

Point Groups and Elastic Properties of Two-Dimensional Quasicrystals

CHENGZHENG HU, RENHUI WANG,* WENGE YANG AND DIHUA DING

Department of Physics, Wuhan University, Wuhan 430072, People's Republic of China

(Received 29 September 1994; accepted 10 October 1995)

Abstract

Possible point groups and elastic properties are discussed for a solid with two-dimensional quasiperiodic and one-dimensional periodic structures. The point groups and Laue classes are given for such structures with Fourier modulus of rank 5. The numbers of independent second-order elastic constants are calculated and all quadratic invariants are derived for all symmetries.

1. Introduction

An ever increasing number of structures with perfect order, but without lattice periodicity, have been found in the past decades. Such structures have been called quasiperiodic. In fact, lattice periodicity is a special case of quasiperiodicity in which the number of integer indices is equal to the dimension of the space. The symmetry description for a quasiperiodic structure (QS) may be given by an embedding into a higher-dimensional space (Bak, 1985; Janssen, 1986). In other words, a quasiperiodic structure in a d -dimensional subspace (the physical space) V_E can be obtained by intersecting this space with a lattice-periodic structure in an n -dimensional embedding space V , which is the direct sum of V_E and V_I . V_I is the orthogonal complement of the physical space. The symmetry groups for three-dimensional (3D) lattice periodic systems have been known for a long time (Hahn, 1983) and their generalizations to higher-dimensional spaces have been studied by a number of scientists. At present, all the symmetry groups have been discussed for $n = 4, 5, 6, 7, 8$ and 9 (Brown, Bulow, Neubuser, Wondratschek & Zassenhaus, 1978; Ryskov, 1972; Plesken & Pohst, 1980). Owing to the distinguished physical subspace, of course, the crystallography of a QS is not strictly the same as nD crystallography. This means that the symmetry groups describing QS are nD , satisfying appropriate additional requirements. Wijnands & Janssen (1993) formulated the additional conditions satisfied by nD crystallographic symmetry groups in order to allow QS. Rabson, Mermin, Rokhsar & Wright (1991) discussed the space groups of axial crystals and quasicrystals with N -fold point groups. Meanwhile, significant progress has also been made in studying the elasticity of quasicrystals. In the density wave picture for quasicrystals, the independent components of the phases can be parametrized by a

phonon field \mathbf{u} and a phason field \mathbf{w} . By standard elasticity theory, the elastic energy can be expressed as a function of gradients of these fields. The expression for the elastic energy of icosahedral quasicrystals and some simple planar quasicrystals have been derived to quadratic order in the fields (Levine *et al.*, 1985; Socolar, 1989).

In this paper, we would like to discuss point groups and elastic properties of all 2D quasicrystals. Here and hereafter, a 2D quasicrystal (QC) refers not to a real plane but to a 3D solid with 2D quasiperiodic and 1D periodic structure unless stated otherwise. Also, we restrict our discussion to 2D QCs with Fourier modulus of rank 5, *i.e.* the quasiperiodic plane of rank 4. This is the case for 2D QCs observed to date. Our work shows that there are ten systems and 57 point groups in this case, which can be divided into two kinds, one with crystallographically allowable operations (the first kind) and the other with crystallographically forbidden operations (the second kind). Six systems and 31 point groups belong to the first kind. The remaining four systems and 26 point groups belong to the second kind. Using group representation theory, we have calculated the numbers of independent elastic constants and the scalar invariants up to second order for all 2D QCs with Fourier modulus of rank 5. Every system with N -fold ($N > 2$) rotation can be divided into two Laue classes and the QCs belonging to the same Laue class possess the same elastic properties.

The following section is devoted to the point groups of 2D QCs. The invariants and elastic constants of 2D QCs are calculated in §3. Some discussions can be found in §4.

