements could be of use. In seismology there is growing recognition of the importance of the elastic anisotropy of the earth and its influence on wave propagation.[11] Whether considering near-field phenomena of far-field asymptotic limits to wave fields radiated by localized sources, the group velocity is a crucial quantity describing signal propagation. Phonon imaging in crystals is another area in which group velocities play a central role.[12] Complex patterns of caustics are observed in phonon images that are derived from the focusing of acoustic ray vectors in certain directions. The caustic patterns of phonon images are governed by the elastic constant ratios, but there does not appear to have been any concerted effort yet to use this technique for elastic constant determinations, although the potential for doing so certainly exists. Fitting *et al.*[13] have developed a method, based on a variable-angle ultrasonic wedge source and an array of phase-insensitive receivers, with which they measure group velocities. Being able to determine the wave normal **n** from the source, however, they are able to obtain the phase velocity, and then follow the familiar inversion route to recover the elastic constants.

The recently developed ultrasonic *point-source–point-receiver* (PS-PR) technique has shown promise as a method for measuring group velocities and determining elastic constants in materials.[14–16] The PS-PR technique has the advantage of flexibility as regards sample geometry, it provides a simultaneous measurement of all three velocities in any number of directions, and its broadband feature proves particularly advantageous in the study of highly attenuating materials. The principle of the PS-PR technique, which has been described in greater detail previously,[14] is illustrated in Fig. 1. Some form of localized excitation, which may, for example, be a pulsed laser beam or a breaking capillary, generates acoustic waves which spread out in all directions in the

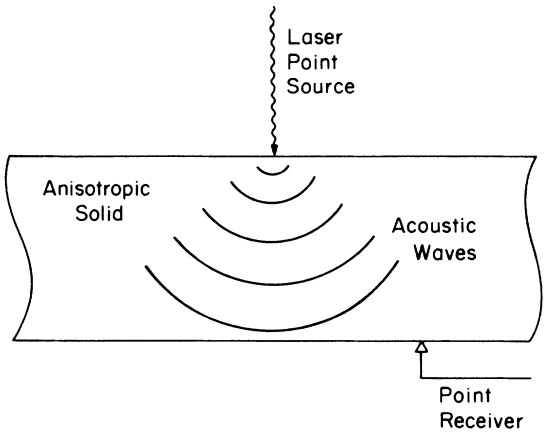

FIG. 1. Schematic diagram of the point-source–point-receiver method.

sample. These waves are then detected by one or more small-aperture sensors located on the surface of the sample. The source position can easily be varied to obtain data for a variety of directions in a specimen. The time dependence of the excitation usually approximates a δ function or a Heaviside step function. In the detected signal one discerns sharp features, such as spikes or discontinuities,[17] that correspond to arrivals of waves that have propagated through the medium at their *group velocity*.[18] In the past, however, the treatment of these wave arrivals has ignored the difference between phase and group velocity.[14,16,19] To determine the elastic constants of an anisotropic material, the arrival times for various source-receiver configurations have been expressed in terms of phase velocities in the respective directions, and the elastic constants were obtained by an optimization method or by use of the simple formulas that apply in the symmetry directions. This approach is valid when applied to materials having a low degree of anisotropy, or where only data pertaining to the neighborhood of certain high-symmetry directions are used. In these situations, the difference between the phase and group velocities is negligible. For more highly anisotropic materials and a wider spread of measuring directions, the phase and group velocities of a wave can differ significantly,[8,20,21] and the elastic constants obtained on the basis of ignoring this difference become progressively less reliable with increasing anisotropy. This fact needs to be recognized even though this earlier approach may continue to serve a useful purpose in providing a relatively simple means of obtaining approximate values of the elastic constants, which for some purposes might be adequate. Indeed, the rigorous algorithm we describe in this paper requires the input of suitable, approximate starting values of the elastic constants, and the above method constitutes one means by which they may be obtained.

There are two main problems in determining the elastic constants from group-velocity data. Firstly, there is no closed-form mathematical expression presently available that relates only the elastic constants and the group velocity, and which might conceivably be manipulated to obtain the elastic constants. Such an expression, if it were to be established, would be of enormous complexity. The only methods that are presently available for calculating the group velocity are based on parametric equations involving quantities such as the phase velocity, wave normal, polarization vector, and slowness vector.[8,20,21] Secondly, the slow transverse (ST) and fast transverse (FT) [but not the outer longitudinal (L)] sheets of the group-velocity surface (ray surface) commonly possess folded regions where the group velocity is multivalued. This poses a severe challenge to the implementation of a computerized optimization scheme. A numerical iteration may go awry, and the resolution of the experimental data may not be adequate to distinguish between different values of the group velocity in a given direction.

In this paper we propose an optimization method for determining the elastic constants of an anisotropic solid from acoustic-wave-group velocities measured in off-symmetry directions, and we point out certain pitfalls which must be avoided in applying the method. We have implemented the method for media of cubic symmetry, developing the appropriate computer coding and processing synthetic computer-generated data for a number of crystals, and have also applied it to experimental data obtained on single crystals of silicon. We demonstrate that, when provided with longitudinal and transverse-mode velocity data, the method is able to accurately recover all three independent elastic constants. When only longitudinal-mode data are provided, C_{11} and the combination $C_{12}+2C_{44}$ can be accurately recovered, but not C_{12} and C_{44} individually.

II. METHOD OF ANALYSIS

A. General considerations

The elastic-wave equation for anisotropic solids admits plane-wave solutions which are governed by the Christoffel equations[8,20,21]

$$(\Gamma_{rs}-\rho v^2\delta_{rs})U_s=0\ , \tag{1}$$

where $\Gamma_{rs}=C_{rlsm}n_l n_m$ is the Christoffel tensor, C_{rlsm} are the second-order elastic constants (in subsequent discussions we will employ the Voigt two-subscript convention,[22] and refer to $C_{\alpha\beta}$), $\mathbf{n}=(n_l)$ is the wave normal, $\mathbf{v}=v\mathbf{n}$ is the phase velocity, $\mathbf{U}=(U_s)$ is the polarization vector of the wave, ρ is the density of the medium, and δ_{rs} is the Kronecker δ. The secular equation for Eq. (1) is

$$|\Gamma_{rs}-\rho v^2\delta_{rs}|=0\ , \tag{2}$$

and is cubic in v^2 and in the elastic constants.

