International Tables for Crystallography (2006). Vol. D, Section 1.10.4, pp. 249–255.

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

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

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

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

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 $\mathbf{r} \rightarrow R\mathbf{r}$. With respect to a basis $\mathbf{a}_i$, the coordinates and basis vectors transform according to

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

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

The metric tensor is invariant under a point group K if

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

On the one hand this formula can be used to determine the symmetry of a lattice with metric tensor g and on the other hand one may use it to determine the general form of a metric tensor invariant under a given point group. This comes down to the determination of the free parameters in g for given group of matrices $\Gamma(K)$. These are the coordinates in the space of invariant tensors.

1.10.4.2. *Tensors in superspace*

The tensors occurring for quasiperiodic structures are defined in a higher-dimensional space, but this space contains as privileged subspace the physical space. Since physical properties are measured in this physical space, the coordinates are not all on the same footing. This implies that sometimes one has to make a distinction between the various tensor elements as well.

The distinction between physical and internal (or perpendicular) coordinates can be made explicit by using a *split basis*. This is a basis for the superspace such that the first d basis vectors span the physical subspace and the other $n-d$ basis vectors the internal space. A lattice basis is, generally, not a split basis.

Let us consider again the metric tensor which is used to characterize higher-dimensional lattices as well, and in particular those corresponding to quasiperiodic structures. The elements $g_{ij} = g(\mathbf{a}_i, \mathbf{a}_j)$ transform according to

$$g'_{ij} = g(\mathbf{a}'_i, \mathbf{a}'_j) = \sum_{kl} R_{ki} R_{lj} g_{kl}.$$

The symmetry of an n-dimensional lattice with metric tensor g is the group of nonsingular $n \times n$ integer matrices S satisfying

$$g = S^T g S, \qquad (1.10.4.5)$$

where ^{T} means the transpose. For a lattice corresponding to a quasiperiodic structure, this group is reducible into a d- and an $(n-d)$-dimensional component, where d is the dimension of physical space. This means that the d-dimensional component, which forms a finite group, is equivalent with a d-dimensional group of orthogonal transformations. In general, however, this does not leave a lattice in physical space invariant. However, it leaves the Fourier module of the quasiperiodic structure invariant. The basis vectors, for which the metric tensor determines the mutual relation, belong to the higher-dimensional superspace. Therefore, in this case the external and internal components of the basis vectors do not need to be treated differently. For the metric tensor g on a split basis one has

$$g_{ij} = 0 \quad \text{if} \;\; i \le d, j > d \;\; \text{or} \;\; i > d, j \le d.$$

A quasiperiodic structure has an n-dimensional lattice embedding such that the intersection of Σ with the physical space V_E does not contain a d-dimensional lattice. Because of the incommensurability, however, there are lattice points of Σ arbitrarily close to V_E. This means that by an arbitrarily small shear deformation one may get a lattice in the physical space. The deformed quasiperiodic structure then becomes periodic. In general, the symmetry of the lattice then changes. This is certainly the case if the point group of the quasiperiodic structure is noncrystallographic, because then there cannot be a lattice in physical space left invariant by such a point group. For a given lattice Σ with symmetry group K one may ask which subgroups allow a deformation of the lattice that gives periodicity in V_E.

Physical tensors give often relations between vectorial or tensorial properties. Then they are multilinear functions of p vectors (and possibly q reciprocal vectors). An example is the dielectric tensor ε that gives the relation between E and D fields. This relation and the corresponding expression for the free energy F are

$$D_i = \sum_j \varepsilon_{ij} E_j \;\; \text{or} \;\; F = \sum_{ij} E_i \varepsilon_{ij} E_j = \varepsilon(\mathbf{E}, \mathbf{E}). \qquad (1.10.4.6)$$

Therefore, the ε tensor is a bilinear function of vectors. The difference from the metric tensor is that here the vectors E and D are physical quantities which have d components and lie in physical space. The transformation properties therefore only depend on the physical-space components R_E of the superspace point group, and not on the full transformations R.