2. Point groups

The symmetry operations used for the description of 2D QCs with Fourier modulus of rank 5 can be derived from the crystallographic operations that act in a 5D space V with a 3D distinguished subspace (the physical space) V_E and the 2D orthogonal complement V_I satisfying some additional conditions (Janssen, 1992). Once the symmetry operations are determined, we can construct the point groups for 2D QCs by the group definition. Consider a 5D lattice Σ in V with its reciprocal lattice Σ^* . A crystallographic operation R that leaves Σ invariant acts on a basis b_i ($i = 1, 2, \dots, 5$) according to

$$Rb_i = \sum_{j=1}^5 \Gamma(R)_{ji} b_j \quad (i = 1, 2, \dots, 5). \quad (1)$$

The matrix $\Gamma(R)$ is integral and of finite order N . Its characteristic polynomial has a unique decomposition in prime factors:

$$f(\lambda) \equiv \det[\Gamma(R) - \lambda E] = \prod f_\mu(\lambda). \quad (2)$$

The roots $\exp(2\pi ip/m_\mu)$ of the prime polynomial $f_\mu(\lambda)$ correspond to eigenspaces which span the space V_μ , where m_μ is a divisor of the order N of $\Gamma(R)$ and p is relative prime to m_μ . Furthermore, we can construct a basis for V_μ that carries $\Gamma(R)$ with characteristic polynomial $f_\mu(\lambda)$. Following the notation used by Hermann (1949), R can now be written as

$$R \simeq \{m_1, m_2, \dots\}, \quad \sum_{\mu} E(m_\mu) = 5. \quad (3)$$

Its order N is the smallest common multiple of the m_μ 's and $E(m_\mu)$ is the Euler function. If R allows a quasi-periodic structure of rank 5 in V_E , R is a non-mixing operation and leaves V_E invariant; besides, the following conditions are satisfied: either V_i carries full spaces V_μ and every corresponding m_μ also occurs in the decomposition of V_E or an invariant subspace of V_μ belongs to V_i whereas the remaining 2D subspace belongs to V_E . All possible 5D crystallographic operations for 3D QCs with Fourier modulus of rank 5 are listed by Janssen (1992). From these operations, we can derive all the point groups of 2D QCs by the group definition provided we notice that in the 3D physical space the symmetry operations may be N -fold proper rotations or inversion rotations or mirrors.

For example, the point group $K_1 = 5$ (C_5) has the representation with

$$\Gamma(R) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (4)$$

The fivefold rotation R is the generator of K_1 , which is of type {15}. This means that the symmetry operation {15} can generate the point group 5. The point group $K_2 = 5m$ (C_{5v}) has the representation with

$$\Gamma(R_1) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Gamma(R_2) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (5)$$

The fivefold rotation R_1 and the mirror R_2 are the generators of K_2 . The former is of type {15} and the latter is of type {11122}. It follows that the symmetry operations {15} and {11122} can generate the point group $5m$. Similarly, the symmetry operations {15} and {21122} can generate the point group 52.

In this way, we can find all point groups of 2D QCs with Fourier modulus of rank 5. It should be noted, however, that a quasiperiodic structure is not necessary to be associated with non-crystallographic point-group symmetry (Janssen, 1992). Thus, it is possible for crystallographic symmetry groups to allow QS. This is the case for the cubic symmetry (Feng, Lu & Withers, 1989; Wang, Qin, Lu, Feng & Xu, 1994). Additionally, since a twofold rotation and a mirror may be along the quasiperiodic plane or the periodic axis, there are six point groups (2, 12, m , $1m$, $2/m$ and $12/m$) in the monoclinic case and four point groups (222 , $2mm$, $mm2$ and $2/mmm$) in the orthorhombic case, as contrasted with conventional crystals which have only three point groups for each system, monoclinic or orthorhombic. The point groups of 2D QCs with Fourier modulus of rank 5 are given in Table 1 (see Appendix A). There are ten systems, *i.e.* triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, pentagonal, decagonal, octagonal and dodecagonal systems, and 57 point groups. Among them, six systems and 31 point groups are crystallographically allowable, four systems and 26 point groups are crystallographically forbidden.

3. Elastic properties

In this section, we calculate the numbers of independent second-order elastic constants and quadratic invariants of 2D QCs with the group representation theory. As we know, to lowest order, the elastic energy density f is composed of quadratic combinations of gradients of the phonon field \mathbf{u} and the phason field \mathbf{w} . Since f is a scalar, these quadratic combinations are form-invariant under all of the point-group operations of the structure considered, *i.e.* they transform according to the identity representation of the group. Thus, if we construct all the invariants, we can determine f . Moreover, the number of such invariants and hence the number of independent elastic constants are just the number of times the identity representation appears in all possible direct product representations under which $\partial_j u_i$ and $\partial_j w_i$ transform. Here it should be noted that: (i) \mathbf{u} is a three-component field and \mathbf{w} is a two-component field; (ii) both \mathbf{u} and \mathbf{w} are only the function of the position vector $\mathbf{r} = (x_1, x_2, x_3)$ in

the physical space (De & Pelcovits, 1987); (iii) the coordinate system is chosen in such a way that the axis x_3 is along the periodic direction and the axes x_1, x_2, x_3 form an orthonormal basis; (iv) for crystallographic symmetries \mathbf{u} and \mathbf{w} , both transform according to the vector-like representation, but for non-crystallographic symmetries \mathbf{u} transforms according to the vector-like representation and \mathbf{w} transforms according to another non-vector-like representation.

