between twinning-related maxima, since it is these intensities which are most useful in the determination of the twinning fraction. A second is that since twin domains may not all be small or may not be evenly distributed throughout a specimen, one should ensure that the volume of the crystal bathed by the X-ray beam is constant throughout data collection.

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The Acoustic Gyrotropic Tensor in Crystals

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Abstract

The acoustic gyrotropic tensor is a fifth-rank tensor characterized by $d_{ij,l} = -d_{jl,l}$, with $i, j = 11, 22, 33, (23, 32), (31, 13), (12, 21)$, $l = 1, 2, 3$, and controls the acoustical activity in crystals. With the employment of group theoretical methods, the number of independent coefficients of this tensor and the character for this tensor under proper and improper rotation are worked out. A classification of the acoustically active classes is given.

Introduction

The phenomenon of acoustical activity refers to the rotation of the plane of polarization of a transverse acoustic wave propagating along the acoustic axis. According to Portigal & Burstein (1968), who predicted this effect, acoustical activity arises due to first-order spatial dispersion contributions to elastic constants, just as optical activity is the result of first-order spatial dispersion contributions to the dielectric constant. Consequently, the velocity degeneracy of the linearly polarized transverse acoustic phonons at $\mathbf{k} = 0$ is lifted at finite $\mathbf{k}$ where $\mathbf{k}$ is the phonon wave vector. The two split modes are left and right circularly polarized along the acoustic axis and they propagate with different phase velocities. This phase-velocity difference leads to the rotation of the plane of polarization.

Direct observation of acoustical activity in α-quartz by Brillouin scattering techniques has been reported by Pine (1970). The splitting of the degenerate optical phonons due to first-order spatial dispersion has also been observed by Pine & Dresselhaus (1969) in the low-temperature Raman spectrum of α-quartz.

Portigal & Burstein (1968) have identified the non-vanishing coefficients of the acoustic gyrotropic tensor for point groups T, T_d and O from symmetry considerations. We have derived the number of non-vanishing coefficients of this tensor and identified

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them for all the 32 point groups employing Bhagavantam's (1966) group-theoretical method.

Acoustic gyrotropic tensor

The effect of first-order spatial dispersion on elastic constants can be expressed as (Portigal & Burstein, 1968)

$$C_{ij}(w,k) = C_{ij}(w) + id_{ij,l}(w)\,k_l + e_{ij,lm}(w)\,k_l k_m + \ldots, \quad (1)$$

with $i, j = 11, 22, 33, (23, 32), (31, 13), (12, 21)$ and $l = 1, 2, 3$. $C_{ij}(w)$ is the contracted notation for the elastic constants C_{pqrs}. $C_{ij}(w)$ is a symmetric fourth-rank tensor. The second term on the right-hand side of (1) is the contribution to elastic constants due to first-order spatial dispersion and acoustical activity arises due to this term. $d_{ij,l}(w)$ is a fifth-rank tensor known as the acoustic gyrotropic tensor. Because of time-reversal invariance, $d_{ij,l} = -d_{ji,l}$.

Being a fifth-rank tensor, $d_{ij,l}$ has 243 coefficients. Since $d_{ij,l} = -d_{ji,l}$, $d_{ij,l} = 0$ for $i = j$. In this way 45 coefficients become zero. Of those remaining, there are only 45 independent coefficients (Table 1).

Number of independent coefficients

Acoustical activity is exhibited only by those crystals that have non-vanishing coefficients $d_{ij,l}$. To determine the number of non-vanishing coefficients $d_{ij,l}$, the character of the reducible representation formed by the transformation matrix of the 45 independent tensor components under a symmetry operation R is derived. The matrix R represents a proper or improper rotation and is given by

$$R = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & \pm 1 \end{bmatrix}. \quad (2)$$

The character of the transformation matrix of the tensor components is obtained by adding the contributions to the character due to each of the 45 independent coefficients mentioned in Table 1, under a transformation R. For example, the contribution to the character, due to one of the independent coefficients d_{11231}, is found from

$$\begin{aligned} d'_{11231} &= a_{11}a_{11}a_{22}a_{33}a_{11}d_{11231} + a_{11}a_{11}a_{23}a_{32}a_{11}d_{11321} \\ &\quad + a_{12}a_{13}a_{21}a_{31}a_{11}d_{23111} \\ &\quad + a_{13}a_{12}a_{21}a_{31}a_{11}d_{32111} = \pm\cos^4\theta\, d_{11231} \quad (3) \end{aligned}$$

to be $\pm\cos^4\theta$. The upper and lower signs correspond to proper and improper rotation respectively. On adding the contributions from all 45 independent coefficients, the character $\chi(R)$ of the reducible representation of the fifth-rank acoustic gyrotropic tensor becomes

$$\chi(R) = \pm 16\cos^4\theta + 24\cos^3\theta \pm 8\cos^2\theta - 2\cos\theta \mp 1. \quad (4)$$

