

The Method of Tensor Invariants and its Application to the Hall Effect in Quasicrystals

BY JIANG YI-JIAN, LIAO LI-JI AND CHEN GANG

Department of Applied Physics, Beijing Polytechnic University, Beijing 100022, People's Republic of China, and
China Center of Advanced Science and Technology, Beijing 100080, People's Republic of China

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Abstract

The method of tensor invariants is systematically summarized and generalized. With the help of the theorem of 'shadow' and the theorem of the number of independent bases, the whole family of isovariant orthogonal basis functions for pentagonal, icosahedral, octagonal, decagonal and dodecagonal point groups is obtained. On the basis of these results, the Hall-coefficient tensors for quasicrystalline point groups are identified and tabulated. The results of this group-theoretical study are briefly discussed and summarized.

Introduction

Since the discovery of quasicrystals (Schechtman, Blech, Gratias & Cahn, 1984), there have been continuous efforts to uncover the influence of the new symmetry on the physical properties of materials. On the theoretical side, Bak (1985) studied the symmetry, stability and elastic properties, phenomenologically, of icosahedral diffraction patterns, and obtained the acoustic phonon and phason modes. Brandmüller & Claus (1988*a,b*) provided the irreducible tensors of ranks 1–4 for all the irreducible representations of the pentagonal and icosahedral point groups. Rama Mohana Rao & Hemagiri Rao (1992, 1993) have worked out the pyromagnetic, magnetoelectric, first- and second-order piezomagnetic polarizability constants and third-order elastic coefficients for the point groups with fivefold rotation axes. The present authors (Jiang, Liao, Chen & Zhang, 1990, 1992; Jiang, Liao, Chen & Shen, 1992) have derived the piezoelectric, elastic, photoelastic and Brillouin tensors corresponding to pentagonal, icosahedral and dodecagonal point groups, and obtained the Raman and hyper-Raman tensors of six octagonal point groups. On the experimental side, not only has anisotropy been observed in the Hall effect (Zhang *et al.*, 1990; Wang, Zhang & Chen, 1993), electric resistivity (Lin *et al.*, 1990), thermopower (Lin *et al.*, 1990) and thermal conductivity (Zhang *et al.*, 1991), but the elasticity of Al–Cu–Li and Al–Cu–Fe quasicrystals has been found to be isotropic through ultrasonic (Reynolds, Golding, Kortan & Parsey, 1990) and

Brillouin scattering (Vanderwal, Zhao & Walton, 1992) studies.

There are many methods of calculating property tensors. Some of them have been further improved and developed by many authors in different approaches to satisfy the requirements of various types of tensors (Fumi & Ripamonti, 1980; Kopsky, 1979; Brandmüller & Winter, 1985; Nye, 1985). Among them, the method of tensor invariants (MTI) is a useful and powerful one. After systematic improvement and generalization in this paper, this method can be applied to the property tensors of quasicrystalline point groups easily and directly just as it was applied in crystal symmetry groups. Here, by the MTI, the Hall-coefficient tensors for pentagonal, icosahedral, octagonal, decagonal and dodecagonal point groups are calculated and presented.

Method of tensor invariants

The mathematical basis of the MTI is the group-theoretical version. It has been proposed and summarized by various authors (Landau & Lifshitz, 1959; Callen, 1968; Lax, 1974; Nye 1985). But in fact at least three problems have not, essentially, been solved. First, there is no general procedure to carry out the calculation. Second, there is no standard to justify whether one has obtained the whole family of independent isovariant orthogonal basis functions of a given irreducible representation (ir). Third, there is no usable group table including all of the independent isovariant orthogonal bases up to rank 3. For these reasons, the method can be used only in some simple case having didactic interest (Fumi & Ripamonti, 1980).

