## **Elastic anisotropy factors for orthorhombic, tetragonal, and hexagonal crystals**

Kei Lau

*570 Washington Street, New York, New York 10080*

A. K. McCurdy

*Department of Electrical and Computer Engineering, Worcester Polytechnic Institute, Worcester, Massachusetts 01609*

(Received 8 January 1998)

Elastic anisotropy factors are derived for each of the three modes of propagation from the special in-plane phonon-focusing considerations arising when wave vectors are constrained to the symmetry planes of orthorhombic, tetragonal, and hexagonal crystals. Elastic anisotropy factors for the pure transverse and quasitransverse modes depend upon the symmetry plane, whereas anisotropy factors for the quasilongitudinal mode depend both upon a symmetry plane and a symmetry axis. These anisotropy factors provide a convenient measure of in-plane phonon focusing.  $[$0163-1829(98)02134-1]$ 

## **I. INTRODUCTION**

Phonon focusing in crystals depends upon the shape of the constant-energy surface in  $\vec{k}$  space.<sup>1,2</sup> In the longwavelength limit the constant-energy surfaces in **k** space are nearly linear in **k** and thus can be determined entirely from the second-order elastic constants of the crystal<sup>2</sup>. The phase velocity  $s = \omega/k$  is parallel to the wave vector **k**, whereas the group velocity  $\mathbf{v} = \partial \omega / \partial \mathbf{k}$  is normal to the constant-energy surface in **k** space. In elastically anisotropic crystals the constant-energy surfaces are nonspherical in the longwavelength elastic limit. As a result, the phase and group velocities are generally no longer parallel. Energy flow is parallel to the group velocity, but momentum is parallel to the wave vector. The angular deviation between the phase and group velocities depends upon the direction of the wave vector **k**, the phonon polarization, and the kind of elastic anisotropy. Phonon focusing arises whenever the direction of the group velocity varies more slowly over solid angle than for an elastically isotropic solid so that an isotropic distribution of wave vectors gives rise to an increased density in group-velocity space. Furthermore, for certain ratios between the elastic constants, two or more wave vectors can give the same group-velocity direction giving the group-velocity surface striking cuspidal features.<sup>3</sup> Phonon focusing has been studied in cubic,  $2.4-8$  hexagonal,<sup>9</sup> tetragonal,<sup>10-12</sup> studied in cubic,  $2,4-8$  hexagonal, tetragonal,  $10-12$ orthorhombic,<sup>10</sup> trigonal,<sup>13,14</sup> monoclinic,<sup>15</sup> and triclinic crystals.<sup>15</sup> Scatter plots of phonon focusing<sup>11,12</sup> provide the most graphic display of this phenomenon. Color scatter plots<sup>16</sup> have also been generated in which the magnitude of the group velocity is converted to a full-color spectrum. This paper derives anisotropy factors for all three propagating modes when wave vectors are restricted to symmetry planes. The results when used with scatter plots of phonon  $focusing$ <sup>11</sup> provide a better understanding of phonon focusing in orthorhombic, tetragonal, hexagonal, and cubic crystals.

## **II. THEORY**

Wave propagation in elastic continuum theory is governed by the well-known Christoffel equations

$$
(\Lambda_{ij} - \rho s^2 \delta_{ij}) u_j = 0,\t\t(1)
$$

where  $u_i$  are the displacement components,  $\delta_{ij}$  is the Kronecker delta,  $s$  is the phase velocity, and  $\rho$  is the density. Note that the Einstein convention is used (i.e., summation over repeated subscripts). The Christoffel coefficients are given by

$$
\Lambda_{ij} = C_{ikjm} n_k n_m, \qquad (2)
$$

where  $C_{ikjm}$  is a fourth-rank tensor describing the elastic constants and  $n_k$  are the direction cosines of the wave vector **k**. Contracted Voigt notation is usually employed to represent the elastic tensor as a  $6\times 6$  matrix  $C_{IJ}$ .

