SHORT COMMUNICATIONS

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The electric susceptibility, piezoelectric, elastic, photoelastic, Brillouin and Raman tensors for point groups with twelvefold rotation axes.

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Abstract

To study the physical properties of two-dimensional dodecagonal quasicrystals, the electric susceptibility, piezoelectric, elastic, photoelastic, Brillouin and Raman tensors for the point groups C_{12}, S_{12}, C_{12h}, C_{12v}, D_{12}, D_{12h} are required. These tensors are tabulated here.

Introduction

With the discovery of two-dimensional dodecagonal quasicrystals (Ishimasa, Nissen & Fukano, 1985), it is useful to calculate the property tensors for the point groups with twelvefold rotation axes. The Raman and hyper-Raman tensors of pentagonal and icosahedral groups have been given by Brandmüller & Claus (1988*a*, *b*) and the piezoelectric, elastic, photoelastic and Brillouin tensors for the point groups with fivefold and eightfold rotation axes have been provided by the present authors (Jiang, Liao, Chen & Zhang, 1990; Jiang, Liao & Chen 1991).

Here, using the method of tensor invariants, the electric susceptibility, piezoelectric, elastic, photoelastic and Raman tensors of point groups C_{12}, S_{12}, C_{12h}, C_{12v}, D_{12} and D_{12h} are obtained. On the basis of these results, the Brillouin tensors with these symmetries are also derived.

Calculation and results

The method of tensor invariants (MTI) is a generalized and powerful method to determine the non-vanishing components of property tensors and has been discussed by many authors (Landau & Lifschitz, 1959; Lax, 1974; Nye, 1985). Recently, it has been further improved and developed by Liao *et al.* (in preparation) so it can be applied not only in determining high-rank static tensors but also in calculating dynamic tensors, such as Raman and hyper-Raman tensors (Jiang, 1990).

The main points of MTI are briefly described in the following.

(1) Determine the number of independent tensor components using a group theoretical method.

(2) Note that the inner product of two sets of isovariant orthogonal bases of the same irreducible representation constitute an independent tensor invariant (ITI) (for static tensors). Also, the inner product of one set of isovariant orthogonal bases with the normal coordinate of the same irreducible representation constitute an ITI (for dynamic tensors).

(3) Multiply the ITIs by different factors and sum them, thus obtaining the general tensor invariant.

(4) Read off the tensor components from the general tensor invariant.

(5) Consider the intrinsic symmetries which have not been included in step (2).

To facilitate the calculation, the isovariant orthogonal bases up to second rank for the point groups with twelvefold rotation axes are constructed with the help of projection operators. They are shown in Table 1.

Table 1. *Isovariant orthogonal bases corresponding to the point groups with twelvefold rotation axes*

Point group	Irreducible representation	1st-rank bases	2nd-rank bases
C_{12}	A	z; Rz	$xx+yy$; zz
	B		
	E_1	(x, y); (Rx, Ry)	(xz, yz); $(-yz, xz)$
	E_2		$(xx-yy, -2xy)$; $(2xy, xx-yy)$
	E_3		
	E_4		
	E_5		
S_{12}	A	Rz	$xx+yy$; zz
	B	z	
	E_1	(x, y)	
	E_2		$(xx-yy, -2xy)$; $(2xy, xx-yy)$
	E_3		
	E_4		
	E_5	(Rx, Ry)	(xz, yz); $(-yz, xz)$
C_{12v}	A_1	z	$xx+yy$; zz
	A_2	Rz	
	B_1		
	B_2		
	E_1	(x, y); (Rx, Ry)	(xz, yz)
	E_2		$(xx-yy, -2xy)$
	E_3		
	E_4		
	E_5		
D_{12}	A_1		$xx+yy$; zz
	A_2	z, Rz	
	B_1		
	B_2		
	E_1	(x, y); (Rx, Ry)	$(yz, -xz)$
	E_2		$(xx-yy, -2xy)$
	E_3		
	E_4		
	E_5		
		$C_{12h}=C_{12}\otimes i$	$D_{12h}=D_{12}\otimes i$

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Table 2. *The electric susceptibility and elastic tensors for the point groups C_{12}, S_{12}, C_{12h}, C_{12v}, D_{12} and D_{12h}*

Electric susceptibility

$$\begin{matrix} \varepsilon_0 & \cdot & \cdot \\ \cdot & \varepsilon_0 & \cdot \\ \cdot & \cdot & \varepsilon_e \end{matrix} \quad (2)$$