An intermediate case occurs for the strain. The strain tensor S gives the relation between a displacement and its origin: the point $\mathbf{r}$ is displaced to $\mathbf{r} + \Delta\mathbf{r}$ with $\Delta\mathbf{r}$ linear in $\mathbf{r}$:

$$\Delta\mathbf{r}_i = \sum_j S_{ij} \mathbf{r}_j.$$

In ordinary elasticity, both $\mathbf{r}$ and $\Delta\mathbf{r}$ belong to the physical space, and the relevant tensor is the symmetric part of S:

$$\tfrac{1}{2}(\partial_i \Delta\mathbf{r}_j + \partial_j \Delta\mathbf{r}_i).$$

For a quasiperiodic structure, $\Delta\mathbf{r}$ may be either a vector in physical space or in superspace and may depend both on physical and internal coordinates. That means that the matrix σ is either $d \times d$, or $n \times d$ or $n \times n$. Displacements in physical space are said to affect the *phonon degrees of freedom*, those in internal space the *phason degrees of freedom*. The phonon and phason displacements are functions of the physical-space coordinates. The transformation of the strain tensor under an element of a superspace group is

$$S'_{ij} = \sum_{k=1}^{d} \sum_{l=1}^{d} R_{Eki} R_{Elj} S_{kl} \;\; \text{for phonon degrees,}$$

$$S'_{ij} = \sum_{k=d+1}^{n} \sum_{l=1}^{d} R_{Iki} R_{Elj} S_{kl} \;\; \text{for phason degrees,}$$

$$S'_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{n} R_{ski} R_{slj} S_{kl} \;\; \text{for the general case.}$$

The first two of these expressions apply only to a split basis, but the third can be written on a lattice basis.

$$\sum_{k,l=1}^{n} \Gamma(R)_{ki} \Gamma(R)_{lj} S_{kl}. \qquad (1.10.4.7)$$

The tensor of elastic stiffnesses c gives the relation between stress T and strain S. The stress tensor is a physical tensor of rank two and dimension three. For the phonon strain one has

$$S_{ij} = \sum_{kl}^{3} c_{ijkl} T_{kl}, \quad (i,j = 1, \ldots, 3). \qquad (1.10.4.8)$$

The phonon part of the elasticity tensor is symmetric under interchange of ij and kl, i and j, and k and l. It can be written in the usual notation $c_{\mu\nu}$ with $\mu, \nu = 1, 2, \ldots, 6$ with $1 = (11)$, $2 = (22)$, $3 = (33)$, $4 = (23)$, $5 = (13)$, $6 = (12)$. Its transformation property under a three-dimensional orthogonal transformation is

$$c'_{ijkl} = \sum_{i'j'k'l'} R_{i'i} R_{j'j} R_{k'k} R_{l'l} c_{i'j'k'l'}.$$

For the phason part a similar elasticity tensor is defined. This and the third elastic contribution, the coupling between phonons and phasons, will be discussed in Section 1.10.4.5.

1.10.4.3. *Inhomogeneous tensors*

A vector field in d-dimensional space assigns a vector to each point of the space. This vector-valued function may, for a quasiperiodic system, have values in physical space or in superspace. In both cases one has the transformation property

$$g\mathbf{f}_i(\mathbf{r}) = \sum_j R_{ji}\mathbf{f}_j(g^{-1}\mathbf{r}). \quad (1.10.4.9)$$

For a vector field in physical space, i and j run over the values 1, 2, 3. This vector field may, however, be quasiperiodic. This means that it may be embedded in superspace. Then

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=1}^{3} R_{Eji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big]. \quad (1.10.4.10)$$

Here $i = 1, 2, 3$. If the vector field has values in superspace, as one can have for a displacement, one has

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=1}^{n} R_{sji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big]. \quad (1.10.4.11)$$

Here $i = 1, \ldots, n$. For Cartesian coordinates with respect to a split basis, R_s acts separately on physical and internal space and one has

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=d+1}^{n} R_{Iji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big] \quad (1.10.4.12)$$

for $i = d+1, \ldots, n$.

Just as for homogeneous tensors, inhomogeneous tensors may be divided into physical tensors with components in physical space only and others that have components with respect to an n-dimensional lattice. A physical tensor of rank two transforms under a space-group element $g = \{R_s|\mathbf{a}_s\}$ as

$$(gT)_{ij}(\mathbf{r}_s) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}[R_E^{-1}(\mathbf{r}_E-\mathbf{a}_E), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)]. \quad (1.10.4.13)$$

This implies the following transformation property for the Fourier components:

$$(g\hat{T})_{ij}(\mathbf{k}) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}(R_E^{-1}\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \quad (1.10.4.14)$$

This gives relations between various Fourier components and restrictions for wavevectors $\mathbf{k}$ for which $R_E\mathbf{k} = \mathbf{k}$:

$$\hat{T}_{ij}(\mathbf{k}) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}(\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \quad (1.10.4.15)$$

For tensors with superspace components, the summation over the indices runs from 1 to n. An invariant tensor then satisfies

$$\hat{T}_{ij}(\mathbf{k}) = \sum_{k=1}^{n}\sum_{l=1}^{n} R_{ski}R_{slj}T_{kl}(\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \quad (1.10.4.16)$$

The generalization to higher-rank tensors is straightforward.