In this paper, the MTI is improved and generalized. It is described as follows:

Property tensors can be defined as $T_{abc...lmn...}$ with j indices of the polar vector a, b, c, \dots and k indices of the axial vector $\bar{l}, \bar{m}, \bar{n}, \dots$ ($a, b, c, \dots, l, m, n, \dots = 1, 2, 3$). Under the operation \hat{R} of a given point group, the tensor components are transformed as

$$\hat{R}[T_{abc...lmn...}] = [\det(\hat{R})]^k \sum_{rst...opq...} R_{ar}R_{bs}R_{ct...}R_{lc}R_{mp}R_{nq...}T_{rst...opq...} \quad (1)$$

where $a, b, c, \dots, l, m, n, \dots, r, s, t, \dots, o, p, q, \dots = 1, 2, 3$, R_{ar} is the element of the transformation matrix of a polar vector and $\det(\hat{R})$ is the determinant of this matrix.

From (1), it is obvious that the tensor components are transformed as a product,

$$X_a X_b X_c \dots X_l X_m X_n \dots$$

so the inner product of $T_{abc\dots lmn\dots}$ and $X_a X_b X_c \dots X_l X_m X_n \dots$ will not change under the operation \hat{R} of the point group. Thus, one has

$$\begin{aligned} \hat{R} \left[\sum_{abc\dots lmn\dots} T_{abc\dots lmn\dots} X_a X_b X_c \dots X_l X_m X_n \dots \right] \\ = \sum_{abc\dots lmn\dots} T_{abc\dots lmn\dots} X_a X_b X_c \dots X_l X_m X_n \dots \end{aligned} \quad (2)$$

Owing to the macroscopic symmetry, Neumann's principle holds good, according to which

$$T_{abc\dots lmn\dots} = \hat{R} [T_{abc\dots lmn\dots}]. \quad (3)$$

So (2) can be considered as an invariant that takes $T_{abc\dots lmn\dots}$ as the coefficients of proportionality of $X_a X_b X_c \dots X_l X_m X_n \dots$. If one has found in any way an invariant of the form

$$\begin{aligned} \hat{R} \left[\sum_{abc\dots lmn\dots} A_{abc\dots lmn\dots} X_a X_b X_c \dots X_l X_m X_n \dots \right] \\ = \sum_{abc\dots lmn\dots} A_{abc\dots lmn\dots} X_a X_b X_c \dots X_l X_m X_n \dots \end{aligned} \quad (4)$$

by comparison with (2), one can obtain the nonzero independent tensor components

$$T_{abc\dots lmn\dots} = A_{abc\dots lmn\dots}. \quad (5)$$

The right-hand side of (4) is defined as the general tensor invariant (GTI) from which the tensor components can be read off as a linear combination of nonzero independent parameters. This is the general principle of the MTI.

In the practical use of the MTI, the following four theorems are very important.

Theorem 1. (Bhagavantam & Venkatarayudu, 1951): The number of nonzero independent components of property tensors is given by

$$n = (1/g) \sum_{\hat{R}} \chi(\hat{R}) \chi^{(A)}(\hat{R}). \quad (6)$$

Here the quantity $\chi^{(A)}(\hat{R})$ denotes the character of the total symmetry ir and $\chi(\hat{R})$ the character of the reducible representation that is formed by the polar or axial property tensor of rank $j+k$ with corresponding intrinsic symmetry. g is the rank of the point group.

Theorem 2. The inner product of two sets of isovariant orthogonal basis functions of the same ir constitutes an independent tensor invariant (ITI).

Theorem 3 (Jiang, 1990). The number of independent basis functions of the i th ir is given by

$$n = (1/g) \sum_{\hat{R}} \chi(\hat{R}) [\chi^{(i)*}(\hat{R})], \quad (7)$$

where $\chi^{(i)}(\hat{R})$ expresses the character of the i th ir for the symmetry operation \hat{R} of the point group, $\chi(\hat{R})$ the character of the representation matrix of the basis function and g the rank of the point group.