The forward motion of points of constant phase in the plane wave is determined by phase velocity $\mathbf{v}$, and it is this quantity, or its inverse, the slowness vector $\mathbf{s}=\mathbf{n}/v$, that is measured in most experiments on nondispersive media. In light scattering or neutron scattering, for example, the information obtained on an acoustic wave or a phonon is its wave vector $\mathbf{k}$ and angular frequency ω, from which $\mathbf{s}=\mathbf{k}/\omega$ follows immediately. In most ul-

trasonic determinations of elastic constants, a plane wave is reflected back and forth between two surfaces which are parallel to the wave fronts and only the phase velocity is measured. Some plane-wave experiments with immersion systems[23,24] involve oblique transmission through a sample, but again, careful analysis shows that it is the phase velocity that is measured.

For a fixed value of $\mathbf{n}$ Eq. (2) represents a relationship between the elastic constants and v. Solving for v yields three velocities, one corresponding to a quasilongitudinal mode and the other two to fast and slow quasitransverse modes. The corresponding inverse problem can be regarded as solving Eq. (2) for the elastic constants when a sufficient number of measured v's are given.

For certain high-symmetry directions, Eq. (2) factorizes, yielding one or more linear equations in the elastic constants and v^2. In some cases, measurements in these directions suffice to determine all the elastic constants. Data pertaining to off-symmetry directions tend to be used, for example, where suitably faceted samples are not available, or where there are additional elastic constants to be determined because of low symmetry, or where higher accuracy is desired. Often in this situation there are more velocity measurements than additional elastic constants to be determined and an optimization method is employed to obtain a least-squares fit. The quantity that is minimized might be the mean-square difference between the calculated and measured velocities,[25,26] or the Euclidean functionals associated with Eq. (2).[9]

The energy of a wave propagates not at its phase velocity $\mathbf{v}$ but at the group velocity $\mathbf{V}$ given by[21]

$$\mathbf{V}=\nabla_{\mathbf{k}}\omega(\mathbf{k})=[v(\mathbf{n})-\mathbf{n}\cdot\nabla_{\mathbf{n}}v(\mathbf{n})]\mathbf{n}+\nabla_{\mathbf{n}}v(\mathbf{n}) . \quad (3)$$

In an elastically anisotropic solid, the phase and group velocities of a wave are not, in general, equal, even in the absence of attenuation and dispersion. It is only in very special (usually high-symmetry) directions that $\mathbf{v}$ and $\mathbf{V}$ are equal. Elsewhere the two velocities may deviate in direction from each other by up to 20° or more, depending on the degree of anisotropy. They are not completely independent of one another, however, being related by[21]

$$\mathbf{V}\cdot\mathbf{n}=v . \quad (4)$$

The inverse problem of obtaining elastic constants from measured group velocities needs to be approached indirectly. There is no equation available, analogous to Eq. (2), that relates the elastic constants and the group velocity, which might conceivably be manipulated to obtain the elastic constants. Analytical arguments[27] indicate that this equation, which for fixed $C_{\alpha\beta}$ would describe the ray or group-velocity surface, could, in the most general case, be of degree as high as 150 in the components of $\mathbf{V}$. The prospect of attempting to construct this equation is daunting. So, at present, there appears to be no closed-form analytical procedure for obtaining the group velocity in a given arbitrary direction. The only presently available methods for calculating $\mathbf{V}$, such as Eq. (3), all involve expressing it parametrically in terms of quantities such as $\mathbf{v}$, $\mathbf{n}$, $\mathbf{s}$, and $\mathbf{U}$. As a result, the determination of elastic constants from group velocities becomes a two-stage process. Given a set of elastic constants, the wave normals $\mathbf{n}$ (or equivalently $\mathbf{v}$ or $\mathbf{s}$) must first be determined such that the associated group velocities are parallel to the observed velocities. The elastic constants are then varied (at each stage adjusting the $\mathbf{n}$'s to keep the directions of the $\mathbf{V}$'s the same) so as to optimize the fit of the calculated to the measured group-velocity magnitudes. Details of the method we have used for calculating these $\mathbf{n}$'s are discussed next.

B. Determination of the wave normals

In principle, if a sufficient number of high-precision measurements were made to accurately map out the entire ray surface, or at least some continuous regions of it, then the wave normals, which are normal to this surface, would follow. These could be obtained, for instance, by piecewise fitting of a low-order polynomial equation

$$\Omega_p(\mathbf{V})=0$$

to small portions of the surface and then obtaining $\mathbf{n}$ from the gradient[20]

$$\mathbf{n}=\nabla_{\mathbf{V}}\Omega_p(\mathbf{V})/|\nabla_{\mathbf{V}}\Omega_p(\mathbf{V})| . \quad (5)$$

However, in a practical situation where the data set is sparse and subject to experimental error, the numerical differentiation of the data required to obtain the normals would generate unacceptably large errors.

We have adopted a different approach. We note that, given the elastic constants of a medium and a direction for the group velocity, it is possible, with certain provisos, to numerically determine, in a systematic way, $\mathbf{n}$, $\mathbf{v}$, and $\mathbf{V}$. We treat this as a minimization problem, varying the polar angular coordinates θ and ϕ of

$$\mathbf{n}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta) ,$$

so as to minimize the angular deviation between the ray vector calculated from $\mathbf{n}$, and the given direction. The quantity that is minimized can be taken to be either

$$F=1-\mathbf{N}_{\text{expt}}\cdot\mathbf{N}_{\text{calc}}$$

or

$$G=(\Theta_{\text{expt}}-\Theta_{\text{calc}})^2+(\Phi_{\text{expt}}-\Phi_{\text{calc}})^2 ,$$

where Θ and Φ are the polar angles of

$$\mathbf{N}=(\sin\Theta\cos\Phi,\sin\Theta\sin\Phi,\cos\Theta) ,$$

which is a unit vector in the direction of $\mathbf{V}$. The subscripts "expt" and "calc" refer to experimental (or input) and calculated (or recovered) values, respectively. An alternative approach would be a constrained minimization with respect to the three components of $\mathbf{n}$ subject to $|\mathbf{n}|=1$. In our computations this minimization was performed with the IMSL subroutine DBCONF, which is based on a quasi-Newton method.

