International Tables for Crystallography (2006). Vol. D, Section 1.10.3, pp. 247–249.

$$\Gamma^*(A) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\Gamma^*(B) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}. \qquad (1.10.2.7)$$

Moreover, there is the central inversion $-E$. The six-dimensional representation of the symmetry group, which is the icosahedral group $\bar{5}\bar{3}m$, is reducible into the sum of two nonequivalent three-dimensional irreducible representations. A basis for this representation in the six-dimensional space is then given by

$$\begin{matrix} (\mathbf{a}_1^*, c\mathbf{a}_1^*) & (\mathbf{a}_2^*, -c\mathbf{a}_2^*) & (\mathbf{a}_3^*, -c\mathbf{a}_4^*) \\ (\mathbf{a}_4^*, -c\mathbf{a}_6^*) & (\mathbf{a}_5^*, -c\mathbf{a}_3^*) & (\mathbf{a}_6^*, -c\mathbf{a}_5^*), \end{matrix} \qquad (1.10.2.8)$$

which projects on the given basis in V_E.

The point-group elements considered here are pairs of orthogonal transformations in physical and internal space. Orthogonal transformations that do not leave these two spaces invariant have not been considered. The reason for this is that the information about the reciprocal lattice comes from its projection on the Fourier module in physical space. By changing the length scale in internal space one does not change the projection but one would break a symmetry that mixes the two spaces. Nevertheless, quasicrystals are often described starting from an n-dimensional periodic structure with a lattice of higher symmetry. For example, the icosahedral 3D Penrose tiling can be obtained from a structure with a hypercubic six-dimensional lattice. Its reciprocal lattice is that spanned by the vectors (1.10.2.8) where one puts $c = 1$. The symmetry of the periodic structure, however, is lower than that of the lattice and has a point group in reducible form. Therefore, we shall consider here only reducible point groups, subgroups of the orthogonal group $O(n)$ which have a d-dimensional invariant subspace, identified with the physical space.

The fact that the spaces V_E and V_I are usually taken as mutually perpendicular does not have any physical relevance. One could as well consider oblique projections of a reciprocal lattice Σ^* on V_E. What is important is that the intersection of the periodic structure with the physical space should be the same in all descriptions. The metric in internal space V_I follows naturally from the fact that there is a finite group K_I.

1.10.2.3. *Superspace groups*

The quasiperiodic function $\rho(\mathbf{r})$ in d dimensions can be embedded as lattice periodic function $\rho_s(\mathbf{r}_s)$ in n dimensions. The symmetry group of the latter is the group of all elements g (1.10.2.4) for which

$$\rho_s(\mathbf{r}_s) = \rho_s(g\mathbf{r}_s) = \rho_s(R_E\mathbf{r} + \mathbf{a}_E, R_I\mathbf{r}_I + \mathbf{a}_I). \qquad (1.10.2.9)$$

This group is an n-dimensional space group G. It has an invariant subgroup of translations, which is formed by the lattice translations Σ, and the quotient G/Σ is isomorphic to the n-dimensional point group K. However, not every n-dimensional space group can occur here because we made the restriction to reducible point groups. For example, the n-dimensional hypercubic groups do not occur in this way as symmetry groups of quasiperiodic systems.

The product of two superspace group elements is

$$\{R_{s1}|\mathbf{a}_{s1}\}\{R_{s2}|\mathbf{a}_{s2}\} = \{R_{s1}R_{s2}|\mathbf{a}_{s1} + R_{s1}\mathbf{a}_{s2}\}. \qquad (1.10.2.10)$$

On a lattice basis for Σ, the orthogonal transformations R_{s1} and R_{s2} are integer $n \times n$ matrices and the translations $\mathbf{a}_{s1}$ and $\mathbf{a}_{s2}$ are column vectors. The orthogonal transformations R_s leave the origin invariant. The translations depend on the choice of this origin. For a symmorphic space group there is a choice of origin such that the translations a are lattice translations.

The point-group elements are reducible, which means that in the physical space one has the usual situation. If $d = 3$ then the only intrinsic nonprimitive translations are those in screw axes or glide planes. An n-dimensional orthogonal transformation can always be written as the sum of a number r of two-dimensional rotations with rotation angle different from π, a p-dimensional total inversion and a q-dimensional identity transformation. The integers r, p, q may be zero and $2r + p + q = n$. The possible intrinsic nonprimitive translations belong to the q-dimensional space in which the identity acts. For the three examples in the previous section, the internal component of the nonprimitive translation for m_x and m_y in the first example can be different from zero, but that for m_z in the same example is zero. For the octagonal case, only the second generator can have an intrinsic nonprimitive translation in the fourth direction, and for the icosahedral case the two generators have one two-dimensional invariant plane and one pointwise invariant line in V_I.