Theorem 4 (Jiang, Liao & Chen, 1992a). If the physical ir that is constituted by two complex conjugate ir's has one set of real bases (a, b) with an orthogonal representation matrix, there is a 'shadow' set $(-b, a)$ that is isovariant with (a, b) .

On the basis of theorem 3 and theorem 4, high-rank isovariant bases can be calculated from lower-rank bases with the help of projection operations. It is necessary to check whether the basis functions are linearly independent and whether they span the same orthogonal transformation matrix.

In this way, the whole family of the isovariant orthogonal bases up to rank 3 for crystal and octagonal point groups and the isovariant orthogonal bases up to rank 2 for point groups with fivefold, tenfold and twelvefold rotation axes have been obtained. The former have been reported by the present authors (Jiang, Liao & Chen, 1992a; Jiang, Liao, Chen & Shen, 1992); the latter are shown in Table 1.

In summary, with the basis functions at hand, one can identify the property tensors by the following steps:

- (1) Determine the number of independent tensor components.
- (2) On the basis of theorem 2, list the whole family of ITI of i th ir.
- (3) Multiply the ITIs by different coefficients and sum them up, thus obtaining the GTI.
- (4) Read off the tensor components from the GTI.
- (5) Consider the intrinsic symmetry that has not been included in step (2).

Hall-coefficient tensors

It can be seen that the phenomenon of the Hall effect is the appearance of an additional electric field \mathbf{E} in the present of a magnetic field \mathbf{H} applied normal to an electric current \mathbf{J} flowing in a conductor, and the Hall coefficients $R_{\mu\nu\lambda}$ of first order are obtained from the governing relation

$$J_\mu = R_{\mu\nu\lambda} E_\nu H_\lambda, \quad (8)$$

with the indices taking the values 1, 2 and 3. Because the symmetry of $R_{\mu\nu\lambda}$ is restricted by Onsager's reciprocity theorem, one has

$$R_{\mu\nu\lambda} = -R_{\nu\mu\lambda}. \quad (9)$$

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

$$S_{10} = C_5 \otimes i, D_{5d} = D_5 \otimes i, I_h = I \otimes i, C_{10h} = C_{10} \otimes i, D_{10h} = D_{10} \otimes i, C_{12h} = C_{12} \otimes i, D_{12h} = D_{10} \otimes i.$$