Elastic

$$\begin{matrix} C_{11} & C_{12} & C_{13} & \cdot & \cdot & \cdot \\ C_{12} & C_{11} & C_{13} & \cdot & \cdot & \cdot \\ C_{13} & C_{13} & C_{33} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & C_{44} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & C_{44} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{2}(C_{11}-C_{12}) \end{matrix} \quad (5)$$

Table 3. *The non-vanishing components of piezoelectric and photoelastic tensors for dodecagonal point groups*

Piezoelectric

C_{12}
$$\begin{matrix} \cdot & \cdot & \cdot & d_{14} & d_{15} & \cdot \\ \cdot & \cdot & \cdot & d_{15} & -d_{14} & \cdot \\ d_{31} & d_{31} & d_{33} & \cdot & \cdot & \cdot \end{matrix} \quad (4)$$

S_{12}, C_{12h} (0)

C_{12v}
$$\begin{matrix} \cdot & \cdot & \cdot & \cdot & d_{15} & \cdot \\ \cdot & \cdot & \cdot & d_{15} & \cdot & \cdot \\ d_{31} & d_{31} & d_{33} & \cdot & \cdot & \cdot \end{matrix} \quad (3)$$

D_{12}
$$\begin{matrix} \cdot & \cdot & \cdot & d_{14} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -d_{14} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{matrix} \quad (1)$$

D_{12h} (0)

Photoelastic

$$\begin{matrix} P_{11} & P_{12} & P_{13} & \cdot & \cdot & P_{16} \\ P_{12} & P_{11} & P_{13} & \cdot & \cdot & -P_{16} \\ P_{31} & P_{31} & P_{33} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & P_{44} & P_{45} & \cdot \\ \cdot & \cdot & \cdot & -P_{45} & P_{44} & \cdot \\ -P_{16} & P_{16} & \cdot & \cdot & \cdot & \frac{1}{2}(P_{11}-P_{12}) \end{matrix} \quad (8)$$

$$\begin{matrix} P_{11} & P_{12} & P_{13} & \cdot & \cdot & \cdot \\ P_{12} & P_{11} & P_{13} & \cdot & \cdot & \cdot \\ P_{31} & P_{31} & P_{33} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & P_{44} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & P_{44} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{2}(P_{11}-P_{12}) \end{matrix} \quad (6)$$

Table 4. *The Raman tensors for dodecagonal point groups*

$$\begin{vmatrix} a & \cdot & \cdot \\ \cdot & a & \cdot \\ \cdot & \cdot & b \end{vmatrix} \quad \begin{vmatrix} \cdot & \cdot & d \\ \cdot & \cdot & e \\ d & e & \cdot \end{vmatrix} \quad \begin{vmatrix} \cdot & \cdot & -e \\ \cdot & \cdot & d \\ -e & d & \cdot \end{vmatrix} \quad \begin{vmatrix} h & i & \cdot \\ i & -h & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix} \quad \begin{vmatrix} i & -h & \cdot \\ -h & -i & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

C_{12}	$A(z, Rz)$	$E_1(x, y; Rx, Ry)$	$E_2(xx-yy, -2xy)$
S_{12}	$A(Rz)$	$E_5(Rx, Ry)$	$E_2(xx-yy, -2xy)$
C_{12h}	$A_g(Rz)$	$E_{1g}(Rx, Ry)$	$E_{2g}(xx-yy, -2xy)$

$$\begin{vmatrix} a & \cdot & \cdot \\ \cdot & a & \cdot \\ \cdot & \cdot & b \end{vmatrix} \quad \begin{vmatrix} \cdot & \cdot & e \\ \cdot & \cdot & \cdot \\ e & \cdot & \cdot \end{vmatrix} \quad \begin{vmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & e \\ \cdot & e & \cdot \end{vmatrix} \quad \begin{vmatrix} f & \cdot & \cdot \\ \cdot & -f & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix} \quad \begin{vmatrix} \cdot & -f & \cdot \\ -f & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

C_{12v}	$A_1(z)$	$E_1(x, y; Rx, Ry)$	$E_2(xx-yy, -2xy)$
D_{12}	A_1	$E_1(y, -x; Ry, -Rx)$	$E_2(xx-yy, -2xy)$
D_{12h}	A_{1g}	$E_{1g}(Ry, -Rx)$	$E_{2g}(xx-yy, -2xy)$