Solutions for the phase velocity *s* is obtained by equating the secular determinant to zero:

$$
|\Lambda_{ij} - \rho s^2 \delta_{ij}| = 0. \tag{3}
$$

Cartesian components of the group velocity can be determined by differentiating the Christoffel equations with respect to  $n_{\alpha}$  and multiplying this result by  $u_i$  using the normalizing condition  $u_i u_j = 1$  to obtain the useful relation

$$
v_{\alpha} = \frac{1}{2\rho s} \frac{\partial \Lambda_{ij}}{\partial n_{\alpha}} u_i u_j. \tag{4}
$$

In the absence of piezoelectricity, $11$  these components can be expressed as

$$
v_i = \frac{C_{ikjm} n_j u_k u_m}{\rho s}.
$$
 (5)

In elastically anisotropic crystals the group velocity is, in general, not parallel to the phase velocity. The phase velocity **s** is parallel to the wave vector *k***n**, but the group velocity **v**  $=$  $\partial \omega / \partial \mathbf{k}$  is normal to the constant-energy surface in *k* space. An equidensity of wave vectors in solid angle gives a corresponding but nonuniform density of group-velocity vectors for each of the three modes of propagation. The resulting scatter plots of group-velocity vectors give a graphic display of the phonon-focusing properties of elastically anisotropic crystals.

The phonon-focusing properties of orthorhombic crystals in the long-wavelength limit are determined by the ratios between the nine second-order elastic constants. One can therefore completely describe and classify such crystals using a eight-dimensional space of elastic constant ratios. Another approach considers the special phonon-focusing properties arising when wave vectors are restricted solely to symmetry planes. In this paper such special phonon-focusing properties will be referred to as in-plane focusing. Winternheimer and McCurdy<sup>10</sup> used this restriction to derive conditions for *cusp-free* in-plane focusing and in-plane cuspidal onset. Although this is a severe restriction on the direction of the wave vectors, this method does have the advantage of analytically identifying the origin of some of the cuspidal features displayed in the phonon-focusing scatter plots. Although this restriction is unable to account for all the cuspidal features in the group-velocity surface in orthorhombic crystals, it, nevertheless, will be shown to be useful in deriving convenient elastic anisotropy factors for the orthorhombic, tetragonal, and hexagonal lattices.

If the wave vectors are confined to a symmetry plane, the solution for the phase-velocity factors into a pure transverse mode  $s_T$ , polarized perpendicular to that symmetry plane, and two mixed (i.e., impure) modes  $s_{\pm}$  [a faster mode (+) and a slower mode  $(-)$ ] orthogonally polarized in that symmetry plane. Results can be expressed in general form as<sup>10</sup>

$$
\rho s_T^2 = a_1 \sin^2 \theta_k + a_2 \cos^2 \theta_k, \qquad (6)
$$

$$
2\rho s_{\pm}^{2} = a_{3}\sin^{2}\theta_{k} + a_{4}\cos^{2}\theta_{k}
$$
  
\n
$$
\pm [(a_{5}\sin^{2}\theta_{k} - a_{6}\cos^{2}\theta_{k})^{2} + (2a_{7}\sin\theta_{k}\cos\theta_{k})^{2}]1/2.
$$
  
\n(7)

Expressions for the generalized elastic constants *ai* are listed in Table I for each of the symmetry planes of the orthorhombic, tetragonal, hexagonal, and cubic lattices. No distinction is made between the tetragonal-6 and tetragonal-7 crystal systems in Table I. When only elastic properties need to be considered (e.g., for cuspidal and focusing properties) the tetragonal-7 elastic constants can be transformed to a tetragonal-6 set by a rotation  $\phi$  of the coordinate system about the four-fold axis<sup>17</sup>. The angle  $\phi$  is defined by

$$
\tan 4\phi = \frac{4C_{16}}{C_{11} - C_{12} - 2C_{66}}\tag{8}
$$

so that the transformed  $C_{16}$  becomes zero. Thus, for tetragonal-7 systems, the elastic constants to be entered in Table I are these *transformed* elastic constants, and no further distinction needs to be made between the two tetragonal systems.