Point group	ir	First-rank bases	Second-rank bases	Point group	ir	First-rank bases	Second-rank bases	
C_5	A	z, Rz	$xx + yy, zz, xy - yx$	C_{12v}	A_1	z	$xx + yy, zz$	
	E_1^*	$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$		A_2	Rz	$xy - yx$	
	E_2^*		$(xx - yy - xy - yx)$		B_1			
C_{5h}	A'	Rz	$xx + yy, zz, xy - yx$	B_2				
	$E_1'^*$	(x, y)		E_1	$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$	$(xz, yz), (zx, zy)$	
	$E_2'^*$		$(xx - yy, -xy - yx)$	E_2		$(xx - yy, -xy - yx)$	$(xx - yy, -xy - yx)$	
	A''	z		E_3				
	$E_1''^*$	(Rx, Ry)	$(xz, yz), (zx, zy)$	E_4				
D_5	$E_2''^*$			E_5				
	A_1		$xx + yy, zz$	D_{12}	A_1		$xx + yy, zz$	
	A_2	z, Rz	$xy - yx$		A_2	z, Rz	$xy - yx$	
	E_1	$(x, y), (Rx, Ry)$	$(yz, -xz), (zy, zx)$		B_1			
E_2		$(xx - yy, -xy - yx)$	B_2					
C_{5v}	A_1	z	$xx + yy, zz$	E_1	$(x, y), (Rx, Ry)$	$(yz, -xz), (zy, -zx)$	$(yz, -xz), (zy, -zx)$	
	A_2	Rz	$xy - yx$	E_2		$(xx - yy, -xy - yx)$	$(xx - yy, -xy - yx)$	
	E_1	$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$	E_3				
	E_2		$(xx - yy, -xy - yx)$	E_4				
D_{5h}	A_1'		$xx + yy, zz$	E_5				
	A_2'	Rz	$xy - yx$	C_{10}	A	z, Rz	$xx + yy, zz, xy - yx$	
	E_1'	(x, y)			B			
	E_2'		$(xx - yy, -xy - yx)$		E_1^*	$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$	$(xz, yz), (zx, zy)$
	A_1''				E_2^*		$(xx - yy, -xy - yx)$	$(xx - yy, -xy - yx)$
	A_2''	z			E_3^*			
E_1''	(Rx, Ry)	$(yz, -xz), (zy, -zx)$	E_4^*					
C_{12}	E_2''			D_{10}	A_1		$xx + yy, zz$	
	A	z, Rz	$xx + yy, zz, xy - yx$		A_2	z, Rz	$xy - yx$	
	B				B_1			
	E_1^*	$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$		B_2			
	E_2^*		$(xx - yy, -xy - yx)$		E_1	$(x, y), (Rx, Ry)$	$(yz, -xz), (zy, -zx)$	$(yz, -xz), (zy, -zx)$
	E_3^*				E_2		$(xx - yy, -xy - yx)$	$(xx - yy, -xy - yx)$
S_{12}	E_4^*			E_3				
	E_5^*			E_4				
	A	Rz	$xx + yy, zz, xy - yx$	C_{10v}	A_1	z	$xx + yy, zz$	
	B	z			A_2	Rz	$xy - yx$	
	E_1^*	(x, y)			B_1			
	E_2^*		$(xx - yy, -xy - yx)$		B_2			
E_3^*			E_1		$(x, y), (Rx, Ry)$	$(xz, yz), (zx, zy)$	$(xz, yz), (zx, zy)$	
E_4^*			E_2			$(xx - yy, -xy - yx)$	$(xx - yy, -xy - yx)$	
I	E_5^*	(Rx, Ry)	$(xz, yz), (zx, zy)$	E_3				
				E_4				
				I	A		$xx + yy + zz$	
					F_1	$(x, y, z), (Rx, Ry, Rz)$	$(yz - zy, zx - xz, xy - yx)$	
					F_2			
					G			
			H					
							$(xx + yy - 2zz,$ $3^{1/2}(xz + zx), 3^{1/2}(xy + yx),$ $3(yz - zy), 3^{1/2}(yz + zy))$	

*Contains shadows.

As the character of the axial vector is given by $1 \pm 2 \cos \theta$ and that of the antisymmetric conductivity by $1 + 2 \cos \theta$, the compound character representing the first-order Hall effect can be expressed as

$$\chi(\hat{R}) = (1 + 2 \cos \theta)(1 \pm 2 \cos \theta). \quad (10)$$

In (10), a positive or negative sign is taken according to whether the symmetry operation \hat{R} in question is a pure rotation or a rotation-reflection through an angle θ . From theorem 1, the number n of independent tensor components required to describe the Hall effect in quasicrystals are obtained; these are listed in Table 2.

The nonvanishing and independent tensor components in respect of each of the quasicrystalline classes for Hall coefficients are identified by the MTI. They are given in Table 3. For the purpose of illustration, the Hall-

Table 2. *Number n of independent tensor components required to describe the Hall effect in quasicrystals*

Pentagonal or icosahedral point group	Octagonal point group	Decagonal point group	Dodecagonal point group
C_5	3	C_{10}	3
C_{5h}	3	C_{10h}	3
S_{10}	3	D_{10}	2
D_5	2	C_{10v}	2
C_{5v}	2	D_{10h}	2
D_{5h}	2		
D_{5d}	2		
I	1		
I_h	1		

coefficient tensor of point group C_{10} is taken as an example.