When applied to the longitudinal modes, we find that this method of minimizing F or G is stable and efficient. Given virtually any direction $\mathbf{N}$ and the starting values and upper and lower bounds for θ and ϕ, the procedure requires only a few tens of iterations to converge to the

correct **n**. This is not surprising since, in the absence of piezoelectric stiffening of the elastic constants, the L sheet of the slowness surface is entirely convex. The ray vector, which is normal to the slowness surface, is rotated towards $\mathbf{N}_{\text{expt}}$ by the numerical procedure, and hence converges to the correct point along a fairly direct path. There is no likelihood of migration to a spurious minimum.

As regards the ST and FT modes, greater care has to be exercised in determining **n**, particularly where the degree of anisotropy is large. The source of the difficulty is illustrated in Fig. 2. Suppose a group velocity is sought having the direction **N**. Because of the folding of the transverse sheets of the group-velocity surface, there are actually three rays, represented by the points a', b', and c' on the ray surface, that point in the required direction. These correspond to similarly labeled points on the slowness surface where the normals are parallel to **N**. The numerical procedure will converge to any one of these three points depending on where the starting point is. If this is a point such as a, then the convergence is towards a' and so on. There are some materials whose ray surfaces are folded to the extent that in some directions there are five or more collinear rays for a particular polarization. It is recognized that it will often not be possible to resolve all of these different velocities in the experimental data. Keeping track of multiple velocities and assigning measured velocities to particular modes is a problem of considerable complexity, particularly when carried out within a computerized optimization scheme in which elastic constants are varied. We have found it expedient therefore to steer a wide berth of folded regions of the ray surface, aiming to fit only data associated with single-valued regions such as the neighborhood of N' in Fig. 2. Even here caution has to be exercised in applying the algorithm that searches for **n**. If the starting value is reasonably close to the correct one, as depicted, for example, by the points d and e in Fig. 2, the numerical procedure converges to the correct value. On the other hand, for a starting value such as f, the procedure migrates to a point of inflection (point of zero Gaussian curvature) on the slowness surface, which corresponds to a cuspidal edge on the ray surface.

Figure 3 shows a $(1\bar{1}0)$ plane section of the ray surface of germanium. It has been constructed by generating a large number of ray vectors from a uniform distribution of wave normals, and sorting out from these rays, ones which lie within an angle of 0.03° of the $(1\bar{1}0)$ plane, and then discarding the small out-of-plane components of these selected rays. Some of these rays are associated with normals which lie very close to the plane. Others, the so-called oblique rays, are associated with normals lying well away from the plane. The arcs labeled ST and FT indicate the single-valued regions of the ST and FT sheets of the ray surface, respectively, whereas elsewhere the surface is folded. In our optimization method for determining the elastic constants, these constants are varied within certain bounds and the folded regions of the ray surface can expand or contract somewhat. Only data well away from the boundaries of the multiple-valued regions is therefore safe to use.

C. Recovery of elastic constants

The successful implementation of the optimization method that we describe here requires that approximate values of the elastic constants be known. These might be obtained, for instance, by treating the measured velocities initially as phase velocities and applying one of the simpler and more direct methods that are available for recovering elastic constants from phase velocities. In cer-

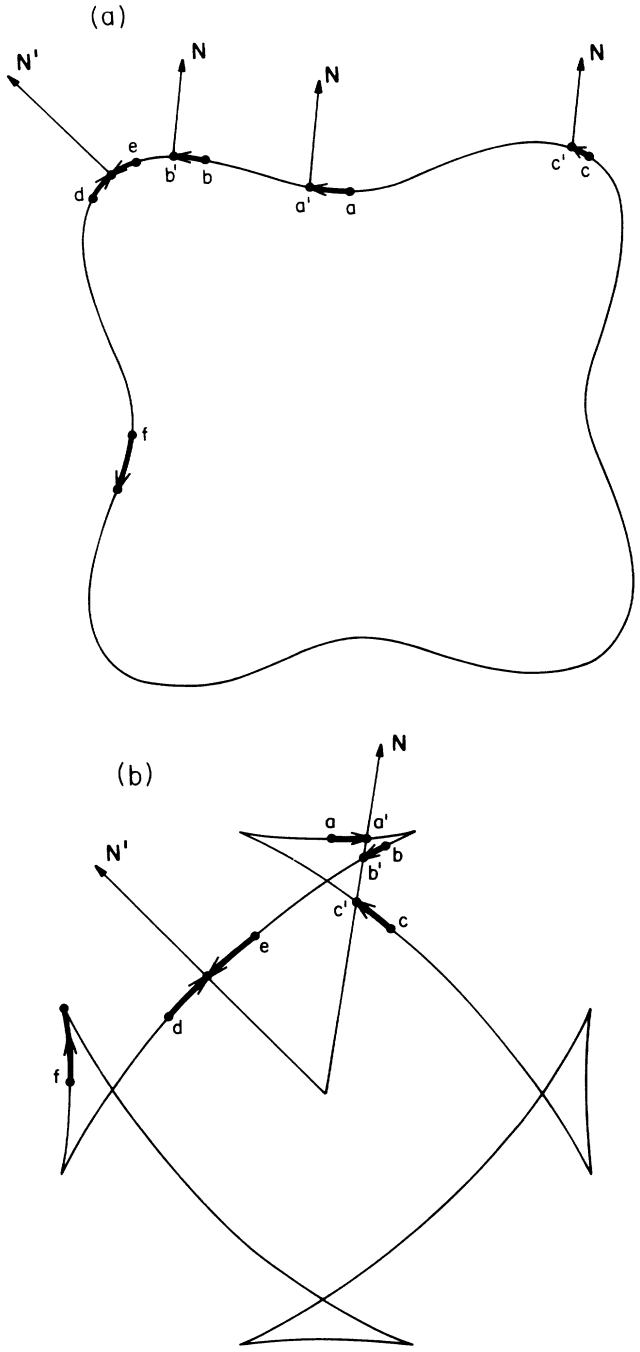

FIG. 2. Two-dimensional schematic of (a) an acoustic slowness surface and (b) the associated group-velocity surface of an anisotropic material.