Values of the generalized constants in Table I are positive for all known materials with only several exceptions: certain cubic manganese-rich Cu-Mn alloys and tetragonal paratellurite.<sup>18</sup> In certain Cu-Mn alloys,  $C_{11}$  <  $C_{44}$  so that  $a_5$ and  $a_6$  are negative in the  $\{100\}$  planes, but only  $a_6 < 0$  in the  $\{110\}$  planes. In paratellurite, however,  $C_{66}$  >  $C_{11}$  so that  $a_5$  and  $a_6$  are negative only in the (001) symmetry plane.

The angle  $\theta_k$  gives the angular direction of the wave vector *k* in a symmetry plane with respect to one of the symmetry axes. This reference axis has been chosen to be the  $\lceil 001 \rceil$ 

TABLE I. Values of the generalized elastic constants in symmetry planes of orthorhombic, tetragonal, hexagonal, and cubic crystals. Angles are measured with respect to the  $[001]$  axis for the  $(010)$ ,  $(100)$ , and  $(110)$  planes. Angles are measured with respect to the [100] axis, however, for the (001) plane. Note that  $a_3 - a_4$  $=a_5-a_6$  so that these generalized constants are not all independent. For tetragonal crystals  $C_L = C_{66} + (C_{11} + C_{12})/2$ , whereas for cubic crystals  $C_L = C_{44} + (C_{11} + C_{12})/2$ . Note, however, that  $C_T$  $=(C_{11}-C_{12})/2$  for both tetragonal and cubic crystals.

Orthorhombic symmetry planes			
$a_i$	(010)	(100)	(001)
a <sub>1</sub>	$\boldsymbol{C}_{66}$	$\boldsymbol{C}_{66}$	$C_{44}$
$a_2$	$C_{44}$	$\boldsymbol{C}_{55}$	$\boldsymbol{C}_{55}$
$a_3$	$C_{11} + C_{55}$	$C_{22}$ + $C_{44}$	$C_{22}$ + $C_{66}$
$a_4$	$C_{33}$ + $C_{55}$	$C_{33}$ + $C_{44}$	$C_{11} + C_{66}$
$a_5$	$C_{11} - C_{55}$	$C_{22} - C_{44}$	$C_{22} - C_{66}$
a <sub>6</sub>	$C_{33} - C_{55}$	$C_{33} - C_{44}$	$C_{11} - C_{66}$
$a_7$	$C_{13} + C_{55}$	$C_{23} + C_{44}$	$C_{12} + C_{66}$
Tetragonal symmetry planes			
$a_i$	$(010)$ or $(100)$	(110)	(001)
a <sub>1</sub>	$C_{66}$	$C_T$	$C_{44}$
$a_2$	$C_{44}$	$C_{44}$	$\boldsymbol{C}_{44}$
$a_3$	$C_{11}$ + $C_{44}$	$C_L + C_{44}$	$C_{11} + C_{66}$
$a_4$	$C_{33}$ + $C_{44}$	$C_{33}$ + $C_{44}$	$C_{11} + C_{66}$
$a_5$	$C_{11}$ – $C_{44}$	$C_L - C_{44}$	$C_{11} - C_{66}$
$a_6$	$C_{33} - C_{44}$	$C_{33} - C_{44}$	$C_{11} - C_{66}$
a <sub>7</sub>	$C_{13} + C_{44}$	$C_{13} + C_{44}$	$C_{12} + C_{66}$
Hexagonal symmetry planes		Cubic symmetry planes	
$a_i$	Containing the [001] axis	$\{100\}$	${110}$
a <sub>1</sub>	$\boldsymbol{C}_{66}$	$C_{\rm 44}$	$\mathcal{C}_T$
$a_2$	$C_{44}$	$C_{44}$	$C_{44}$
$a_3$	$C_{11}$ + $C_{44}$	$C_{11} + C_{44}$	$C_L + C_{44}$
$a_4$	$C_{33}$ + $C_{44}$	$C_{11} + C_{44}$	$C_{11}$ + $C_{44}$
$a_5$	$C_{11} - C_{44}$	$C_{11} - C_{44}$	$C_L - C_{44}$
$a_6$	$C_{33} - C_{44}$	$C_{11} - C_{44}$	$C_{11}$ – $C_{44}$
$a_7$	$C_{13} + C_{44}$	$C_{12} + C_{44}$	$C_{12} + C_{44}$