The Hall-coefficient tensor is a third-rank axial tensor. According to its intrinsic symmetry, the ITI should take

Table 3. Non-vanishing and independent tensor components of Hall coefficients for quasicrystalline point groups

Point group	Hall coefficients
$C_5, C_{5h}, S_{10}, C_8, C_{8h}, S_8,$ $C_{10}, C_{10h}, C_{12}, C_{12h}, S_{12}$	$R_{123} = -R_{213},$ $R_{231} = R_{312} = -R_{321} = -R_{132},$ $R_{311} = R_{322} = -R_{131} = -R_{232}$
$D_5, C_{5v}, D_{5h}, D_{5d}, D_8, C_{8v}, D_{8h},$ $D_{10}, C_{10v}, D_{10h}, D_{12}, C_{12v}, D_{12h}$	$R_{123} = -R_{213},$ $R_{231} = R_{312} = -R_{321} = -R_{132}$
I, I_h	$R_{123} = R_{231} = R_{312}$ $= -R_{132} = -R_{213} = -R_{321}$

the form of the product of one axial vector and one second-rank basis function. From Table 1, we have

$$A: Rz; \quad xx + yy, \quad zz, \quad xy - yx.$$

$$E_1: (Rx, Ry); \quad (xz, yz), \quad (zx, zy), \quad (-yz, xz),$$

$$\quad \quad \quad (-zy, zx).$$

So the ITI of A is

$$xxRz + yyRz, \quad zzRz, \quad xyRz - yxRz.$$

and the ITI of E_1 is

$$xzRx + yzRy, \quad zxRx + zyRy, \quad -yzRx + xzRy,$$

$$-zyRx + zxRy.$$

$$GTI = A(xxRz + yyRz) + BzzRz + C(xyRz - yxRz)$$

$$+ D(xzRx + yzRy) + E(zxRx + zyRy)$$

$$+ F(-yzRx + xzRy) + G(-zyRx + zxRy).$$

Compared with (4), we have:

$$R_{113} = R_{223} = A, \quad R_{333} = B, \quad R_{123} = -R_{213}C,$$

$$R_{131} = R_{232} = D, \quad R_{311} = R_{322} = E,$$

$$R_{132} = -R_{231} = F, \quad R_{312} = -R_{321} = G.$$

With consideration of (8), we can obtain

$$A = B = 0, \quad D = -E \quad \text{and} \quad F = -G.$$

So the nonvanishing and independent tensor components are

$$R_{123} = -R_{213}, \quad R_{231} = R_{312} = -R_{321} = -R_{132},$$

$$R_{131} = R_{232} = -R_{311} = -R_{322}.$$

Discussion

It can be seen that the MTI is a general and powerful method that can be used not only in determining various polar and axial tensors of crystalline point groups but also in calculating property tensors of quasicrystalline classes. With the third-rank basis functions at hand, one can calculate the acoustic gyrotropic, acoustic electrogyration and third-order elastic tensors without any difficulty (Jiang, Liao & Chen, 1992b).

It can be observed that, for the Hall effect, the 26 quasicrystalline point groups can be divided into three categories.

(a) The point groups C_n , S_n and C_{nh} require three coefficients each, as do those in tetragonal, hexagonal and trigonal crystal systems.

(b) The point groups D_n , C_{nv} , D_{nh} and D_{nd} require two coefficients each, as do those in tetragonal, hexagonal and trigonal crystal systems.

(c) The two icosahedral point groups require only one coefficient each, as do those in cubic crystal systems.

The results summarized above can be understood on the basis of Ripamonti's (1987) conclusion that, for $n < N$, an n th-rank tensor, which is invariant under a cyclic rotation group C_N along a direction z , is actually isotropic about z , and that, if two (or more) directions of rotation symmetry C_N ($N > n$) exist for the symmetry group G , then the tensor is fully (*i.e.* in three dimensions) isotropic.

