Elastic Anisotropy Factors for Orthorhombic, Tetragonal and Hexagonal Crystals[1]

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ABSTRACT

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 (T) and quasi-transverse (QT) modes depend upon the symmetry plane, whereas anisotropy factors for the quasi-longitudinal (QL) mode depend both upon a symmetry plane and a symmetry axis. These anisotropy factors provide a convenient measure of in-plane phonon focusing.

KEY WORDS: anisotropy factors; elastic anisotropy; elastic constants; group velocities; hexagonal crystals; orthorhombic crystals; phonon focusing; tetragonal crystals.

1. INTRODUCTION

Phonon focusing in crystals depends upon the shape of the constant-energy surface in $\mathbf{k}$ space [1,2]. In the long-wavelength limit the constant-energy surfaces in $\mathbf{k}$ space are nearly linear in $\mathbf{k}$ and thus can be determined entirely from the second-order elastic constants of the crystal [2]. The phase velocity $s = \omega/k$ and is parallel to the wave vector $\mathbf{k}$, whereas the group velocity $\mathbf{v} = \partial\omega/\partial\mathbf{k}$ is normal to the constant energy surface in $\mathbf{k}$ space. In elastically anisotropic crystals the constant energy surfaces are nonspherical in the long-wavelength 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 $\mathbf{k}$, 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 [3]. Phonon focusing has been studied in cubic [2,4-8], hexagonal [9], tetragonal [10-12], orthorhombic [10], trigonal [13,14], monoclinic [15] and triclinic crystals [15]. Scatter plots of phonon focusing [11,12] provide the most graphic display of this phenomenon. Color scatter plots [16] 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 [11] provide a better understanding of phonon focusing in orthorhombic, tetragonal, hexagonal and cubic crystals.

2. THEORY

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

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

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

$$\Lambda_{ij} = C_{ikjm} n_k n_m \tag{2}$$

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

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

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

If the wave vectors are confined to a symmetry plane the solution 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. When the (001) plane, for example, is a symmetry plane then $n_3 = 0$ and $\Lambda_{23} = \Lambda_{13} = 0$. The solutions for the phase velocity then factor to:

$$\rho s_T^2 = \Lambda_{33} \tag{4}$$

$$2\rho s_\pm^2 = \Lambda_{11} + \Lambda_{22} \pm [(\Lambda_{11} - \Lambda_{22})^2 + 4\Lambda_{12}^2]^{\frac{1}{2}}. \tag{5}$$

If, however, the $(1\bar{1}0)$ is a symmetry plane, so that $n_1 = n_2$ and $\Lambda_{11} = \Lambda_{22}, \Lambda_{13} = \Lambda_{23}$, the solutions for the phase velocity then factors to:

$$\rho s_T^2 = \Lambda_{11} - \Lambda_{12} \tag{6}$$

$$2\rho s^2 \pm = \Lambda_{11} + \Lambda_{12} + \Lambda_{33} \pm [(\Lambda_{11} + \Lambda_{12} - \Lambda_{33})^2 + 8\Lambda_{23}^2]^{\frac{1}{2}}. \tag{7}$$

The group velocity is defined as $\mathbf{v} = \partial\omega/\partial\mathbf{k}$. In the absence of dispersion this becomes:

$$\mathbf{v} = \frac{\partial s}{\partial \mathbf{n}}. \tag{8}$$

so that the Cartesian components of the group velocity can be expressed as:

$$v_x = \frac{\partial s}{\partial n_x},\ v_y = \frac{\partial s}{\partial n_y},\ v_z = \frac{\partial s}{\partial n_z}. \tag{9}$$

Differentiating the Christoffel equations with respect to n_α and multiplying this result by u_j using the normalizing condition $u_j u_j = 1$ one obtains the useful result:

$$v_\alpha = \frac{1}{2\rho s}\frac{\partial \Lambda_{ij}}{\partial n_\alpha} u_i u_j. \tag{10}$$

In the absence of piezoelectricity [11], these components can be expressed as:

$$v_i = \frac{C_{ikjm} n_j u_k u_m}{\rho s}. \tag{11}$$

In elastically anisotropic crystals the group velocity is, in general, not parallel to the phase velocity. The phase velocity $\mathbf{s}$ is parallel to the wave vector $k\mathbf{n}$, but the group velocity $\mathbf{v} = \partial\omega/\partial\mathbf{k}$ 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 9 second-order elastic constants. One can therefore completely describe and classify such crystals using a 8-dimensional space of elastic constant ratios. Another approach considers the special phonon-focusing properties arising when wave vectors are restricted soley to symmetry planes. In this paper such special phonon focusing properties will be referred to as in-plane focusing. Winternheimer *et al* [10] 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.