axis for the (010), (100), and ( $1\bar{1}0$ ) symmetry planes in Table I. For the (001) symmetry plane, however, the reference axis was chosen as the  $[100]$  direction. The direction  $\theta_n$  of the group velocity in each of the symmetry planes can be expressed  $as<sup>10</sup>$ 

$$
\tan \theta_v = v_\perp / v_\parallel, \tag{9}
$$

where  $v_{\parallel} = \partial s / \partial(\cos \theta_k)$  and  $v_{\perp} = \partial s / \partial(\sin \theta_k)$ .

Using these equations one can calculate the phase- and group-velocity directions in symmetry planes for each mode. Note that in elastically anisotropic crystals these velocities can be collinear for all three modes only when the wave vector is parallel or perpendicular to the reference axis. There is also a collinear axis  $\theta$  for the slower mixed mode  $s_$  that is quasitransverse near  $\theta_$  for<sup>10</sup>

$$
\tan \theta_- = [(a_6 + a_7)/(a_5 + a_7)]^{1/2}, \quad (10)
$$

and a collinear axis  $\theta_+$  for the faster mixed mode  $s_+$  that is pure longitudinal at  $\theta_+$  for <sup>10</sup>

$$
\tan \theta_{+} = \left[ (a_6 - a_7)/(a_5 - a_7) \right]^{1/2}.
$$
 (11)

Note that Eq.  $(11)$  also gives the axis along that which a pure longitudinal and two pure transverse waves propagate.

For certain ratios between the elastic constants there are values of  $\theta$ <sub>v</sub> about a collinear axis that permit more than one corresponding value of  $\theta_k$ . In these regions the values of  $\theta_k$ can be double or triple valued and the group velocity exhibits cuspidal features. Conditions for elastic stability<sup>10</sup> restrict such cuspidal features in nonpiezoelectric materials to the slower mixed mode (provided the wave vectors are constrained to symmetry planes). Winternheimer and McCurdy<sup>10</sup> have shown that when wave vectors are restricted to symmetry planes the corresponding groupvelocity locus for each of the three modes is cusp free if

$$
\frac{d\,\theta_k}{d\,\theta_v} > 0\tag{12}
$$

and the locus exhibits special cusp-free in-plane focusing in that same plane whenever:

$$
\frac{d\theta_k}{d\theta_v} > 1.
$$
\n(13)

Conditions for *cusp-free* in-plane focusing about collinear axes have been derived by Winternheimer and McCurdy, $10$ and from these results phonon amplification factors were derived. Special cusp-free in-plane focusing occurs along the reference axis in the  $s_$  mode when  $a_6$ >0 if

$$
a_7^2 > a_5 a_6 \tag{14}
$$

but, if  $a_6$ <0, it occurs when

TABLE II. Anisotropy factors  $A_{-}$  derived from the phonon-focusing properties of the slower mixed mode  $s<sub>2</sub>$  for each of the symmetry planes of orthorhombic, tetragonal, hexagonal, and cubic crystals. For tetragonal crystals  $C_L = C_{66} + (C_{11} + C_{12})/2$ , whereas for cubic crystals  $C_L = C_{44} + (C_{11} + C_{12})/2$ . Because of the transverse isotropy condition  $C_{12} = C_{11} - 2C_{66}$ , results for hexagonal crystals are valid for any plane containing the  $[001]$  axis. Note that for cubic symmetry only the entries  $A<sub>-</sub>$  for the (010), (100), and (001) planes for the orthorhombic and tetragonal lattices reduce to  $A = 2C_{44}/(C_{11}-C_{12})$ . The value of  $A_{-}$  for the  $\{110\}$ planes of the cubic lattice is not independent of *A*, but does reduce to *A* for conditions of elastic isotropy, i.e.,  $2C_{44} = C_{11} - C_{12}$ . See Discussion for special cases.