It is obvious that all phonon strains $\partial_j u_i$ and phason strains $\partial_j w_i$ are centrosymmetric, *i.e.* under the action of the symmetry operation 'inversion' ($x_i \rightarrow -x_i$, and hence $u_i \rightarrow -u_i$, $w_i \rightarrow -w_i$, $\partial_i \rightarrow -\partial_i$) they remain to be unchanged. Therefore, elastic properties possess an intrinsic (or inherent) centrosymmetry, and hence all point groups belonging to the same Laue class (Hahn, 1983), *i.e.* those point groups that would become identical when a centre of symmetry is added to them, possess the same elastic properties. Tables 1 and 2 of the present paper are therefore arranged according to Laue classes.

The numbers n_C , n_K and n_R of independent elastic constants C_{ijkl} , K_{ijkl} and R_{ijkl} (Ding, Yang, Hu & Wang, 1993) for each Laue class have been calculated by the method proposed by Yang, Ding, Hu & Wang (1994) and listed in Table 1.

To determine the invariants, let us consider the point group $K = 5$ (C_5) generated by a fivefold rotation. Obviously, for the phonon field, nine components of $\partial_j u_i$ transform under

$$(\Gamma_1 + \Gamma_2) \times (\Gamma_1 + \Gamma_2) = 3\Gamma_1 + 2\Gamma_2 + \Gamma_3, \quad (6)$$

where Γ_1 is the identity representation, and Γ_2 and Γ_3 are two 2D representations. The former is the vector-like representation and the latter non-vector-like, but each of them is the direct sum of two 1D conjugate representations. Since the antisymmetric components $\partial_1 u_2 - \partial_2 u_1$, $\partial_2 u_3 - \partial_3 u_2$ and $\partial_3 u_1 - \partial_1 u_3$ transform under $\Gamma_1 + \Gamma_2$ corresponding to rigid rotations, they do not change the elastic energy. Associated with the remaining constituent representations are two linear invariants

$$E_{33}, \quad E_{11} + E_{22}, \quad (7)$$

and two quadratic invariants

$$(E_{11} - E_{22})^2 + 4E_{12}^2, \quad E_{13}^2 + E_{23}^2, \quad (8)$$

where $E_{ij} = (\partial_j u_i + \partial_i u_j)/2$. Thus, five quadratic invariants are

$$(E_{11} + E_{22})^2, \quad E_{33}^2, \quad E_{33}(E_{11} + E_{22}), \quad (9)$$

$$E_{13}^2 + E_{23}^2, \quad E_{11}E_{22} - E_{12}^2,$$

among which the first three are products of two linear invariants (7). From (9), it follows that non-vanishing elastic constants are

$$C_{1111} = C_{2222}, \quad C_{1133} = C_{2233}, \quad C_{3333}, \quad C_{2323} = C_{1313},$$

$$C_{1122}, \quad 2C_{1212} = C_{1111} - C_{1122}. \quad (10)$$

The number of independent constants $n_c = 5$. For the phason field, six components of $\partial_j w_i$ transform under

$$(\Gamma_1 + \Gamma_2) \times \Gamma_3 = \Gamma_2 + 2\Gamma_3 \quad (11)$$

producing five quadratic invariants, *i.e.*

$$(W_{21} + W_{12})^2 + (W_{11} - W_{22})^2,$$

$$W_{13}(W_{21} - W_{12}) + W_{23}(W_{11} + W_{22}),$$

$$W_{13}(W_{11} + W_{22}) - W_{23}(W_{21} - W_{12}), \quad (12)$$

$$W_{13}^2 + W_{23}^2,$$

$$(W_{11} + W_{22})^2 + (W_{21} - W_{12})^2,$$

where $W_{ij} = \partial_j w_i$. Non-vanishing elastic constants are

$$K_{1111} = K_{2222} = K_{1212} = K_{2121}, \quad K_{1313} = K_{2323},$$

$$K_{1113} = K_{1322} = K_{1223} = -K_{2123}, \quad K_{1221} = -K_{1122},$$

$$K_{1123} = K_{2223} = K_{1321} = -K_{1213}. \quad (13)$$

The number of independent constants $n_K = 5$. Moreover, there are six quadratic invariants coupling \mathbf{u} to \mathbf{w} , *i.e.*