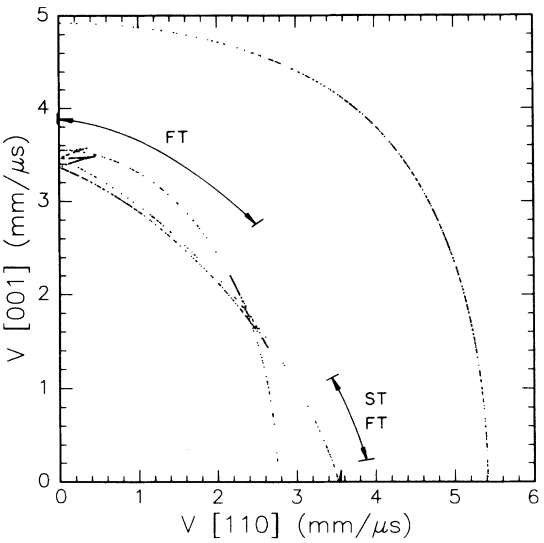

FIG. 3. A $(1\bar{1}0)$ section of the ray surface of germanium. Elastic constants for the calculation are from Ref. 8.

tain high-symmetry directions, the values of the phase and group velocities are identical, and data acquired for these directions will generally, with minimal effort, yield fairly reliable estimates of some or all of the elastic constants. Using the approximate elastic constants, one then calculates the ray surface using Eqs. (2) and (3) and identifies the folded regions of the transverse sheets that are to be avoided.

Our optimization method for determining the accurate elastic constants $C_{\alpha\beta}$ of an anisotropic medium is as follows.

(1) A set of r group velocities $\mathbf{V}^1_{\text{expt}}, \ldots, V^r_{\text{expt}}$ (with directions $\mathbf{N}^1, \ldots, \mathbf{N}^r$) are measured. These velocities may correspond to L modes in any direction or to transverse modes associated with unfolded regions of the ray surface. For an accurate determination of all the elastic constants, both longitudinal and transverse velocities are required in general.

(2) Using a trial set of elastic constants $C^0_{\alpha\beta}$ the method of Sec. II B is used to determine a calculated set of wave normals $\mathbf{n}^1, \ldots, \mathbf{n}^r$ whose associated group velocities (of the appropriate polarization) $\mathbf{V}^1_{\text{calc}}, \ldots, \mathbf{V}^r_{\text{calc}}$ point in the directions $\mathbf{N}^1, \ldots, \mathbf{N}^r$. The calculation of the $\mathbf{n}$'s can be done with any required degree of precision, since two parameters θ and ϕ are being varied to fit two quantities Θ and Φ.

(3) The magnitudes of the calculated and measured group velocities will differ. The closer the $C^0_{\alpha\beta}$ are to the "correct" values of the elastic constants, the smaller, on average, the differences between the two velocities will be. At this point we follow the customary practice of resorting to a least-squares fit, varying the trial elastic constants so as to minimize

$$\chi^2 = \frac{1}{r} \sum_{j=1}^{r} (V^j_{\text{expt}} - V^j_{\text{calc}})^2 . \tag{6}$$

(4) At each step of this minimization the $\mathbf{n}$'s are recalculated using the current values of the elastic constants.

In our implementation of this procedure we have used the IMSL subroutine DBCLSF which is based on a modified Levenberg-Marquardt algorithm and a finite difference Jacobian.

D. Formulation for cubic symmetry

For a medium of cubic symmetry there are three independent elastic constants C_{11}, C_{12}, and C_{44}, and the Christoffel tensor takes on the form[8]

$$\Gamma_{rs} = \begin{cases} (C_{12}+C_{44})n_r n_s , & r \neq s , \\ C_{11}n_r^2 + C_{44}(n^2 - n_r^2) , & r = s . \end{cases} \tag{7}$$

In our computations we have made use of a closed-form solution to Eq. (2) for calculating v, and have obtained $\mathbf{V}$ from Eq. (3) by implicit differentation of Eq. (2).[26]

The computer program we have set up for recovering the elastic constants from supplied velocity data consists of a number of modules. The starting values and bounds for the elastic constants are required. Based on the initial values of the elastic constants, a set of wave normals that yield the required ray directions is determined. To be certain of identifying the correct normals, a coarse grid search is conducted first to obtain approximate values. These are then provided as starting values to the minimization procedure DBCONF which, in conjunction with a fitting routine, does the accurate determination. We will call this the reference set of normals. They are used as starting values in subsequent callings of DBCONF.

The IMSL optimization procedure DBCLSF is then invoked. It repeatedly calls a subroutine FITT which it provides with a succession of values for the elastic constants. FITT, in turn, calls DBCONF to calculate the wave normals, using the current values of the elastic constants. Since the elastic constants vary by no more than about $\pm 10\%$ in the optimization process, the wave normals at each stage of the optimization are expected to be reasonably close to the reference set and so the coarse grid search is dispensed with and DBCONF is run using the reference set starting values. FITT returns a set of calculated group velocities, which have the same directions as the measured velocities, to DBCLSF. By a numerical convergence process, DBCLSF then arrives at values of the elastic constants that minimize the mean-square deviation of the observed from the calculated group-velocity magnitudes.

We have written this program in FORTRAN and run it on a Convex C210 supercomputer. The number of iterations to convergence averages about 50. The CPU time varies depending on the size of the data set. We have found that when 15 measured velocities are fit, the computational time is seldom more than about 2 min.