Symmetry plane	Anisotropy factor $A_{-}$		
	Orthorhombic		
(010)	$C_{55}(C_{11}+2C_{13}+C_{33})/(C_{11}C_{33}-C_{13}^2)$		
(100)	$C_{44}(C_{22}+2C_{23}+C_{33})/(C_{22}C_{33}-C_{23}^2)$		
(001)	$C_{66}(C_{11}+2C_{12}+C_{22})/(C_{11}C_{22}-C_{12}^2)$		
	Tetragonal		
$(010)$ or $(100)$	$C_{44}(C_{11}+2C_{13}+C_{33})/(C_{11}C_{33}-C_{13}^2)$		
(110)	$C_{44}(C_1+2C_{13}+C_{33})/(C_1C_{33}-C_{13}^2)$		
(001)	$2C_{66}/(C_{11}-C_{12})$		
	Hexagonal		
Planes containing the $\lceil 001 \rceil$ axis	$C_{44}(C_{11}+2C_{13}+C_{33})/(C_{11}C_{33}-C_{13}^2)$		
	Cubic		
${100}$	$2C_{44}/(C_{11}-C_{12})$		
${110}$	$C_{44}(C_1+2C_{12}+C_{11})/(C_1C_{11}-C_{12}^2)$		

$$
a_7^2 > a_6^2. \tag{15}
$$

Cusp-free in-plane focusing occurs perpendicular to the reference axis in the  $s_$  mode when  $a_5$ >0 if

$$
a_7^2 > a_5 a_6,\tag{16}
$$

but, if  $a_5$ <0, it occurs when

$$
a_7^2 > a_5^2. \t\t(17)
$$

Cusp-free in-plane focusing occurs along the  $\theta$  axis in the  $s$ <sub>-</sub> mode if<sup>10</sup>

$$
a_7^2 < a_5 a_6. \tag{18}
$$

Consider, for example, the (010) plane of orthorhombic crystals where  $[001]$  is the reference axis. For  $a_6 > 0$  and from Table I the in-plane focusing condition becomes

$$
(C_{13} + C_{55})^2 > (C_{11} - C_{55})(C_{33} - C_{55}).
$$
 (19)

Since  $C_{1,1}C_{33} - C_{13}^2 > 0$  is one of the conditions for elastic stability,<sup>10</sup> the inequality [Eq.  $(19)$ ] can be rewritten as

$$
C_{55}[(C_{11}+C_{13})+(C_{33}+C_{13})]>C_{11}C_{33}-C_{13}^2.
$$
 (20)

An elastic anisotropy factor can be defined for this symmetry plane and reference axis  $as^{16,19}$ 

$$
A_{-}(010) = \frac{C_{55}[(C_{11} + C_{13}) + (C_{33} + C_{13})]}{C_{11}C_{33} - C_{13}^{2}},
$$
 (21)

so that cusp-free in-plane focusing occurs in the  $s_$  mode along the  $\lceil 001 \rceil$  and  $\lceil 100 \rceil$  axes when  $A_-(010) > 1$ . This is, however, accompanied by in-plane defocusing in this same mode<sup>10</sup> along  $\theta$ <sub>-</sub>. When  $A_-(010)$  < 1, however, cusp-free in-plane focusing occurs in the  $s$ <sub>-</sub> mode<sup>10</sup> along  $\theta$ <sub>-</sub> with defocusing along  $[001]$  and  $[100]$ . The value of this anisotropy factor thus gives one useful information about the inplane focusing conditions about collinear axes. Anisotropy factors for the  $s_$  mode are given for each of the symmetry planes of orthorhombic, tetragonal, and hexagonal crystals in Table II for the usual case where  $a_5$  and  $a_6$  are positive.