In the diffraction pattern of an IC phase one can distinguish between main reflections and satellites. A symmetry operation cannot transform a main reflection into a satellite. This implies that for these structures the reciprocal lattice of the basic structure is left invariant by the point group, and consequently the latter must be a three-dimensional crystallographic point group. Therefore, the point groups for IC phases are the same as those for lattice periodic systems. They act in superspace as a representation of a three-dimensional crystallographic point group. This is not true for an arbitrary quasiperiodic structure. The restriction in the general case comes from the requirement that the three-dimensional point group must have a faithful integer matrix representation in superspace. There is a mathematical statement to the effect that the lowest dimension in which a p-fold rotation can be represented as an integer matrix is given by the Euler function, the number of integers smaller than p that do not divide p. For example, for a prime number p this number is $p - 1$. This implies that if one restricts the rank of the Fourier module (*i.e.* the dimension of the superspace) to six, only values 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14 and 18 are possible for p. The values 7, 9, 14 and 18 only occur for two-dimensional quasiperiodic structures of rank six. Therefore, the allowable three-dimensional point groups for systems up to rank six are limited to the groups given in Table 1.10.2.1. The possible superspace groups for IC modulated phases of rank four are given in Chapter 9.8 of Volume C of *International Tables* (1999). Superspace groups for quasicrystals of rank $n \leq 6$ are given in Janssen (1988).

The notation of higher-dimensional symmetry groups is discussed in two IUCr reports (Janssen *et al.*, 1999, 2002).

1.10.3. Action of the symmetry group

1.10.3.1. *Action of superspace groups*

The action of the symmetry group on the periodic density function ρ_s in n dimensions is given by (1.10.2.9). The real physical structure, however, lives in physical space. One can derive from the action of the superspace group on the periodic structure its action on the quasiperiodic d-dimensional one. One knows that the density function in V_E is just the restriction of that in V_s. The same holds for the transformed function.

$$g\rho_s(\mathbf{r}_s) = \rho_s(g^{-1}\mathbf{r}_s) \rightarrow g\rho(\mathbf{r}) = \rho_s[R^{-1}(\mathbf{r} - \mathbf{a}_E), -R_I^{-1}\mathbf{a}_I]. \tag{1.10.3.1}$$

This transformation property differs from that under an n-dimensional Euclidean transformation by the 'phase shift' $-R_I^{-1}\mathbf{a}_I$. Take for example the IC phase with a sinusoidal modulation. If the positions of the atoms are given by

$$\mathbf{n} + \mathbf{r}_j + \mathbf{A}_j \cos(2\pi\mathbf{Q} \cdot \mathbf{n} + \varphi_j),$$

then the transformed positions are

$$R(\mathbf{n} + \mathbf{r}_j) + R\mathbf{A}_j \cos(2\pi\mathbf{Q} \cdot \mathbf{n} + \varphi_j - R_I^{-1}\mathbf{a}_I) + \mathbf{a}_E. \tag{1.10.3.2}$$

If the transformation g is a symmetry operation, this means that the original and the transformed positions are the same.

$$R(\mathbf{n} + \mathbf{r}_j) + \mathbf{a}_E = \mathbf{n}' + \mathbf{r}_{j'}$$

and

$$R\mathbf{A}_j \cos(2\pi\mathbf{Q} \cdot \mathbf{n} + \varphi_j - R_I^{-1}\mathbf{a}_I) = \mathbf{A}_{j'} \cos(2\pi\mathbf{Q} \cdot \mathbf{n}' + \varphi_{j'}).$$

This puts, in general, restrictions on the modulation.

Another view of the same transformation property is given by Fourier transforming (1.10.2.9). The result for the Fourier transform is

$$g\hat{\rho}_s(\mathbf{k}_s) = \hat{\rho}_s(R_s^{-1}\mathbf{k}_s) \exp(-i\mathbf{k}_s \cdot \mathbf{a}_s) \tag{1.10.3.3}$$

and because there is a one-to-one correspondence between the vectors $\mathbf{k}_s$ in the reciprocal lattice and the vectors $\mathbf{k}$ in the Fourier module one can rewrite this as

$$g\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{a}_E - \mathbf{k}_I \cdot \mathbf{a}_I). \tag{1.10.3.4}$$

For a symmetry element one has $g\hat{\rho}(\mathbf{k}) = \hat{\rho}(\mathbf{k})$. Therefore, the superspace group element g is a symmetry transformation of the quasiperiodic function ρ if