As pointed out in Sec. II B, transverse velocities need to be selected well away from folded regions of the ray surface. The topology of the ray surface of cubic crystals and its variation with degree of anisotropy has been studied in great detail by Every[28] and by Hurley and Wolfe.[29]

When the anisotropy is low there are only small regions where the transverse sheets of the surface are folded. These regions grow in extent as the anisotropy increases.

Figure 4 shows polar plots of the distributions of ST and FT rays associated with a uniform distribution of wave normals. The calculation is based on the elastic constants of CsBr, a moderately anisotropic crystal for which $(C_{11}-C_{12})/2 > C_{44}$. In the context of phonon imaging, a plot of this type is known as a phonon focusing pattern. The cuspidal edges of the ray surface are revealed as caustics or lines of accumulation of the rays. These delimit regions where the ray surface is folded and where velocity measurements are to be avoided. The regions from which data can safely be taken are: ST modes in the proximity of the $\{100\}$ planes and FT modes in the proximity of $\langle 100 \rangle$ directions.

Figure 5 shows polar plots of the ray distributions for Ge, a moderately anisotropic crystal for which $(C_{11}-C_{12})/2 < C_{44}$. The regions in the FT patterns that are devoid of rays lie inside circles of conical refraction surrounding the $\langle 111 \rangle$ directions. It is self-evident that FT velocities cannot be specified in these lacunas, and ST rays in these regions should also be avoided. CsBr possesses similar lacunas, but they are partly obscured by the folding of the ray surface of that material. Folded regions of the ray surface of Ge are evident in Fig. 5. The regions from which data can safely be taken are ST modes in the proximity of $\langle 110 \rangle$ directions and FT modes away from the $\{100\}$ planes and the $\langle 111 \rangle$ directions.

Application of the method described here presupposes knowledge of the approximate values of the elastic con-

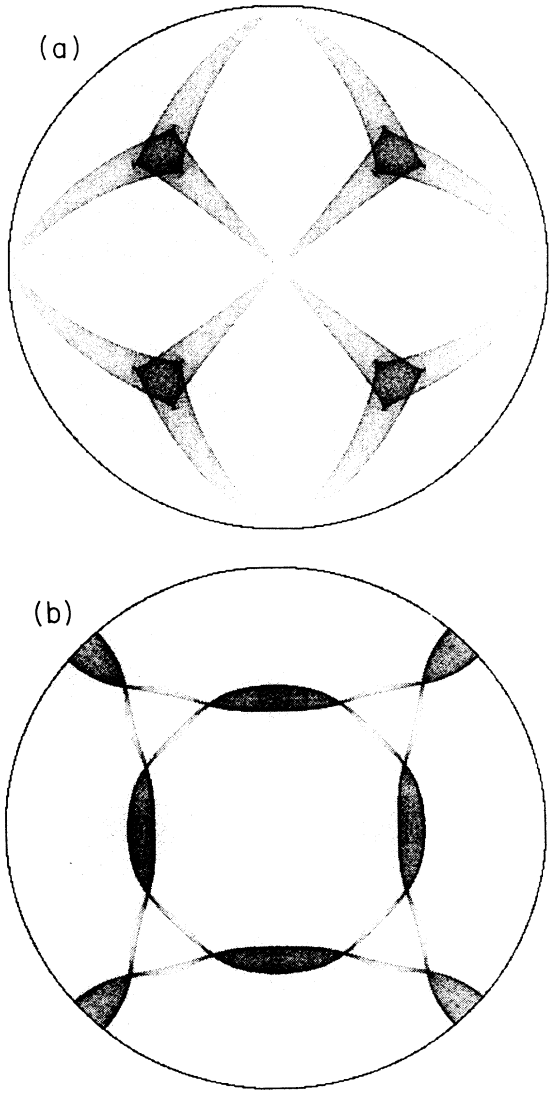

FIG. 4. Polar plot of the (a) ST and (b) FT ray distributions of CsBr for a uniform distribution of wave normals. Elastic constants for the calculation are from Ref. 30. The [001] direction lies at the center of the plot.

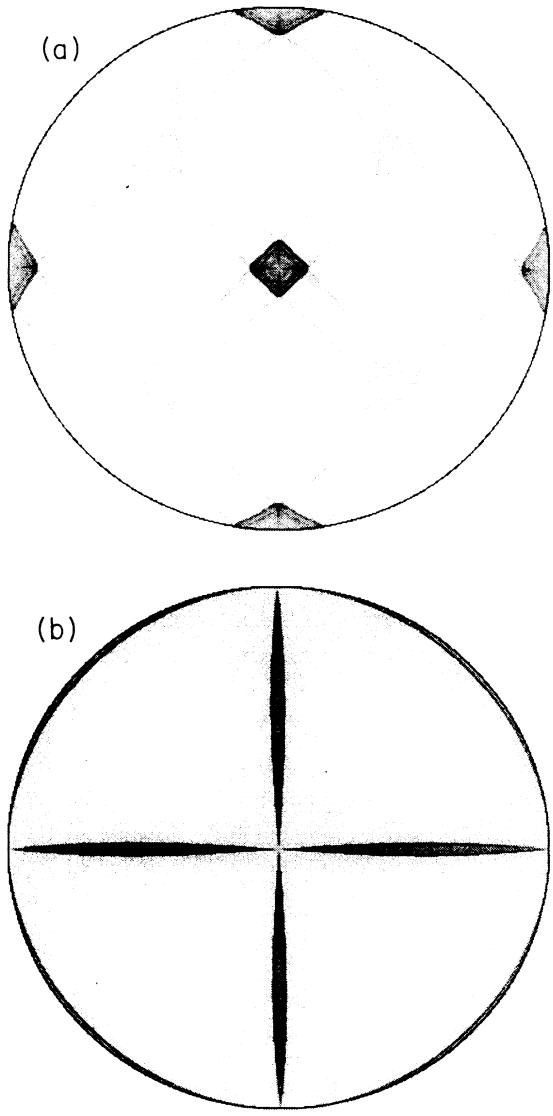

FIG. 5. Polar plot of the (a) ST and (b) FT ray distributions of germanium for a uniform distribution of wave normals. Elastic constants for the calculation are from Ref. 8.

stants of the medium under investigation. These are used to calculate the ray distribution patterns so that safe regions for data input can be identified.