Certain crystals exhibit unusual in-plane focusing conditions in one or both of the cusp-free  $s_T$  or  $s_+$  modes so corresponding anisotropy factors are useful for these cases. If  $a_6$ >0 then in-plane focusing occurs in the  $s_+$  mode about the reference axis when

$$
a_6^2 > a_7^2,\tag{22}
$$

but, if  $a_6$ <0, it occurs when

$$
a_5 a_6 > a_7^2. \t\t(23)
$$

In-plane focusing occurs in the  $s_+$  mode perpendicular to the reference axis when  $a_5$ >0 providing

$$
a_5^2 > a_7^2,\tag{24}
$$

but, if  $a_5 < 0$ , it occurs when

$$
a_5 a_6 > a_7^2. \t\t(25)
$$

In-plane focusing occurs in the  $s_+$  mode along  $\theta_+$  (when this exists) if<sup>10</sup>

$$
a_7^2 > a_5 a_6. \t\t(26)
$$

Consider again the (010) plane of orthorhombic crystals where  $[001]$  is the reference axis. For  $a_6 > 0$  and from Table I the in-plane focusing condition becomes

$$
(C_{33} - C_{55})^2 > (C_{13} + C_{55})^2. \tag{27}
$$

This inequality can be rewritten as

$$
C_{33} - C_{13} > 2C_{55}.
$$
 (28)

In analogy with the anisotropy factor of a cubic crystal, i.e.,  $A=2C_{44}/(C_{11}-C_{12})$ , an elastic anisotropy factor can be defined for this symmetry plane and reference axis  $as^{16,19}$ 

$$
A_{+}[001],(010) = \frac{2C_{55}}{(C_{33} - C_{13})}.
$$
 (29)

Thus, in-plane defocusing occurs in the  $s_+$  mode along [001] in the (010) plane for  $a_6 > 0$  when  $A_+$ [001],(010) $> 1$  provided  $C_{33}$  $>C_{13}$ . In a similar manner the anisotropy factor in the  $s_+$  mode along the [100] axis in the (010) plane is

$$
A_{+}[100],(010) = \frac{2C_{55}}{(C_{11} - C_{13})}.
$$
 (30)

Thus, in-plane defocusing occurs when  $A_{+}[100]$ , (010) > 1 provided  $C_{11} > C_{13}$ . For the rare case where  $C_{33} < C_{13}$  or  $C_{11}$   $<$   $C_{13}$ , but  $C_{11}C_{33}$   $C_{13}^2$   $>$  0,  $A_+$  becomes negative and only defocusing is possible along the  $[001]$  or  $[100]$  axes, respectively, in the (010) plane. Note that in-plane focusing (or defocusing) must occur along both of these axes if an additional collinear axis  $\theta_+$  is to exist in this symmetry plane.<sup>10</sup> Finally, note that in-plane focusing information for the  $s_+$  mode requires a total of six different anisotropy fac-

TABLE III. Anisotropy factors  $A_+$  derived from the phononfocusing properties of the faster mixed mode  $s<sub>+</sub>$  for each of the symmetry axes and symmetry planes of orthorhombic, tetragonal, and hexagonal crystals. For tetragonal crystals  $C_L = C_{66} + (C_{11})$  $+C_{12}/2$ . Because of the transverse isotropy condition:  $C_{12} = C_{11}$  $-2C_{66}$  results for hexagonal crystals are valid for any plane containing the  $\lceil 001 \rceil$  axis. Note that for cubic symmetry entry  $A_+$  for the [110],(1<sup> $\overline{1}$ </sup>) reduces to  $2C_{44}/(C_{L}-C_{12})$  and thus is not independent of *A*. All other entries for cubic symmetry reduce to the elastic anisotropy factor  $A = 2C_{44}/(C_{11}-C_{12})$  for cubic crystals. See Discussion for special cases.



tors: one for each of the two mutually orthogonal symmetry planes defining each of the three mutually perpendicular principal axes. Values of the anisotropy factors for each of the principal axes and related symmetry planes are listed in Table III for the usual case where  $a_5$  and  $a_6$  are positive.