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{a}_E - \mathbf{k}_I \cdot \mathbf{a}_I). \tag{1.10.3.5}$$

This relation is at the basis of the *systematic extinctions*. If one has an orthogonal transformation R such that this in combination with a translation $(\mathbf{a}_E, \mathbf{a}_I)$ is a symmetry element and such that $R\mathbf{k} = \mathbf{k}$, then

$$\hat{\rho}(\mathbf{k}) = 0 \;\; \text{if} \;\; \mathbf{k} \cdot \mathbf{a}_E + \mathbf{k}_I \cdot \mathbf{a}_I \neq 2\pi \times \text{ integer}. \tag{1.10.3.6}$$

Because the structure factor is the Fourier transform of a density function which consists of δ functions on the positions of the atoms, for a quasiperiodic crystal it is the Fourier transform of a quasiperiodic function $\rho(\mathbf{r})$. Therefore, symmetry-determined absence of Fourier components leads to zero intensity of the corresponding diffraction peaks. Therefore, although there is no lattice periodicity for aperiodic crystals, systematic extinctions follow in the same way from the symmetry as in lattice periodic systems if one considers the n-dimensional space group as the symmetry group.

1.10.3.2. *Compensating gauge transformations*

The transformation property of the Fourier transform of the density given in the previous section can be formulated in another way. Consider a function $\rho(\mathbf{r})$ which is invariant under a d-dimensional Euclidean transformation $\{R|\mathbf{a}\}$ in physical space. Then its Fourier transform satisfies

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{a}). \tag{1.10.3.7}$$

Conversely, if the Fourier transform satisfies this relation, the Euclidean transformation is a symmetry operation for $\rho(\mathbf{r})$. The two equations (1.10.3.5) and (1.10.3.7) are closely related. One can also write (1.10.3.5) as

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{a}) \exp[i\Phi(R, \mathbf{k})], \tag{1.10.3.8}$$

where $\Phi(R, \mathbf{k})$ can be considered as a gauge transformation that compensates for the phase shift: it is a *compensating gauge transformation*. It is a function that is linear in $\mathbf{k}$,

$$\Phi(R, \mathbf{k} + \mathbf{k}') = \Phi(R, \mathbf{k}) + \Phi(R, \mathbf{k}') \;(\text{mod } 2\pi), \tag{1.10.3.9}$$

and satisfies a relation closely related to the one satisfied by nonprimitive translations.

$$\Phi(R, \mathbf{k}) + \Phi(S, R\mathbf{k}) = \Phi(RS, \mathbf{k}) \;(\text{mod } 2\pi). \tag{1.10.3.10}$$

[Recall that a system of nonprimitive translations $\mathbf{u}(R)$ satisfies $\mathbf{u}(R) + R\mathbf{u}(S) = \mathbf{u}(RS)$ modulo lattice translations.] Therefore, the Euclidean transformation $\{R|\mathbf{a}\}$ combined with the compensating gauge transformation with gauge function $\Phi(R, \mathbf{k})$ is a symmetry transformation for $\rho(\mathbf{r})$ if equation (1.10.3.8) is satisfied. This is a three-dimensional formulation of the superspace group symmetry relation (1.10.3.5).

Table 1.10.2.1. *Allowable three-dimensional point groups for systems up to rank six*

Isomorphism class	Order	Three-dimensional point groups
C_1	1	1
C_2	2	$2, \bar{1}, m$
C_3	3	3
C_4	4	$4, \bar{4}$
C_5	5	5
C_6	6	$6, \bar{6}, \bar{3}$
C_8	8	$8, \bar{8}$
C_{10}	10	$10, \overline{10}, \bar{5}$
C_{12}	12	$12, \overline{12}$
D_2	4	$222, 2/m, 2mm$
D_3	6	$32, 3m$
D_4	8	$422, 4mm, \bar{4}2m$
D_5	10	$52, 5m$
D_6	12	$622, \bar{3}m, 6mm, \bar{6}2m$
D_8	16	$822, 8mm, \bar{8}2m$
D_{10}	20	$10\,22, 10\,mm, \overline{10}\,2m, \bar{5}m$
D_{12}	24	$12\,22, 12\,mm, \overline{12}\,2m$
$C_4 \times C_2$	8	$4/m$
$C_6 \times C_2$	12	$6/m$
$C_8 \times C_2$	16	$8/m$
$C_{10} \times C_2$	20	$10/m$
$C_{12} \times C_2$	24	$12/m$
$D_2 \times C_2$	8	mmm
$D_4 \times C_2$	16	$4/mmm$
$D_6 \times C_2$	24	$6/mmm$
$D_8 \times C_2$	32	$8/mmm$
$D_{10} \times C_2$	40	$10/mmm$
$D_{12} \times C_2$	48	$12/mmm$
T	12	23
O	24	$432, \bar{4}3m$
I	60	532
$T \times C_2$	24	$m\bar{3}$
$O \times C_2$	48	$m\bar{3}m$
$I \times C_2$	120	$\bar{5}\bar{3}m$

1.10.3.3. *Irreducible representations of three-dimensional space groups*

A third way to describe the symmetry of a quasiperiodic function is by means of irreducible representations of a space group. For the theory of these representations we refer to Chapter 1.2 on representations of crystallographic groups.