Solutions for the phase velocity in symmetry planes can be expressed in general form as [10]:

$$\rho s_T^2 = a_1 \sin^2\theta_k + a_2 \cos^2\theta_k \tag{12}$$

$$2\rho s_{\pm}^2 = a_3 \sin^2\theta_k + a_4 \cos^2\theta_k \pm [(a_5 \sin^2\theta_k - a_6 \cos^2\theta_k)^2 + (2a_7 \sin\theta_k \cos\theta_k)^2]^{\frac{1}{2}}. \quad (13)$$

Expressions for the generalized elastic constants a_i 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 ϕ of the coordinate system about the 4-fold axis [17]. The angle ϕ is defined by:

$$\tan 4\phi = \frac{4C_{16}}{C_{11} - C_{12} - 2C_{66}} \quad (14)$$

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 [18]. 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 θ_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 [001] 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, θ_v, of the group velocity in each of the symmetry planes can be expressed as [10]:

$$\tan\theta_v = v_{\perp}/v_{\parallel} \quad (15)$$

where $v_{\parallel} = \partial s/\partial(\cos\theta_k)$ and $v_{\perp} = \partial s/\partial(\sin\theta_k)$. For the pure transverse mode s_T this becomes:

$$\tan\theta_v = (a_1/a_2)\tan\theta_k \quad (16)$$

or for directions nearly perpendicular to the reference axis:

$$\cot\theta_v = (a_2/a_1)\cot\theta_k. \quad (17)$$

Table I. Values of the generalized elastic constants in symmetry planes of orthorhombic, tetragonal, hexagonal, and cubic crystals. Angles are measured with respect the the [001] axis for the (010), (100), and $(1\bar{1}0)$ 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_1	C_{66}	C_{66}	C_{44}
a_2	C_{44}	C_{55}	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_6	$C_{33}-C_{55}$	$C_{33}-C_{44}$	$C_{11}-C_{66}$
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_1	C_{66}	C_T	C_{44}
a_2	C_{44}	C_{44}	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_7	$C_{13}+C_{44}$	$C_{13}+C_{44}$	$C_{12}+C_{66}$

	Hexagonal Symmetry Planes	Cubic Symmetry Planes	
a_i	Containing the [001] Axis	{100}	{110}
a_1	C_{66}	C_{44}	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	$C_{13}+C_{44}$	$C_{12}+C_{44}$	$C_{12}+C_{44}$

For the two mixed modes $s_\pm$ the results can be expressed as:

$$\tan\theta_v = (u/v)\tan\theta_k \tag{18}$$

where

$$u = a_3 \pm \frac{a_5^2\tan^2\theta_k + (2a_7^2 - a_5a_6)}{[(a_5\tan^2\theta_k - a_6)^2 + (2a_7\tan\theta_k)^2]^{\frac{1}{2}}}, \tag{19}$$

$$v = a_4 \pm \frac{(2a_7^2 - a_5a_6)\tan^2\theta_k + a_6^2}{[(a_5\tan^2\theta_k - a_6)^2 + (2a_7\tan\theta_k)^2]^{\frac{1}{2}}}. \tag{20}$$

For directions nearly perpendicular to the reference axis it is more convenient to use:

$$\cot\theta_v = (u'/v')\cot\theta_k \tag{21}$$

where u' is u and v' is v, but with a_3 and a_4 interchanged, a_5 and a_6 interchanged, and with $\cot\theta_k$ replacing $\tan\theta_k$.

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 3 modes only when the wave vector is parallel or perpendicular to the reference axis. The phase and group velocities can also be collinear when [10]:

$$\tan^2\theta_k = (a_6 + a_7)/(a_5 + a_7) \tag{22}$$

and when

$$\tan^2\theta_k = (a_6 - a_7)/(a_5 - a_7). \tag{23}$$

The collinear axis θ_- for the slower mixed mode s_- which is quasi-transverse near θ_- is:

$$\tan\theta_- = [(a_6 + a_7)/(a_5 + a_7)]^{\frac{1}{2}} \tag{24}$$

and the collinear axis θ_+ for the faster mixed mode s_+ which is pure longitudinal at θ_+ is:

$$\tan\theta_+ = [(a_6 - a_7)/(a_5 - a_7)]^{\frac{1}{2}}. \tag{25}$$

Note that Eq. (25) gives the collinear axis along which a pure longitudinal and two pure transverse waves propagate.