$$2W_{13}E_{12} + W_{23}(E_{11} - E_{22}),$$

$$W_{13}(E_{11} - E_{22}) - 2W_{23}E_{12},$$

$$(W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}, \quad (14)$$

$$2(W_{11} + W_{22})E_{12} - (W_{21} - W_{12})(E_{11} - E_{22}),$$

$$(W_{21} + W_{12})E_{13} + (W_{11} - W_{22})E_{23},$$

$$(W_{21} + W_{12})E_{23} - (W_{11} - W_{22})E_{13}.$$

Non-vanishing elastic constants are

$$R_{1111} = R_{2211} = R_{2112} = -R_{2222} = -R_{1122} = -R_{1212},$$

$$R_{1112} = R_{1211} = R_{2122} = R_{2212} = -R_{1222} = -R_{2111},$$

$$R_{1223} = R_{2213} = R_{2123} = -R_{1113},$$

$$R_{1311} = -R_{1322} = -R_{2312}, \quad (15)$$

$$R_{1123} = R_{1213} = R_{2113} = -R_{2223},$$

$$R_{1312} = R_{2311} = -R_{2322}.$$

The number of independent constants $n_R = 6$. Thus, it can be seen that there are 16 quadratic invariants and hence 16 independent second-order elastic constants for $K = 5$ symmetry. Among them, five constants are due to the phonon field, five constants due to the phason field and six constants associated with the phonon-phason coupling.

In a similar manner, we can construct all invariants for all Laue classes of 2D QCs, as listed in Table 2 (see Appendix A), where those quadratic invariants that can be written as the product of linear invariants are omitted. From these results, one can easily obtain the expression for the elastic energy of 2D QCs.

4. Concluding remarks and discussion

We have given the point groups for 2D QCs with Fourier modulus of rank 5. It is shown that there are ten systems, 18 Laue classes and 57 point groups in this case. Since the structures with perfect order, but without lattice periodicity, may have crystallographically allowable symmetries, a 2D crystallographic point group also belongs to the point groups of 2D QCs. There are six systems, ten Laue classes and 31 point groups known to crystallography. The remaining four systems, eight Laue classes and 26 point groups are relevant for non-crystallographic symmetries. We have also calculated the numbers of independent second-order elastic constants and quadratic invariants for all Laue classes of 2D QCs. All the results are given in Appendix A.

In this paper, we have discussed only those 2D QCs with the quasiperiodic plane of rank 4. If rank 6 is

included, 7-, 9-, 14- and 18-fold axes are allowable (Hu, Ding, Yang & Wang, 1994). The extension of the above treatment to such structures is straightforward.

Brandmüller & Claus (1988) derived the forms of irreducible tensors of rank 1 to 4 without intrinsic symmetries for point groups $5, \bar{5}, \bar{10}, \bar{10}m2, 52, \bar{5}m$ and $5m$. However, they did not consider the phason strains in their derivation and hence the results are not appropriate for elastic properties of QCs. According to Brandmüller & Claus (1988), the numbers of independent components of the fourth-rank tensor without any intrinsic symmetry are 19, 19, 10 and 10 for the Laue classes $\bar{5}, 10/m, \bar{5}m$ and $10/mmm$, respectively. By considering the intrinsic symmetry for elastic constants C_{ijkl} ($= C_{jikl} = C_{ijlk} = C_{klij}$), all these numbers reduce to 5 and the corresponding non-vanishing C_{ijkl} are $C_{1111} = C_{2222}, C_{3333}, C_{1133} = C_{2233}, C_{1313} = C_{2323}, 2C_{1212} = C_{1111} - C_{1122}$. These results are in good agreement with our results ($n_C = 5$) for independent elastic constants C_{ijkl} related to the phonon strains as listed in Table 1 and equation (10) of the present paper.

This work was supported by the National Natural Science Foundation of China.