The results given in Table 3 can be extended to other tensors. For the point groups with fivefold, eightfold, tenfold and twelfold rotation axes, any one of the antisymmetric axial tensors of rank three, such as the magneto-optical tensor and the magnetic-field-induced force constant, has the same form as that given in Table 3.

Recently, experimental investigations of single decagonal quasicrystals (Al-Ni-Co, Al-Cu-Co, and Al-Si-Cu-Co) show that the anisotropy of the Hall coefficient is quite universal for these structures. Both the sign and the temperature dependence of $R_{\mu\nu\lambda}$ changes when the magnetic field rotates by 90° from the tenfold axis (Wang, Zhang & Chen, 1993). This can be explained not only on the basis of the macroscopic property tensor of the D_{10h} point group but also in the framework of the interaction of the Fermi surface with the quasi-Brillouin zone boundaries that are determined by the structural symmetry.

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X-ray Diffraction Profiles in Strained Crystals Undergoing Ultrasonic Excitation. The Laue Case

BY E. ZOLOTAYABKO AND B. SANDER

Department of Materials Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel

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Abstract

A new approach for the calculation of diffraction profiles in strained crystals is developed, based on the visual concepts of the dispersion surface and Poynting vectors. By this approach, analytical expressions have been obtained for diffraction profiles for the case of a constant strain gradient without, as well as with, ultrasonic excitation. Calculations of acoustically induced modifications in diffraction spectra explain in detail the anomalous dependence of integrated intensity on ultrasound amplitude, a dependence that was recently found in the Laue scattering geometry.

1. Introduction

The sensitivity of X-ray diffraction to static strain fields in single crystals is traditionally used to study lattice distortions related to crystal defects. Recently, attention has been given to X-ray diffraction under dynamic deformations created by high-frequency ultrasound (US) (Kohler, Mohling & Peibst, 1974; Entin, 1977, 1979; Entin & Assur, 1981; Chapman, Colella & Bray, 1983) as a result of the new possibilities of measuring weak US fields (Cerva & Graff, 1984; Andreev, Ponomarev & Smolin, 1988; Zolotoyabko, Panov & Schvarkov, 1993; Zolotoyabko, Jacobsohn, Shechtman, Kantor & Salzman, 1993) and of acoustically controlling X-ray beams in space and time (Kikuta, Takahashi & Nakatani, 1984; Kocharyan, Sukiasyan, Megrabyan & Sarkisyan, 1989;

Roshchupkin, Brunel, Bergevin & Erko, 1992). Moreover, it turns out that diffraction processes in the presence of combined static and dynamic deformation fields are of great interest, because of the high sensitivity of US-induced diffraction effects to small intrinsic strains in the samples. Few works (Entin, Khrupa & Datsenko, 1990; Khrupa, Entin & Datsenko, 1991; Zolotoyabko, Polikarpov, Panov & Schvarkov, 1992; Raranskii, Fodchuk, Novikov & Korovyanko, 1993) have been devoted to the development of new methods for the characterization of the structural quality of semiconductor crystals using the high sensitivity mentioned. The application of these methods is limited, however, by insufficient knowledge about diffraction phenomena in complex static and dynamic deformation fields in real crystals with defects and subsequent difficulties related to the interpretation of experimental data. A comprehensive analysis can be performed for crystals homogeneously bent by a constant strain gradient (Iolin, 1987; Iolin, Raitman, Kuvaldin & Zolotoyabko, 1988; Zolotoyabko & Panov, 1992; Chukhovskii, Nosik & Iolin, 1993). Even in this model case interesting effects such as a new type of *Pendellösung* fringe (Zolotoyabko & Panov, 1992) and the anomalous behaviour of the integrated diffraction intensity S (Iolin, Raitman, Kuvaldin & Zolotoyabko, 1988; Zolotoyabko & Panov, 1992) were observed under US excitation. These effects shed some light on the mechanisms of X-ray–acoustic interaction in strained crystals. For example, the anomalous behaviour of S consists of a substantial decrease (by up to 50%) of S