The number of independent non-zero coefficients (Table 2) is determined for each point group using the well-known formula

$$n = \frac{1}{N}\sum_{\varrho=1}^{K} h_\varrho \chi_\varrho(R)\,\chi_i(R), \quad (5)$$

where N is the total number of group elements in the given point group. h_ϱ is the number of group elements in the class, K being the total number of classes in the group. $\chi_i(R)$ is the character of the totally symmetric irreducible representation and it is equal to unity for all the group operations. $\chi(R)$ is the character of the reducible representation for the fifth-rank tensor.

The non-vanishing coefficients

Once the number of non-vanishing independent coefficients have been determined, the coefficients can be identified by applying Neumann's method. Since the coefficients of the fifth-rank acoustic gyrotropic tensor are responsible for acoustical activity, the coefficients should have the symmetry of the point group of the crystal, if the crystal is to exhibit acoustical activity. Therefore all the 45 independent coefficients are subjected to each point-group operation successively. Only those coefficients will survive that remain invariant under all the point-group operations. The non-zero independent coefficients for each point group as derived by the above method are given in Table 2. All the coefficients are zero for centrosymmetric crystal classes which, therefore, are acoustically inactive.

Table 1. 45 *independent coefficients of* $d_{ij,l}$ ($l = 1, 2, 3$)

d_{12l}	d_{23l}	d_{35l}
d_{13l}	d_{24l}	d_{36l}
d_{14l}	d_{25l}	d_{45l}
d_{15l}	d_{26l}	d_{46l}
d_{16l}	d_{34l}	d_{56l}

Conclusion

Only those crystals which belong to non-centrosymmetric classes can exhibit acoustical activity. The