III. APPLICATION TO SYNTHETIC DATA ON CUBIC CRYSTALS

Because of the complications encountered in dealing with the transverse sheets of the ray surface, it is worth investigating what information can be obtained on the elastic constants solely from L-mode-velocity measurements. A further motivation for addressing this question is that, in the experimental signals obtained with the PS-PR technique, the L-wave arrivals are generally more distinct and easier to measure accurately than the ST- and FT-wave arrivals. For ablative sources or buried thermoacoustic sources,[31,32] the L signals are also the most intense.

In the three principal directions ⟨100⟩, ⟨110⟩, and ⟨111⟩, the L-mode velocities depend not on all three independent elastic constants, but only on C_{11} and the combination $C_l = C_{12} + 2C_{44}$. Phase and group velocities coincide in these directions and are given by[8]

$$\rho v^2_{\langle 100\rangle} = C_{11} ,$$
$$\rho v^2_{\langle 110\rangle} = (C_{11} + C_l)/2 , \tag{8}$$

and

$$\rho v^2_{\langle 111\rangle} = (C_{11} + 2C_l)/3 .$$

Using L-mode-velocity measurements in these directions, the individual values of C_{12} and C_{44} cannot be determined, only their combination C_l. Away from these symmetry directions, the phase and group velocities differ. The L-mode velocities are still mainly determined by C_{11} and C_l, but now they also have a slight dependence on C_{12} and C_{44} individually. Except in cases of extreme anisotropy, this dependence on C_{12} and C_{44} is too weak, however, to allow these constants to be determined with any reasonable degree of accuracy. Similar considerations apply to the transverse modes whose velocities are determined mainly by C_{44} and $C_t = (C_{11} - C_{12})/2$.

Table I presents some results we have obtained on germanium and other cubic crystals from computer-generated velocity data. The first row lists the elastic constants we have taken for Ge.[8] On the basis of these values we have calculated group velocities in various directions for the three polarizations. We have then applied our optimization method to this data in an effort to recover the elastic constants. The density ρ has not been specified since it scales the computed velocities but does not affect the calculated elastic constants.

The second row of Table I shows values of the elastic constants that have been obtained from a grid of 7 L velocities, and 3 ST and 4 FT velocities randomly chosen outside the folded regions of the ray surface. All velocities were calculated and supplied to the fitting program with eight-figure accuracy. This is much higher accuracy than is attained in practice, and has merely been used to test the method. As can be seen, the original elastic constants have all been recovered to six- or seven-figure accuracy. In running the program we have randomized the starting values of the elastic constants by up to ±5%, and have found that for this material this affects only the seventh or eight figures in the final results.

The third row shows typical values of the elastic constants that have been obtained by fitting to a grid of 15 L velocities covering the irreducible sector ($\frac{1}{48}$th of the unit sphere that is replicated into the whole sphere by the symmetry operations of the cube). No transverse velocities have been used here. Again the velocities were supplied with eight-figure accuracy. We see that C_{11} and C_l have been determined to four figures, but the optimization procedure has not been able to drive C_{12}, C_{44}, and C_t to their correct values in spite of the very high accuracy of the calculations. In successive runs with different starting values, a similar pattern was found. It is significant that, although all the elastic constants are inextricably involved in determining all three velocities (unlike in the high-symmetry directions where there is exact separation), C_{11} and C_l can be fairly accurately obtained from the L velocities even though the other elastic constants remain poorly known.

The fourth row shows the values obtained when the 15 calculated L velocities are randomly varied within an interval ±0.5% to simulate statistical errors. Again we see that C_{11} and C_l have been determined with reasonable accuracy, but the other three elastic constants have not been successfully recovered.

TABLE I. Recovery of elastic constants of cubic crystals from computer-generated velocity data. The input elastic constants for Ge and Al are from Ref. 8, and those for Cu are from Ref. 30.

	Elastic constants in GPa				
	C_{11}	C_{12}	C_{44}	C_l	C_t
Germanium data					
a	128.9	48.3	67.1	182.5	40.3
b	128.9000	48.3000	67.1000	182.5000	40.3000
c	128.9	49.3	66.6	182.5	39.8
d	128.8	46.9	68.1	183.1	40.9
e	128.7	49.1	66.9	182.9	39.8
Aluminum data					
a	108.0	61.3	28.5	118.3	23.35
d	108.1	60.0	29.0	118.1	24.0
Copper data					
a	169	122	75.3	272.6	23.5
d	168.5	119.8	76.2	272.1	24.4

[a]Values used in calculating group velocities.
[b]Values recovered from grid of 7 L velocities and 3 ST and 4 FT velocities, all supplied with eight-figure accuracy.
[c]Values recovered from grid of 15 L velocities, all with eight-figure accuracy.
[d]Values recovered from grid of 15 L velocities, randomly scattered in interval of ±0.5%.
[e]Values recovered from grid 15 L, 1 ST, and 2 FT velocities, randomly scattered in interval ±0.5%.

The fifth row shows the elastic constants obtained by fitting to 15 L velocities, 1 ST velocity, and 2 FT velocities, all with statisitcal scatter in a ±0.5% interval. All the elastic constants are now determined with a fair degree of accuracy, but C_{11} and C_l are still more accurate than the others, reflecting the fact that more longitudinal than transverse velocities have been used.

We have carried out similar calculations for a number of other materials and find that whether they are fairly isotropic (like aluminum) or fairly anisotropic (like copper), the conclusions are essentially the same. When only L data are used C_{11} and C_l can be accurately determined, as shown in Table I for Al and Cu, but not the other elastic constants. The inclusion of transverse velocity data allows C_{12}, C_{44}, and C_t to also be obtained with reasonable accuracy.