APPENDIX A

Table 1. Point groups, Laue classes and numbers of independent elastic constants of 2D QCs

System	No. of Laue classes	Point groups	No. of elastic constants			
			n_C	n_K	n_R	Sum
Triclinic	1	1, $\bar{1}$	21	21	36	78
Monoclinic	2	2, $m, 2/m$	13	13	20	46
	3	12, $1m, 12/m$	13	12	18	43
Orthorhombic	4	2mm, 222, mmm, mm2	9	8	10	27
Tetragonal	5	4, $\bar{4}, 4/m$	7	7	10	24
	6	4mm, 422, $\bar{4}m2, 4/mmm$	6	5	5	16
Trigonal	7	3, $\bar{3}$	7	7	12	26
	8	3m, 32, $\bar{3}m$	6	5	6	17
Hexagonal	9	6, $\bar{6}, 6/m$	5	5	8	18
	10	6mm, 622, $\bar{6}m2, 6/mmm$	5	4	4	13
Pentagonal	11	5, $\bar{5}$	5	5	6	16
	12	5m, 52, $\bar{5}m$	5	4	3	12
Decagonal	13	10, $\bar{10}, 10/m$	5	3	2	10
	14	10mm, 1022, $\bar{10}m2, 10/mmm$	5	3	1	9
Octagonal	15	8, $\bar{8}, 8/m$	5	5	2	12
	16	8mm, 822, $\bar{8}m2, 8/mmm$	5	4	1	10
Dodecagonal	17	12, $\bar{12}, 12/m$	5	5	0	10
	18	12mm, 1222, $\bar{12}m2, 12/mmm$	5	4	0	9

Table 2. Scalar invariants

No. of Laue classes	Phonon field	Phason field	Phonon-phason coupling
1	$E_{11}, E_{22}, E_{33}, E_{12}, E_{13}, E_{23}$,	$W_{11}, W_{22}, W_{13}, W_{23}, W_{12}, W_{21}$	
2	$E_{11}, E_{22}, E_{33}, E_{12}, E_{13}^2, E_{23}^2,$ $E_{13}E_{23}$	$W_{11}, W_{22}, W_{12}, W_{21}, W_{13}^2, W_{23}^2, W_{13}W_{23}$	$W_{13}E_{13}, W_{13}E_{23}, W_{23}E_{13}, W_{23}E_{23}$
3	$E_{11}, E_{22}, E_{33}, E_{23}, E_{12}^2, E_{13}^2,$ $E_{12}E_{13}$	$W_{11}, W_{22}, W_{23}, W_{13}^2, W_{12}^2, W_{21}^2, W_{13}W_{12},$ $W_{13}W_{21}, W_{12}W_{21}$	$W_{13}E_{12}, W_{13}E_{13}, W_{21}E_{12}, W_{21}E_{13}, W_{12}E_{12}, W_{12}E_{13}$

Table 2 (cont.)