For certain ratios between the elastic constants there are values of θ_v about a collinear axis which permit more than one corresponding value of θ_k. In these regions the values of θ_k can be double or triple-valued and the group velocity exhibits cuspidal features. Conditions for elastic stability [10] restrict such cuspidal features in nonpiezoelectric materials to the slower mixed mode (provided the wave vectors are constrained to symmetry planes). Winternheimer *et al* [10] has shown that when wave vectors are restricted to symmetery planes the corresponding group-velocity locus for each of the three modes is cusp free if:

$$\frac{d\theta_k}{d\theta_v} > 0 \tag{26}$$

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

$$\frac{d\theta_k}{d\theta_v} > 1. \tag{27}$$

Conditions for *cusp-free* in-plane focusing about collinear axes have been derived by Winternheimer *et al* [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:

$$a_7^2 > a_5 a_6 \tag{28}$$

but if $a_6 < 0$ occurs when:

$$a_7^2 > a_6^2. \tag{29}$$

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

$$a_7^2 > a_5 a_6 \tag{30}$$

but if $a_5 < 0$ occurs when:

$$a_7^2 > a_5^2. \tag{31}$$

Cusp-free in-plane focusing occurs along the θ_- axis in the s_- mode if [10]:

$$a_7^2 < a_5 a_6. \tag{32}$$

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:

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

Since $C_{11}C_{33} - C_{13}^2 > 0$ is one of the conditions for elastic stability [10] inequality (33) can be rewritten as:

$$C_{55}[(C_{11} + C_{13}) + (C_{33} + C_{13})] > C_{11}C_{33} - C_{13}^2. \tag{34}$$

An elastic anisotropy factor can be defined for this symmetry plane and reference axis as [16,19]:

$$A_-(010) = \frac{C_{55}[(C_{11} + C_{13}) + (C_{33} + C_{13})]}{C_{11}C_{33} - C_{13}^2}, \tag{35}$$

so that cusp-free in-plane focusing occurs in the s_- mode along the [001] and [100] axes when $A_-(010) > 1$. This is, however, accompanied by in-plane defocusing in this same mode [10] along θ_-. When $A_-(010) < 1$, however, cusp-free in-plane focusing occurs in the s_- mode [10] along θ_- with defocusing along [001] and [100]. The value of this anisotropy factor thus gives one useful information about the in-plane 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 Table II. Anisotropy factors A_- derived from the phonon-focusing properties of the slower mixed mode s_- for each of the symmetry planes of orthorhombic, tetragonal, hexagonal, and cubic crystals [16,19]. 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_- 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., $2C_{44} = C_{11} - C_{12}$.

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)	$C_{44}(C_{11}+2C_{13}+C_{33})/(C_{11}C_{33}-C_{13}^2)$
$(1\bar{1}0)$	$C_{44}(C_L+2C_{13}+C_{33})/(C_LC_{33}-C_{13}^2)$
(001)	$2C_{66}/(C_{11}-C_{12})$
Hexagonal	
Planes Containing the [001] 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}	$C_{44}(C_L+2C_{12}+C_{11})/(C_LC_{11}-C_{12}^2)$

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:

$$a_6^2 > a_7^2 \tag{36}$$

but if $a_6 < 0$ occurs when:

$$a_5 a_6 > a_7^2. \tag{37}$$

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

$$a_5^2 > a_7^2 \tag{38}$$

but if $a_5 < 0$ occurs when:

$$a_5 a_6 > a_7^2. \tag{39}$$

In-plane focusing occurs in the s_+ mode along θ_+ (when this exists) if [10]:

$$a_7^2 > a_5 a_6. \tag{40}$$

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:

$$(C_{33} - C_{55})^2 > (C_{13} + C_{55})^2. \tag{41}$$

This inequality can be rewritten as:

$$C_{33} - C_{13} > 2C_{55}. \tag{42}$$

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]:

$$A_+[001]\&(010) = \frac{2C_{55}}{(C_{33} - C_{13})}. \tag{43}$$

Thus in-plane focusing occurs in the s_+ mode along [001] in the (010) plane for $a_6 > 0$ when $A_+[001]\&(010) < 1$. In a similar manner the anisotropy factor in the s_+ mode along the [100] axis in the (010) plane is:

$$A_+[100]\&(010) = \frac{2C_{55}}{(C_{11} - C_{13})}, \tag{44}$$

thus in-plane focusing occurs when $A_+[100]\&(010) < 1$. Note that in-plane focusing (or defocusing) must occur along both of these axes if an additional collinear axes θ_+ is to exist in this symmetry plane [10]. Furthermore, for this mode to be cusp free both anisotropy factors must be positive. This requires: $C_{33} - C_{13} > 0$ and $C_{11} - C_{13} > 0$ and is more stringent than the elastic stability condition: $C_{11}C_{33} > C_{13}^2$. Finally, note that in-plane focusing information for the s_+ mode requires a total of 6 different anisotropy factors: one for each of the two mutually orthogonal symmetry planes defining each of the 3 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:

$$a_2 > a_1 \tag{45}$$

and perpendicular to the reference axis when:

$$a_1 > a_2. \tag{46}$$

Such phonon-focusing predictions, however, are most relevant for hexagonal crystals which exhibit transverse isotropy perpendicular to the c axis. In orthorhombic crys-

Table III. Anisotropy factors A_+ derived from the phonon-focusing properties of the faster mixed mode s_+ for each of the symmetry axes and symmetry planes of orthorhombic, tetragonal, and hexagonal crystals [16,19]. 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 [001] axis. Note that for cubic symmetry entry A_+ for the $[110]\&(1\bar{1}0)$ 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.

Reference Axis & Symmetry Plane	Anisotropy Factor A_+
Orthorhombic	
[100]&(010)	$2C_{55}/(C_{11}-C_{13})$
[001]&(010)	$2C_{55}/(C_{33}-C_{13})$
[010]&(100)	$2C_{44}/(C_{22}-C_{23})$
[001]&(100)	$2C_{44}/(C_{33}-C_{23})$
[100]&(001)	$2C_{66}/(C_{11}-C_{12})$
[010]&(001)	$2C_{66}/(C_{22}-C_{12})$
Tetragonal	
[100]&(010) or [010]&(100)	$2C_{44}/(C_{11}-C_{13})$
[001]&(010) or [001]&(100)	$2C_{44}/(C_{33}-C_{13})$
[110]&($1\bar{1}0$)	$2C_{44}/(C_L-C_{13})$
[001]&($1\bar{1}0$)	$2C_{44}/(C_{33}-C_{13})$
[100]&(001) or [010]&(001)	$2C_{66}/(C_{11}-C_{12})$
Hexagonal	
[100]&(010)	$2C_{44}/(C_{11}-C_{13})$
[001]&(010)	$2C_{44}/(C_{33}-C_{13})$

tals 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 [16,19]:

$$A_T(010) = a_2/a_1 = C_{44}/C_{66}. \tag{47}$$

Thus when $A_T(010) > 1$ the pure transverse mode exhibits in-plane focusing along the [001] axis, but in-plane defocusing along [100] 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:

$$A_T(1\bar{1}0) = a_2/a_1 = 2C_{44}/(C_{11}-C_{12}) \tag{48}$$

Table IV. Anisotropy factors A_T derived from the phonon-focusing properties of the pure transverse mode s_T for each of the symmetry planes of tetragonal, hexagonal, and cubic crystals [16,19]. 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.

Symmetry Plane	Anisotropy Factor A_T
Tetragonal	
(010) or (100)	C_{44}/C_{66}
$(1\bar{1}0)$	$2C_{44}/(C_{11}-C_{12})$
Hexagonal	
Planes Containing the [001] Axis	C_{44}/C_{66}
Cubic	
{110}	$2C_{44}/(C_{11}-C_{12})$

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.

3. 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 (29)-(31) 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 $[001]\&(1\bar{1}0)$ becomes $2C_{44}/(C_{11}-C_{12})$, A_- for the $[110]\&(1\bar{1}0)$ becomes $C_{44}(C_L+2C_{12}+C_{11})/(C_LC_{11}-C_{12}^2)$, A_+ for the $[001]\&(1\bar{1}0)$ becomes $C_{44}(C_L+2C_{12}+C_{11})/(C_LC_{11}-C_{12}^2)$, and A_+ for the $[110]\&(1\bar{1}0)$ becomes $2C_{44}/(C_L-C_{12})$.

In-plane cuspidal features can be inferred from the values of A_-. Cuspidal features about a principal axis require A_- to be somewhat greater than unity, whereas cuspidal features about θ_- require values of A_- 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. Values of A_+ less than unity indicate in-plane focusing, whereas values greater than unity indicate in-plane defocusing about that principal axis. Note that a θ_+ 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 θ_+.

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 s_+ mode, however, provide the most useful information for orthorhombic crystals.

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