IV. APPLICATION TO EXPERIMENTAL DATA ON SILICON

The experimental data reported in this section were obtained using a scanned broadband ultrasonic PS-PR technique based on laser excitation and piezoelectric sensing. The method has previously been described in greater detail.[14] The beam of a Q-switched Nd:YAG (yttrium aluminum garnet) laser (wavelength = 1.06 μm, pulse duration $\simeq$ 4 ns, energy $\simeq$ 10 mJ) is focused down to a diameter of $\simeq$0.5 mm on one face of a disk-shaped single crystal of silicon. This acts as a thermoelastic source generating waves which spread out in all directions in the sample. The waves are detected with a small (1.3-mm-diam) PZT piezoelectric transducer mounted on the opposite face of the sample. Signal onsets are registered at the arrival times of longitudinal and transverse waves which have propagated through the sample at their group velocities.[18]

Two disk-shaped silicon single crystals, both of diameter 7.5 cm, have been studied. The first one has faces parallel to the (001) plane, and is of thickness 9.906 mm. The excitation was carried out at a series of points lying in a line along the [100] direction and passing through epicenter, i.e., the point directly opposite the detector. In this sample only the L and ST waves were observed. The reasons for this have been discussed elsewhere.[18] The first 6 L velocities and the 2 ST velocities listed in Table II are measurements made on this sample. The second sample has faces parallel to the $(\bar{1}10)$ plane and is of thickness 9.970 mm. The excitation was carried out at a series of points lying along the $[11\bar{2}]$ direction and passing through epicenter. In this sample only the L and FT waves were observed. The remaining L and the FT velocities listed in Table II were obtained with this sample.

The elastic constants we have obtained for silicon using our optimization method on this data are listed in the first row of Table II. For comparison, the second row lists published values for this material.[33] The agreement between the two sets is within 2% for all the constants. Table II also shows the calculated angular coordinates of the wave normals and the calculated values of the group

TABLE II. Elastic constants of silicon determined from 16 group-velocity measurements made on ⟨100⟩ and ⟨110⟩ oriented single crystals. The density has been taken to be 2.332 g/cm^3. Measured (m) and calculated (c) data on the group velocities is given. Θ,Φ—polar angles of **V**; θ,ϕ—polar angles of **n**.

	Elastic constants in GPa					
	C_{11}	C_{12}	C_{44}	C_l	C_t	
a	165.1	65.0	80.2	225.5	50.0	
b	165.7	63.9	79.6	223.1	50.9	
	Angles in degrees				Velocities in mm/μs	
Branch	Θ_m	Φ_m	θ_c	ϕ_c	V_m	V_c
L	90.0	0.6	90.0	0.3	8.26	8.41
L	90.0	33.7	90.0	25.2	8.93	9.00
L	90.0	39.8	90.0	35.0	9.20	9.11
L	90.0	31.9	90.0	22.9	9.06	8.96
L	90.0	25.9	90.0	16.3	8.89	8.80
L	90.0	19.2	90.0	10.9	8.72	8.64
L	89.5	44.7	89.7	44.3	8.93	9.15
L	66.1	26.7	72.6	18.6	9.23	9.07
L	76.7	35.4	80.4	28.2	9.28	9.11
L	85.9	42.1	86.9	39.3	9.29	9.14
L	87.4	43.2	88.1	41.4	9.26	9.15
ST	90.0	22.5	90.0	36.8	4.95	4.87
ST	90.0	32.0	90.0	40.5	4.77	4.71
FT	77.2	35.8	61.8	40.0	5.40	5.48
FT	72.7	32.3	59.9	39.5	5.35	5.40
FT	67.7	28.1	58.4	39.0	5.36	5.36

[a]This investigation.

[b]Published values from Ref. 33.

velocities. The agreement between calculated and measured group velocities is better than 1% in all but one case. The importance of distinguishing between phase and group velocity is highlighted by the angular separation between the measured **V**'s and their calculated **n**'s. For the L-mode data this angle ranges up to 9.6°, while for the FT modes it reaches 14.4°.

We have not attempted at this stage to do a detailed statistical analysis of the experimental errors or the effect they have on the elastic constants. A few comments are, however, in order. The accuracy of the time measurements in these experiments is limited by the wave-form sampling period, which is 16.7 ns. Most of the transit times exceeded 1.67 μs, and so the time measurements are at best accurate to $\simeq 1\%$. The major source of error in the path lengths is the finite size of the detecting transducer. Near epicenter and far from epicenter this introduces a negligible error, but in between, it leads to a fractional error in the path length of $(d/4l)\sin 2\beta$, where $d \simeq 1.3$ mm is the diameter of the sensor, $l \simeq 10$ mm is the specimen thickness, and β is the angle between the source-receiver direction and the normal to the surface. Taking an average value of $\sin 2\beta \simeq 0.5$, one obtains an error of $\simeq 1.6\%$ for the path length. The errors in the measured group velocities are therefore about 2%, and the errors in the elastic constants might be expected to be comparable.

V. CONCLUSIONS

We have described a method that permits the determination of the elastic constants of an anisotropic solid from measurements of the group velocities of acoustic waves traveling in off-symmetry directions in the specimen. The method is necessarily an indirect one, since there is no explicit equation available, or easily derivable, that relates only elastic constants and group velocities, and which might be manipulated to yield the elastic constants. The method we have presented is based on the following: (1) A minimization procedure to calculate the wave normals associated with the given velocities. (2) An optimization procedure that varies the elastic constants to minimize the mean-square deviation of the measured from the calculated group-velocity magnitudes.

In order to apply the method, reasonable estimates of the elastic constants of the medium must be known, so that the approximate ray surface can be calculated and suitable regions for data input identified, and also to provide starting values for the optimization procedure. Application of this method is simplest when only L data are used. All directions are available in this case since the L sheet of the wave surface is single valued and the procedure is more robust, tolerating much wider bounds and more remote starting values for the elastic constants. However, when only L data are used, not all the elastic constants can be determined.