Table 5. *The Brillouin tensors for dodecagonal point groups*

C_{12} S_{12} C_{12h}

1. x phonon $\mathbf{q} = (1, 0, 0)$

$\rho v^2 = C_{11}$

$\mathbf{u}(1, 0, 0)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{11} & -\varepsilon_0^2 P_{16} & \cdot \\ -\varepsilon_0^2 P_{16} & \varepsilon_0^2 P_{12} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{31} \end{vmatrix}$$

$\rho v^2 = C_{66}$

$\mathbf{u} = (0, 1, 0)$ (T_1)
$$\begin{vmatrix} \varepsilon_0^2 P_{16} & \varepsilon_0^2 P_{66} & \cdot \\ \varepsilon_0^2 P_{66} & -\varepsilon_0^2 P_{16} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 0, 1)$ (T_2)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & P_{45} \\ P_{44} & P_{45} & \cdot \end{vmatrix}$$

2. y phonon $\mathbf{q} = (0, 1, 0)$

$\rho v^2 = C_{11}$

$\mathbf{u} = (0, 1, 0)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{12} & \varepsilon_0^2 P_{16} & \cdot \\ \varepsilon_0^2 P_{16} & \varepsilon_0^2 P_{11} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{31} \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 0, 1)$ (T_1)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & -P_{45} \\ \cdot & \cdot & P_{44} \\ -P_{45} & P_{44} & \cdot \end{vmatrix}$$

$\rho v^2 = C_{66}$

$\mathbf{u} = (1, 0, 0)$ (T_2)
$$\varepsilon_0^2 \begin{vmatrix} P_{16} & P_{66} & \cdot \\ P_{66} & -P_{16} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

3. z phonon $\mathbf{q} = (0, 0, 1)$

$\rho v^2 = C_{33}$

$\mathbf{u} = (0, 0, 1)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{13} & \cdot & \cdot \\ \cdot & \varepsilon_0^2 P_{13} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{33} \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (1, 0, 0)$ (T_1)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & P_{45} \\ P_{44} & P_{45} & \cdot \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 1, 0)$ (T_2)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & -P_{45} \\ \cdot & \cdot & P_{44} \\ -P_{45} & P_{44} & \cdot \end{vmatrix}$$

D_{12} C_{12v} D_{12h}

1. x phonon $\mathbf{q} = (1, 0, 0)$

$\rho v^2 = C_{11}$

$\mathbf{u} = (1, 0, 0)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{11} & \cdot & \cdot \\ \cdot & \varepsilon_0^2 P_{12} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{31} \end{vmatrix}$$

$\rho v^2 = C_{66}$

$\mathbf{u} = (0, 1, 0)$ (T_1)
$$\begin{vmatrix} \cdot & \varepsilon_0^2 P_{66} & \cdot \\ \varepsilon_0^2 P_{66} & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 0, 1)$ (T_2)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & \cdot \\ P_{44} & \cdot & \cdot \end{vmatrix}$$

2. y phonon $\mathbf{q} = (0, 1, 0)$

$\rho v^2 = C_{11}$

$\mathbf{u} = (0, 1, 0)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{12} & \cdot & \cdot \\ \cdot & \varepsilon_0^2 P_{11} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{31} \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 0, 1)$ (T_1)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & P_{44} \\ \cdot & P_{44} & \cdot \end{vmatrix}$$

$\rho v^2 = C_{66}$

$\mathbf{u} = (1, 0, 0)$ (T_2)
$$\varepsilon_0^2 \begin{vmatrix} \cdot & P_{66} & \cdot \\ P_{66} & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

3. z phonon $\mathbf{q} = (0, 0, 1)$

$\rho v^2 = C_{33}$

$\mathbf{u} = (0, 0, 1)$ (L)
$$\begin{vmatrix} \varepsilon_0^2 P_{13} & \cdot & \cdot \\ \cdot & \varepsilon_0^2 P_{13} & \cdot \\ \cdot & \cdot & \varepsilon_e^2 P_{33} \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (1, 0, 0)$ (T_1)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & \cdot \\ P_{44} & \cdot & \cdot \end{vmatrix}$$

$\rho v^2 = C_{44}$

$\mathbf{u} = (0, 1, 0)$ (T_2)
$$\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & P_{44} \\ \cdot & P_{44} & \cdot \end{vmatrix}$$

Table 5 (*cont.*)