In-plane focusing occurs for the pure transverse mode  $s_T$ along the reference axis if

$$
a_2 > a_1 \tag{31}
$$

and occurs perpendicular to the reference axis when

$$
a_1 > a_2. \tag{32}
$$

Such phonon-focusing predictions, however, are most relevant for hexagonal crystals that exhibit transverse isotropy perpendicular to the *c* axis. In orthorhombic crystals this anisotropy factor has little relevance to phonon-focusing scatter plots because of much stronger focusing effects which arise when this constant-energy surface in **k** space no longer has wave vectors constrained to the symmetry plane. As a result, entries for orthorhombic crystals are omitted from Table IV.

Consider, therefore, the hexagonal lattice and any plane containing the  $c$  axis [e.g.,  $(010)$ ]. One can define a single anisotropy factor for the pure transverse mode<sup>16,19</sup>

$$
A_T(010) = a_2/a_1 = C_{44}/C_{66}.
$$
 (33)

Thus, when  $A_T(010) > 1$ , the pure transverse mode exhibits in-plane focusing along the  $[001]$  axis, but in-plane defocus-

TABLE IV. Anisotropy factors  $A_T$  derived from the phononfocusing properties of the pure transverse mode  $s<sub>T</sub>$  for each of the symmetry planes of tetragonal, hexagonal, and cubic crystals. Note that in tetragonal crystals the pure transverse mode is isotropic in the (001) plane (i.e.,  $A_T=1$ ). Similarly, the  $s_T$  mode is isotropic in cubic crystals in  ${100}$  planes. Because of the transverse isotropy condition  $C_{12} = C_{11} - 2C_{66}$  results for hexagonal crystals are valid for any plane containing the  $[001]$  axis.



ing along  $\lceil 100 \rceil$  and all other directions perpendicular to the *c* axis. Note that the corresponding anisotropy factor for the  $(1\bar{1}0)$  plane of tetragonal crystals (see Table I) is

$$
A_T(1\bar{1}0) = a_2/a_1 = 2C_{44}/(C_{11} - C_{12}),
$$
 (34)

and thus is identical to the anisotropy factor *A* for cubic crystals. Selected anisotropy factors for the  $s_T$  mode are listed for tetragonal, hexagonal, and cubic lattices in Table IV.

## **III. DISCUSSION**

Tables II and III give useful anisotropy factors for the usual conditions where  $a_5 > 0$  and  $a_6 > 0$ . Note, however, that inequalities [Eqs.  $(15)–(17)$ ] are equivalent whenever  $a_5 = a_6$ . As a result, there is no change in the entries of Tables II and III when  $a_5 = a_6 < 0$ , and, thus, no change for the  $\{100\}$  planes of certain Cu-Mn alloys or for the  $(001)$ plane of tetragonal paratellurite. The  $\{110\}$  plane of certain cubic Cu-Mn alloys where  $a_5$ >0, but  $a_6$ <0, requires special treatment. Here, the value of  $A_{-}$  for the  $[001]$ ,  $(11\overline{1}0)$ becomes  $2C_{44}/(C_{11}-C_{12})$ , *A* for the [110],(11<sup> $\overline{1}$ 0) be-</sup> comes  $C_{44}(C_L+2C_{12}+C_{11})/(C_LC_{11}-C_{12}^2)$ ,  $A_+$  for the  $[001]$ , (1<sup>T</sup>O) becomes  $C_{44}(C_L+2C_{12}+C_{11})/(C_LC_{11}-C_{12}^2)$ , and  $A_+$  for the [110],(1<sup> $\overline{1}$ </sup>) becomes  $2C_{44}/(C_L-C_{12})$ .