We have applied this method to media of cubic symmetry and have shown in this case that when data on longitudinal and transverse velocities are provided, all the elastic constants can be accurately recovered. When only L data are provided, C_{11} and C_l can be accurately determined, but the other elastic constants cannot be recovered.

In many situations the optimum strategy for recovery of elastic constants will probably be a hybrid approach, in which some of the elastic constants are determined using data measured along certain high-symmetry directions where the phase and group velocities are equal, and the remaining elastic constants are then determined by the optimization procedure described here.

One of the main objectives of this paper has been to draw attention to the fact that there are a number of techniques that deliver group-velocity rather than phase-velocity data on acoustic waves. When determining elastic constants from such data, the distinction between phase and group velocity should be borne in mind, even though in certain cases it might be expedient to ignore this distinction in order to easily arrive at approximate values of the elastic constants. We have shown that recognizing that the wave-speed data refer to group velocities does not lead to an intractable problem, but rather to one that can be solved numerically in a systematic way.

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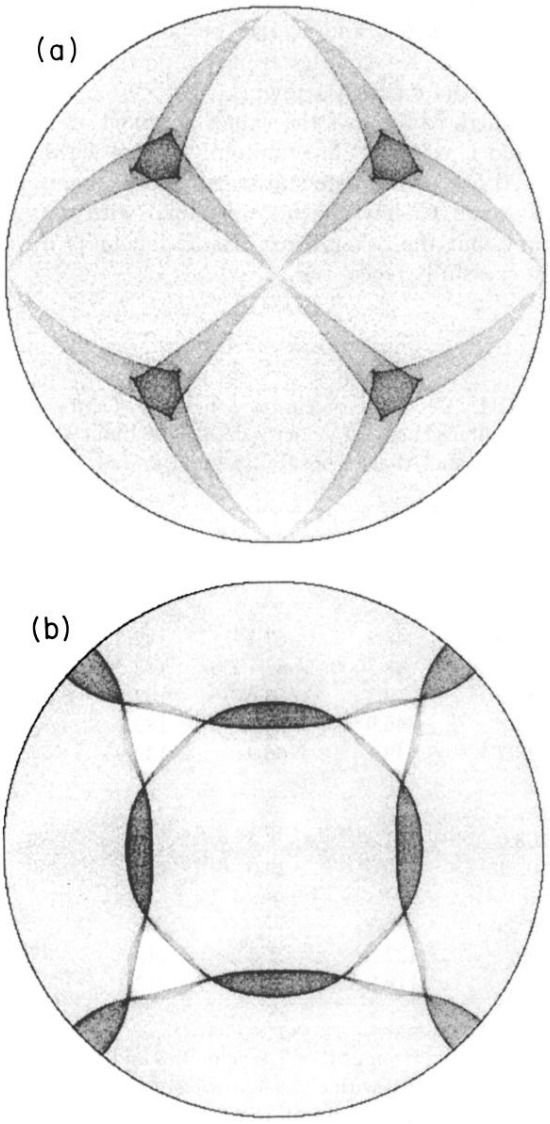

FIG. 4. Polar plot of the (a) ST and (b) FT ray distributions of CsBr for a uniform distribution of wave normals. Elastic constants for the calculation are from Ref. 30. The [001] direction lies at the center of the plot.

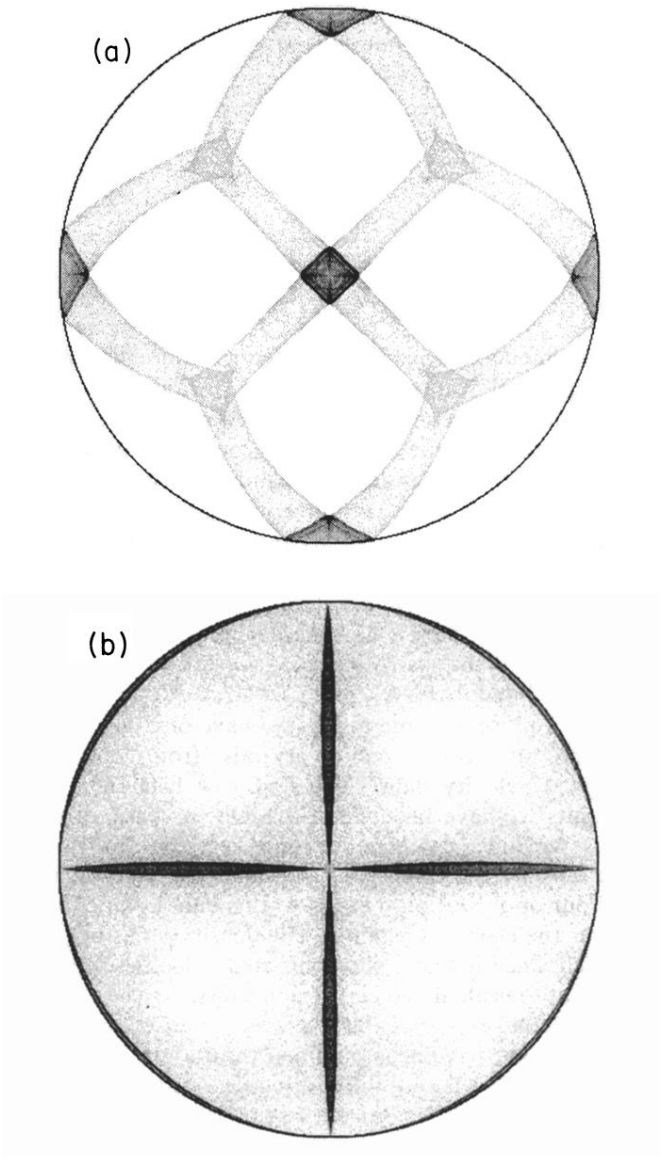

FIG. 5. Polar plot of the (a) ST and (b) FT ray distributions of germanium for a uniform distribution of wave normals. Elastic constants for the calculation are from Ref. 8.