No. of Laue classes	Phonon field	Phason field	Phonon-phason coupling
4	$E_{11}, E_{22}, E_{33}, E_{12}^2, E_{13}^2, E_{23}^2$	$W_{11}, W_{22}, W_{13}^2, W_{23}^2, W_{12}^2, W_{21}^2, W_{12}W_{21}$	$W_{12}E_{12}, W_{12}E_{12}, W_{13}E_{13}, W_{23}E_{23}$
5	$E_{33}, E_{11} + E_{22}, E_{12}^2, (E_{11} - E_{22})^2, E_{13}^2 + E_{23}^2, E_{12}(E_{11} - E_{22})$	$W_{11} + W_{22}, W_{21} - W_{12}, (W_{11} - W_{22})^2, (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} - W_{22})(W_{21} + W_{12})$	$W_{13}E_{13} + W_{23}E_{23}, W_{13}E_{23} - W_{23}E_{13}, (W_{11} - W_{22})E_{12}, (W_{11} - W_{22})(E_{11} - E_{22}), (W_{21} + W_{12})E_{12}, (W_{21} + W_{12})(E_{11} - E_{22})$
6	$E_{33}, E_{11} + E_{22}, (E_{11} - E_{22})^2, (E_{12} + E_{21})^2, E_{13}^2 + E_{23}^2$	$W_{11} + W_{22}, (W_{11} - W_{22})^2, (W_{21} + W_{12})^2, (W_{21} - W_{12})^2, W_{13}^2 + W_{23}^2$	$W_{13}E_{13} + W_{23}E_{23}, (W_{11} - W_{22})(E_{11} - E_{22}), (W_{21} + W_{12})E_{12}$
7	$E_{33}, E_{11} + E_{22}, 2E_{13}E_{12} + E_{23}(E_{11} - E_{22}), E_{13}(E_{11} - E_{22}) - 2E_{23}E_{12}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$W_{11} + W_{22}, (W_{21} - W_{12}), W_{13}^2 + W_{23}^2, (W_{21} + W_{12})^2 + (W_{11} - W_{22})^2, W_{13}(W_{21} + W_{12}) + W_{23}(W_{11} - W_{22}), W_{13}(W_{11} - W_{22}) - W_{23}(W_{21} + W_{12})$	$2(W_{21} + W_{12})E_{12} + (W_{11} - W_{22})(E_{11} - E_{22}), (W_{21} + W_{12})(E_{11} - E_{22}) - 2(W_{11} - W_{22})E_{12}, W_{13}E_{12} + W_{23}(E_{11} - E_{22}), W_{13}(E_{11} - E_{22}) - 2W_{23}E_{12}, W_{13}E_{13} + W_{23}E_{23}, W_{13}E_{23} - W_{23}E_{13}, (W_{21} + W_{12})E_{13} + (W_{11} - W_{22})E_{23}, (W_{21} + W_{12})E_{23} - (W_{11} - W_{22})E_{13}$
8	$E_{33}, E_{11} + E_{22}, 2E_{13}E_{12} + E_{23}(E_{11} - E_{22}), E_{11}E_{22} - E_{12}^2, E_{13}^2 + E_{23}^2$	$W_{11} + W_{22}, (W_{21} - W_{12})^2, W_{13}^2 + W_{23}^2, (W_{21} + W_{12})^2 + (W_{11} - W_{22})^2, W_{13}(W_{21} + W_{12}) + W_{23}(W_{11} - W_{22})$	$(W_{21} + W_{12})E_{13} + (W_{11} - W_{22})E_{23}, 2W_{13}E_{12} + W_{23}(E_{11} - E_{22}), 2(W_{21} + W_{12})E_{12} + (W_{11} - W_{22})(E_{11} - E_{22}), W_{13}E_{13} + W_{23}E_{23}$
9	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$W_{11} + W_{22}, W_{21} - W_{12}, W_{13}^2 + W_{23}^2, (W_{11} - W_{22})^2 + (W_{21} + W_{12})^2$	$(W_{11} - W_{22})(E_{11} - E_{22}) + 2(W_{21} + W_{12})E_{12}, 2(W_{11} - W_{22})E_{12} - (W_{21} + W_{12})(E_{11} - E_{22}), W_{13}E_{23} - W_{23}E_{13}, W_{13}E_{13} + W_{23}E_{23}$
10	$E_{33}, E_{11} + E_{22}, E_{11}E_{22} - E_{12}^2, E_{13}^2 + E_{23}^2$	$W_{11} + W_{22}, (W_{21} - W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} - W_{22})^2 + (W_{21} + W_{12})^2$	$(W_{11} - W_{22})(E_{11} - E_{22}) + 2(W_{21} + W_{12})E_{12}, W_{13}E_{13} + W_{23}E_{23}$
11	$E_{33}, E_{11} + E_{22}, E_{11}E_{22} - E_{12}^2, E_{13}^2 + E_{23}^2$	$(W_{11} + W_{22})^2 + (W_{21} - W_{12})^2, (W_{21} + W_{12})^2 + (W_{11} - W_{22})^2, W_{13}(W_{11} + W_{22}) - W_{23}(W_{21} - W_{12}), W_{13}(W_{21} - W_{12}) + W_{23}(W_{11} + W_{22}), W_{13}^2 + W_{23}^2$	$2W_{13}E_{12} + W_{23}(E_{11} - E_{22}), W_{13}(E_{11} - E_{22}) - 2W_{23}E_{12}, (W_{21} + W_{12})E_{13} + (W_{11} - W_{22})E_{23}, (W_{21} + W_{12})E_{23} - (W_{11} - W_{22})E_{13}, (W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}, 2(W_{11} + W_{22})E_{12} - (W_{21} - W_{12})(E_{11} - E_{22})$
12	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} + W_{22})^2 + (W_{21} - W_{12})^2, (W_{21} + W_{12})^2 + (W_{11} - W_{22})^2, W_{13}^2 + W_{23}^2, W_{13}(W_{21} - W_{12}) + W_{23}(W_{11} + W_{22})$	$2W_{13}E_{12} + W_{23}(E_{11} - E_{22}), (W_{21} + W_{12})E_{13} + (W_{11} - W_{22})E_{23}, (W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}$
13	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} + W_{22})^2 + (W_{21} - W_{12})^2, (W_{11} - W_{22})^2 + (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2$	$(W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}, 2(W_{11} + W_{22})E_{12} - (W_{21} - W_{12})(E_{11} - E_{22})$
14	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$W_{13}^2 + W_{23}^2, (W_{11} - W_{22})^2 + (W_{21} + W_{12})^2, (W_{11} + W_{22})^2 + (W_{21} - W_{12})^2$	$(W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}$
15	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} - W_{22})^2, (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} - W_{22})(W_{21} + W_{12}), (W_{11} + W_{22})^2 + (W_{21} - W_{12})^2$	$(W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}, 2(W_{11} + W_{22})E_{12} - (W_{21} - W_{12})(E_{11} - E_{22})$
16	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} - W_{22})^2, (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} + W_{22})^2 + (W_{21} - W_{12})^2$	$(W_{11} + W_{22})(E_{11} - E_{22}) + 2(W_{21} - W_{12})E_{12}$
17	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} - W_{22})^2, (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} + W_{22})^2 + (W_{21} - W_{12})^2, (W_{11} - W_{22})(W_{21} + W_{12})^2$	
18	$E_{33}, E_{11} + E_{22}, E_{13}^2 + E_{23}^2, E_{11}E_{22} - E_{12}^2$	$(W_{11} - W_{22})^2, (W_{21} + W_{12})^2, W_{13}^2 + W_{23}^2, (W_{11} + W_{22})^2 + (W_{21} - W_{12})^2$	