In-plane cuspidal features can be inferred from the values of *A*<sup>2</sup> . Cuspidal features about a principal axis require *A*<sup>2</sup> to be somewhat greater than unity, whereas cuspidal features about  $\theta$ <sub>-</sub> require values of  $A$ <sub>-</sub> to be significantly less than unity. The onset and precise shape of these in-plane cuspidal features are, however, also determined by two other elastic constant ratios.

In-plane focusing for the  $s_+$  mode can be determined directly from the two anisotropy factors  $A_+$  defined for each principal axis. Positive values of  $A_+$  less than unity indicate in-plane focusing, whereas values greater than unity indicate in-plane defocusing about that principal axis. For the rare case where  $A_+$  is negative, however, only in-plane defocusing is possible about that principal axis. Note that a  $\theta_+$  exists only if in-plane focusing (or defocusing) occurs about both principal axes in the symmetry plane. In-plane focusing (or defocusing) about either principal axis gives in-plane defocusing (or focusing), respectively, about  $\theta_+$ .

Anisotropy factors are easy to calculate and provide important in-plane phonon-focusing information. The three anisotropy factors for the  $s_$  mode and the six anisotropy factors for the  $s_+$  mode, however, provide the most useful information for orthorhombic crystals.

- 1B. Taylor, H. J. Maris, and C. Elbaum, Phys. Rev. B **3**, 1462  $(1971).$
- <sup>2</sup>H. J. Maris, J. Acoust. Soc. Am. **50**, 812 (1971).
- $3<sup>3</sup>M$ . J. P. Musgrave, Proc. Cambridge Philos. Soc. **53**, 897 (1957).
- $^{4}$ A. G. Every, Phys. Rev. B 22, 1746 (1980).
- ${}^5$ A. G. Every, Phys. Rev. B 24, 3456 (1981).
- ${}^{6}$ A. K. McCurdy, Phys. Rev. B **26**, 6971 (1982).
- ${}^{7}$ A. G. Every and A. J. Stoddart, Phys. Rev. B 32, 1319 (1985).
- ${}^{8}$ D. C. Hurley and J. P. Wolfe, Phys. Rev. B 32, 2568 (1985).
- $^{9}$ A. K. McCurdy, Phys. Rev. B 9, 466 (1974).
- 10C. G. Winternheimer and A. K. McCurdy, Phys. Rev. B **18**, 6576 (1978). Note that phonon-amplification factors for the transverse modes were derived for *cusp-free* conditions in both symmetry planes defining each of the respective axes.
- $11$  A. G. Every and A. K. McCurdy, Phys. Rev. B 36, 1432 (1987).
- $12$  A. G. Every, Phys. Rev. B 37, 9964 (1988).
- 13A. G. Every, G. L. Koos, and J. P. Wolfe, Phys. Rev. B **29**, 2190  $(1984).$
- 14A. K. McCurdy and A. G. Every, in *Thermal Conductivity 20*, edited by D. P. H. Hasselman and J. R. Thomas, Jr. (Plenum, New York, 1989), p. 243.
- $15$  J. Thomas (unpublished)
- $16$ K. Lau and A. K. McCurdy (unpublished).
- <sup>17</sup> F. I. Federov, *Theory of Elastic Waves in Crystals* (Plenum, New York, 1968), p. 27.
- 18A. G. Every and A. K. McCurdy, in *Second and Higher Order Elastic Constants*, edited by O. Madelung and D. F. Nelson, Landolt-Bornstein, New Series, Group III, Vol. 29, pt. a (Springer-Verlag, Berlin, 1992), pp. 23, 101, and 168.
- $19$ K. Lau and A. K. McCurdy (unpublished).