Table 2. *Non-vanishing coefficients of* $d_{ij,l}$

Crystal system	Point group International	Point group Schönflies	No. of independent coefficients	Non-vanishing coefficients
Triclinic	1	C_1	45	All
Monoclinic	m	C_s	22	$d_{121}, d_{122}, d_{143}, d_{153}, d_{161}, d_{162}, d_{131}, d_{132}, d_{231}, d_{232}, d_{243}, d_{253}, d_{261}, d_{262}, d_{343}, d_{353}, d_{361}, d_{362}, d_{451}, d_{452}, d_{463}, d_{563}$
	2	C_2	23	$d_{123}, d_{133}, d_{141}, d_{142}, d_{151}, d_{152}, d_{163}, d_{233}, d_{241}, d_{242}, d_{251}, d_{252}, d_{263}, d_{341}, d_{342}, d_{351}, d_{352}, d_{363}, d_{453}, d_{461}, d_{462}, d_{561}, d_{562}$
Orthorhombic	$2mm$	C_{2v}	11	$d_{123}, d_{133}, d_{142}, d_{151}, d_{233}, d_{242}, d_{251}, d_{342}, d_{351}, d_{461}, d_{562}$
	222	D_2	12	$d_{141}, d_{152}, d_{163}, d_{241}, d_{252}, d_{263}, d_{341}, d_{352}, d_{363}, d_{453}, d_{462}, d_{561}$
Tetragonal	4	C_4	11	$d_{133} = d_{233}, d_{141} = -d_{252}, d_{142} = d_{251}, d_{151} = d_{242}, d_{152} = -d_{241}, d_{163} = -d_{263}, d_{341} = -d_{352}, d_{342} = d_{351}, d_{453}, d_{461} = d_{562}, d_{462} = -d_{561}$
	$\bar{4}$	S_4	12	$d_{123}, d_{133} = -d_{233}, d_{141} = d_{252}, d_{142} = -d_{251}, d_{151} = -d_{242}, d_{152} = d_{241}, d_{163} = d_{263}, d_{341} = d_{352}, d_{342} = -d_{351}, d_{363}, d_{461} = -d_{562}, d_{462} = d_{561}$
	$4mm$	C_{4v}	5	$d_{133} = d_{233}, d_{142} = d_{251}, d_{151} = d_{242}, d_{342} = d_{351}, d_{461} = d_{562}$
	$\bar{4}2m$	D_{2d}	6	$d_{141} = d_{252}, d_{152} = d_{241}, d_{163} = d_{263}, d_{341} = d_{352}, d_{363}, d_{462} = d_{561}$
	422	D_4	6	$d_{141} = -d_{252}, d_{152} = -d_{241}, d_{163} = -d_{263}, d_{341} = -d_{352}, d_{453}, d_{462} = -d_{561}$
Rhombohedral	3	C_3	15	$d_{121} = 2d_{162} = 2d_{262}, d_{122} = -2d_{161} = -2d_{261}, d_{163} = -d_{263}, d_{133} = d_{233}, d_{352} = -d_{341}, d_{351} = d_{342}, d_{361} = -d_{132} = d_{232}, d_{362} = d_{131} = -d_{231}, d_{143} = -d_{243} = -d_{563}, d_{253} = -d_{463} = -d_{153}, d_{453}, d_{241} - d_{141} = -2d_{561} = 2d_{462} = d_{252} - d_{152}$ with $d_{141} = -d_{252}$ and $d_{241} = -d_{152}$; $d_{242} - d_{142} = -2d_{562} = -2d_{461} = d_{151} - d_{251}$ with $d_{142} = d_{251}$ and $d_{242} = d_{151}$
	$3m$	C_{3v}	7	$d_{122} = -2d_{161} = -2d_{261}, d_{133} = d_{233}, d_{351} = d_{342}, d_{361} = -d_{132} = d_{232}, d_{143} = -d_{243} = -d_{563}, d_{242} - d_{142} = -2d_{562} = -2d_{461} = d_{151} - d_{251}$ with $d_{142} = d_{251}$ and $d_{242} = d_{151}$
	32	D_3	8	$d_{121} = 2d_{162} = 2d_{262}, d_{163} = -d_{263}, d_{352} = -d_{341}, d_{362} = d_{131} = -d_{231}, d_{253} = -d_{463} = -d_{153}, d_{453}, d_{241} - d_{141} = -2d_{561} = 2d_{462} = d_{252} - d_{152}$ with $d_{141} = -d_{252}$ and $d_{241} = -d_{152}$
Hexagonal	$\bar{6}$	C_{3h}	6	$d_{121} = 2d_{162} = 2d_{262}, d_{122} = -2d_{161} = -2d_{261}, d_{361} = -d_{132} = d_{232}, d_{362} = d_{131} = -d_{231}, d_{143} = -d_{243} = -d_{563}, d_{253} = -d_{463} = -d_{153}$
	6	C_6	9	$d_{163} = -d_{263}, d_{133} = d_{233}, d_{352} = -d_{341}, d_{351} = d_{342}, d_{453}, d_{241} - d_{141} = -2d_{561} = 2d_{462} = d_{252} - d_{152}$ with $d_{141} = -d_{252}$ and $d_{241} = -d_{152}$; $d_{242} - d_{142} = -2d_{562} = -2d_{461} = d_{151} - d_{251}$ with $d_{142} = d_{251}$ and $d_{242} = d_{151}$
	$\bar{6}m2$	D_{3h}	3	$d_{122} = -2d_{161} = -2d_{261}, d_{361} = -d_{132} = d_{232}, d_{143} = -d_{243} = -d_{563}$
	$6mm$	C_{6v}	4	$d_{133} = d_{233}, d_{351} = d_{342}, d_{242} - d_{142} = -2d_{562} = -2d_{461} = d_{151} - d_{251}$ with $d_{142} = d_{251}$ and d_{242} and d_{151}
	622	D_6	5	$d_{163} = -d_{263}, d_{352} = -d_{341}, d_{453}, d_{241} - d_{141} = -2d_{561} = 2d_{462} = d_{252} - d_{152}$ with $d_{141} = -d_{252}$ and $d_{241} = -d_{152}$
Cubic	23	T	4	$d_{141} = d_{252} = d_{363}, d_{152} = d_{263} = d_{341}, d_{163} = d_{241} = d_{352}, d_{453} = d_{561} = -d_{462}$
	$\bar{4}3m$	T_d	2	$d_{141} = d_{252} = d_{363}, d_{152} = d_{263} = d_{341} = d_{163} = d_{241} = d_{352}$
	432	O	2	$d_{453} = d_{561} = -d_{462}, d_{152} = d_{263} = d_{341} = -d_{163} = -d_{241} = -d_{352}$

All centro-symmetric crystals 0

non-vanishing coefficients as determined by the general group-theoretical method agree with those determined by Portigal & Burstein (1968) for the point groups T, T_d and O. The identification of the non-vanishing coefficients of the acoustic gyrotropic tensor for all non-centrosymmetric point groups will be of great help to experimentalists in high-resolution spectroscopy studying acoustical activity. It would be interesting to study the elastic wave propagation along various directions in acoustically active crystals and such a study is in progress.

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