C_{12} S_{12} C_{12h}

4. $x \pm y$ phonon $\mathbf{q} = (1, \pm 1, 0)/\sqrt{2}$

$$\rho v^2 = (C_{11} - C_{12})/2$$

$$\mathbf{u} = (1, \pm 1, 0)/\sqrt{2} \quad (L)$$

$$\begin{vmatrix} \frac{1}{2}\varepsilon_0^2(P_{11} + P_{12} \pm 2P_{16}) & \pm\varepsilon_0^2 P_{66} & \cdot \\ \pm\varepsilon_0^2 P_{66} & \frac{1}{2}\varepsilon_0^2(P_{11} + P_{12} \mp 2P_{16}) & \cdot \\ \cdot & \cdot & 2\varepsilon_e^2 P_{31} \end{vmatrix}$$

$$\rho v^2 = C_{11}$$

$$\mathbf{u} = (1, \mp 1, 0)/\sqrt{2} \quad (T_1)$$

$$\varepsilon_0^2 \begin{vmatrix} P_{66} & -P_{16} & \cdot \\ -P_{16} & -P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

$$\rho v^2 = C_{44}$$

$$\mathbf{u} = (0, 0, 1) \quad (T_2)$$

$$\frac{\varepsilon_e \varepsilon_0}{\sqrt{2}} \begin{vmatrix} \cdot & \cdot & \mp P_{45} + P_{44} \\ \cdot & \cdot & \pm P_{44} + P_{45} \\ \mp P_{45} + P_{44} & \pm P_{44} + P_{45} & \cdot \end{vmatrix}$$

D_{12} C_{12v} D_{12h}

4. $x \pm y$ phonon $\mathbf{q} = (1, \pm 1, 0)/\sqrt{2}$

$$\rho v^2 = (C_{11} - C_{12})/2$$

$$\mathbf{u} = (1, \pm 1, 0)/\sqrt{2} \quad (L)$$

$$\begin{vmatrix} \frac{1}{2}\varepsilon_0^2(P_{11} + P_{12}) & \pm\varepsilon_0^2 P_{66} & \cdot \\ \pm\varepsilon_0^2 P_{66} & \frac{1}{2}\varepsilon_0^2(P_{11} + P_{12}) & \cdot \\ \cdot & \cdot & 2\varepsilon_e^2 P_{31} \end{vmatrix}$$

$$\rho v^2 = C_{11}$$

$$\mathbf{u} = (1, \mp 1, 0)/\sqrt{2} \quad (T_1)$$

$$\varepsilon_0^2 \begin{vmatrix} P_{66} & \cdot & \cdot \\ \cdot & -P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$$

$$\rho v^2 = C_{44}$$

$$\mathbf{u} = (0, 0, 1) \quad (T_2)$$

$$\frac{\varepsilon_e \varepsilon_0}{\sqrt{2}} \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & \pm P_{44} \\ P_{44} & \pm P_{44} & \cdot \end{vmatrix}$$

Once the basis functions are available, with the use of the MTI, the electric susceptibility, elastic, piezoelectric, photoelastic and Raman tensors of dodecagonal point groups may be identified. They are tabulated in Tables 2-4.

The Christoffel matrices of the point groups with twelve-fold rotation axes may be calculated and the velocities of sound waves may be obtained by solving the secular equations (Auld, 1973). Based upon these results, the Brillouin tensors for dodecagonal point groups can be derived, following Cummius & Schoen (1972), to characterize the coupling between acoustic phonons and electric polarizability in quasicrystals. The results are presented in Table 5.

Discussion

The results given above can be extended to other tensors. For the point groups of C_{12}, C_{12h}, S_{12}, C_{12v}, D_{12} and D_{12h}, any one of the polar tensors of rank 2, such as the electric conductivity, strain and stress, has the same form as that given in Table 2. On the other hand, based upon the lists of Table 2 and Table 3, any one of the polar tensors of rank 3 or rank 4 can be easily determined by considering its intrinsic symmetry. Examples of such tensors are the linear electric-optic and the non-linear dielectric susceptibility and electrostriction tensors. We hope these results may be helpful to studies of the physical properties of quasicrystals.

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Notes & News

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Oxford Cryosystems Award during ECM-14

During the 14th European Crystallographic Meeting, to be held 2-7 August 1992 in Enschede, The Netherlands, the Oxford Cryosystems Award for the most outstanding presentation (oral or poster) in the use of low temperatures for crystallography or the design of equipment or techniques in low-temperature crystallography will be presented. An independent jury appointed by the Programme Committee of ECM-14 will judge candidate presentations. The prize (250 pound sterling) is donated by Oxford Cryosystems.

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