Consider first a modulated IC phase. Suppose the positions of the atoms are given by

$$\mathbf{n} + \mathbf{r}_j + \mathbf{u}_{\mathbf{n}j}, \tag{1.10.3.11}$$

where $\mathbf{n}$ belongs to the lattice, $\mathbf{r}_j$ is a position inside the unit cell and $\mathbf{u}_{\mathbf{n}j}$ is a displacement. If the structure is quasiperiodic with

Fourier module M^*, the vectors $\mathbf{u}_{\mathbf{n}j}$ can be written as a superposition of normal modes.

$$\mathbf{u}_{\mathbf{n}j} = \sum_{\mathbf{k}\in M^*,\nu} Q_{k\nu}\boldsymbol{\varepsilon}(\mathbf{k}\nu|j)e^{i\mathbf{k}\cdot\mathbf{n}} + c.c., \qquad (1.10.3.12)$$

where the coefficient $Q_{\mathbf{k}\nu}$ is a normal coordinate, ν denotes the band index and $\boldsymbol{\varepsilon}(\mathbf{k}\nu|j)$ denotes the polarization of the normal mode. The normal coordinates transform under a space group according to one of its irreducible representations. The relevant space group here is that of the basic structure. For the simple case of a one-dimensional irreducible representation, for each $\mathbf{k}$ the effect is simply multiplication by a factor of absolute value unity. For example, for the modulated phase with basic space group $Pcmn$ and wavevector $\mathbf{k} = \gamma\mathbf{c}^*$ there are four non-equivalent one-dimensional representations. It depends on the band index which representation occurs in the decomposition. The space-group element $\{R|\mathbf{a}\}$, for which $R\mathbf{q} = \mathbf{q}$ (modulo reciprocal lattice) acts on $Q_{\mathbf{k}\nu}$ according to

$$Q_{\mathbf{k}\nu} \to Q_{\mathbf{k}\nu}\exp(i\mathbf{k}.\cdot\mathbf{a})\chi_\nu(R),$$

where $\chi_\nu(R)$ is the character of R in an irreducible representation associated with the branch ν. Because the character of a one-dimensional representation is of absolute value unity, one may write it as $\exp[i\varphi_\nu(R,\mathbf{k})]$. Consequently, if the decomposition of the displacement contains only the vectors $\pm\mathbf{k}$, the factor $\exp[i\varphi_\nu(R,\mathbf{k})]$ describes a shift in the modulation function.

Consider again as an example a basic structure with space group $Pcmn$ and a modulation wavevector $\gamma\mathbf{c}^*$. The point group $K_{\mathbf{k}}$ that leaves the modulation wavevector invariant is generated by m_y and m_x. This point group $mm2$ has four elements and four irreducible representations, all one-dimensional. One of them has for the character $\chi(m_x) = +1$, $\chi(m_y) = -1$. If the displacements of the atoms are described by a normal mode belonging to this irreducible representation, then the compensating phase shifts for c_x and m_y are, respectively, 0 and π. In the notation for superspace groups, this is the group $Pcmn(00\gamma)1s\bar{1}$. The same structure can be described by the irreducible representation characterized as Δ_3, because the modulation wavevector is the point Δ in the Brillouin zone and the irreducible representation Γ_3 has the character mentioned above.

In this way there is a correspondence between superspace groups for $(3+1)$-dimensional modulated structures and two-dimensional irreducible representations of three-dimensional space groups.