References

- Bak, P. (1985). *Phys. Rev. B*, **32**, 5764–5772.
 Brandmüller, J. & Claus, R. (1988). *Croat. Chem. Acta*, **61**, 267–300.
 Brown, H., Bulow, R., Neubuser, J., Wondratschek, H. & Zassenhaus, H. (1978). *The Crystallographic Groups of Four-Dimensional Space*. Dordrecht: Kluwer.
 De, P. & Pelcovits, P. A. (1987). *Phys. Rev. B*, **35**, 8609.
 Ding, D., Yang, W., Hu, C. & Wang, R. (1993). *Phys. Rev. B*, **48**, 7003–7010.

- Feng, Y., Lu, G. & Withers, R. L. (1989). *J. Phys. C*, **1**, 3695–3700.
- Hahn, T. (1983). *International Tables for Crystallography*, Vol. A. Boston: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- Hermann, C. (1949). *Acta Cryst.* **2**, 139–145.
- Hu, C., Ding, D., Yang, W. & Wang, R. (1994). *Phys. Rev. B*, **49**, 9423–9427.
- Janssen, T. (1986). *Acta Cryst.* **A42**, 261–271.
- Janssen, T. (1992). *Z. Kristallogr.* **198**, 17–32.
- Levine, D., Lubensky, T. C., Ostlund, S., Ramaswamy, S., Steinhardt, P. J. & Toner, J. (1985). *Phys. Rev. Lett.* **54**, 1520–1523.
- Plesken, W. & Pohst, M. (1980). *Math. Comput.* **34**, 245–258.
- Rabson, D. A., Mermin, N. D., Rokhsar, D. S. & Wright, D. C. (1991). *Rev. Mod. Phys.* **63**, 699–733.
- Ryskov, S. (1972). *Dokl. Akad. Nauk SSSR*, **204**, 561–564; Engl. transl: *Sov. Math. Dokl.* **13**, 720–724.
- Socolar, J. E. S. (1989). *Phys. Rev. B*, **39**, 10519–10551.
- Wang, R., Qin, C., Lu, G., Feng, Y. & Xu, S. (1994). *Acta Cryst.* **A50**, 366–375.
- Wijnands, F. & Janssen, T. (1993). *Acta Cryst.* **A49**, 315–324.
- Yang, W., Ding, D., Hu, C. & Wang, R. (1994). *Phys. Rev. B*, **49**, 12656–12661.