1.10.4. Tensors

1.10.4.1. *Tensors in higher-dimensional spaces*

A vector in an n-dimensional space V transforms under an element of a point group as $\mathbf{r} \to R\mathbf{r}$. With respect to a basis $\mathbf{a}_i$, the coordinates and basis vectors transform according to

$$\mathbf{a}'_i = \sum_{j=1}^n R_{ji}\mathbf{a}_j$$

$$\mathbf{r} = \sum_{i=1}^n x_i\mathbf{a}_i \to \mathbf{r}' = \sum_{i=1}^n x'_i\mathbf{a}_i, \quad x'_i = \sum_{j=1}^n R_{ij}x_j$$

and the reciprocal basis vectors and coordinates in reciprocal space according to

$$\mathbf{a}^*_i = \sum_{j=1}^n R_{ij}\mathbf{a}^{*'}_j$$

$$\mathbf{k} = \sum_{i=1}^n \kappa_i\mathbf{a}^*_i \to \mathbf{k}' = \sum_{i=1}^n \kappa'_i\mathbf{a}^*_i, \quad \kappa'_i = \sum_{j=1}^n R^{-1}_{ji}\kappa_j.$$

With respect to an orthonormal basis in V the transformations are represented by orthogonal matrices. For orthogonal matrices $R^{-1} = R^T$, the vectors in reciprocal space transform in exactly the same way as in direct space:

$$\mathbf{r} = \sum_{i=1}^n x_i\mathbf{e}_i \to \mathbf{r}' = \sum_{i=1}^n x'_i\mathbf{e}_i \quad x'_i = \sum_{i=1}^n R_{ij}x_i$$

$$\mathbf{k} = \sum_{i=1}^n \kappa_i\mathbf{e}^*_i \to \mathbf{k}' = \sum_{i=1}^n \kappa'_i\mathbf{e}^*_i \quad \kappa'_i = \sum_{i=1}^n R_{ij}\kappa_j.$$

As discussed in Section 1.2.4, a tensor is a multilinear function of vectors and reciprocal vectors. Consider for example a tensor of rank two, the metric tensor g. It is a function of two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ which results in the scalar product of the two.

$$g(\mathbf{r}_1,\mathbf{r}_2) = \mathbf{r}_1\cdot\mathbf{r}_2.$$

It clearly is a symmetric function because $g(\mathbf{r}_1,\mathbf{r}_2) = g(\mathbf{r}_2,\mathbf{r}_1)$. It is a function that is linear in each of its arguments and therefore

$$g(\mathbf{r}_1,\mathbf{r}_2) = g\left(\sum_{i=1}^n x_i\mathbf{e}_i, \sum_{j=1}^n y_j\mathbf{e}_j\right) = \sum_{ij} x_iy_j\delta_{ij} = \sum_i x_iy_j$$

if x_i and y_j are Cartesian coordinates of $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. For another basis, for example a lattice basis, one has coordinates ξ_i and η_j, and the same function becomes

$$g(\mathbf{r}_1,\mathbf{r}_2) = g\left(\sum_{i=1}^n \xi_i\mathbf{a}_i, \sum_{j=1}^n \eta_j\mathbf{a}_j\right) = \sum_{ij}\xi_i\eta_jg_{ij} \qquad (1.10.4.1)$$

with $g_{ij} = g(\mathbf{a}_i,\mathbf{a}_j)$. The relation between the Cartesian tensor components and the lattice tensor components follows from the basis transformation from orthonormal to a lattice basis. If

$$\mathbf{a}_j = \sum_k S_{kj}\mathbf{e}_k, \qquad (1.10.4.2)$$

then the lattice tensor components are

$$g_{ij} = \sum_k S_{ki}S_{kj}.$$

For example, in the two-dimensional plane a lattice spanned by $a(1,0)$ and $a(-\frac{1}{2},\frac{1}{2}\sqrt{3})$ has a basis obtained from an orthonormal basis by the basis transformation

$$S = a\begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{1}{2}\sqrt{3}\end{pmatrix}$$

and consequently the tensor components in lattice coordinates are

$$g_{ij} = \begin{pmatrix} a^2 & -\frac{1}{2}a^2 \\ -\frac{1}{2}a^2 & a^2\end{pmatrix}.$$

The transformation of the tensor g under an orthogonal transformation follows from its definition. The transformation of the Cartesian tensor under the orthogonal transformation R is

$$g'_{ij} = \sum_{kl} R_{ki}R_{lj}g_{kl} = \sum_{kl} R_{ki}R_{lj}\delta_{kl} = \delta_{ij}$$

because of the fact that the matrix R_{ij} is orthogonal. The transformation of the tensor components with respect to the lattice basis, on which R is given by $\Gamma(R)$, is

$$g'_{ij} = \sum_{kl}\Gamma(R)_{ki}\Gamma(R)_{lj}g_{kl}, \qquad (1.10.4.3)$$

or in matrix form $g' = \Gamma(R)^Tg\Gamma(R)$.

The metric tensor is invariant under a point group K if

$$g_{ij} = \sum_{kl}\Gamma(R)_{ki}\Gamma(R)_{lj}g_{kl} \quad \forall\, R\in K. \qquad (1.10.4.4)$$

references