1.10.4.4. *Irreducible representations*

For the characterization of vectors and tensors one needs the irreducible and vector representations of the point groups. If the point group is crystallographic in three dimensions, these can be found in Chapter 1.2. All point groups for IC phases or composite structures belong to this category. Exceptions are the point groups for quasicrystals. For the finite point groups for structures up to rank six these are given in Table 1.10.5.1. This table presents:

(1) The character tables for the point groups

$5, \bar{5}, 5m, 52, \bar{5}m$

$10, \overline{10}, 10/m, 10mm, 1022, \overline{10}2m, 10/mmm$

$8, \bar{8}, 8/m, 8mm, 822, \bar{8}2m, 8/mmm$

$12, \overline{12}, 12/m, 12mm, 1222, \overline{12}2m, 12/mmm$

$532, \bar{5}\bar{3}m.$

(2) Matrices for the generators in the irreducible representations of the groups

$$\bar{5}m, 10/mmm, 8/mmm, 12/mmm, \bar{5}\bar{3}m.$$

(3) The vector representations and some tensor representations for the groups in the systems

$$\bar{5}m, 10/mmm, 8/mmm, 12/mmm, \bar{5}\bar{3}m.$$

The character tables can be used to determine the number of independent tensor elements. This is the dimension of subspace of tensors transforming with the identity representation. Tensors transform according to (properly symmetrized or antisymmetrized) tensor products of vector representations. The number of times the identity representation occurs in the decomposition of the tensor product into irreducible components is equal to the number of independent tensor elements and can be calculated with the multiplicity formula. A number of examples are given in the following section.

1.10.4.5. *Determining the number of independent tensor elements*

1.10.4.5.1. *Piezoelectric tensor*

(See Sections 1.1.4.4.3 and 1.1.4.10.1.) The strain in a crystal is determined by its displacement field. For a quasiperiodic crystal, this displacement can have components in the physical space V_E as well as in the internal space V_I. The first implies a local displacement of the material, the latter corresponds to a local deformation because of the shift in the internal coordinate, which is, for example, the phase of a modulation wave or a phason jump for a quasicrystal. The displacement in the point $\mathbf{r}$ is $u = [u_E(\mathbf{r}), u_I(\mathbf{r})]$. Denote u_E by $\mathbf{v}$ and u_I by $\mathbf{w}$. The strain tensor then is given by $\partial_i v_j$ and by $\partial_i w_k$. Here i and j run from 1 to the physical dimension d, and k from 1 to the internal dimension $n-d$. The antisymmetric part of $\partial_i v_j$ corresponds to a global rotation, which does not lead to an energy change. Therefore, the relevant tensors are

$$e_{ij} = (\partial_i v_j + \partial_j v_i)/2, \quad f_{ik} = \partial_i w_k,$$
$$(i, j = 1, \ldots, d;\ k = 1, \ldots, n-d). \quad (1.10.4.17)$$

Both the phonon part e and the phason part f may be coupled to an external electric field E. A linear coupling is given by the piezoelectric tensor p_{ijk}. The free energy is given by

$$F = \int \mathrm{d}r \left(\sum_{ijk} p^e_{ijk}e_{ij}E_k + \sum_{ijk} p^f_{ijk}f_{ij}E_k\right).$$

The tensor e transforms with the symmetrized square of the vector representation in physical space, the tensor f according to the product of the vector representations in physical and internal space. Then p^e and p^f transform according to the product of these two representations with the vector representation in physical space, because E is a physical vector.

As an example, consider the decagonal phase with point group $10\,mm(10^3\,mm)$. The physical space is three-dimensional and

Table 1.10.4.1. *Characters of the point group* $10\,mm(10^3\,mm)$ *for representations relevant for elasticity*

$\tau = (\sqrt{5} - 1)/2$.

Representation	Classes E 1	A 12	A^2 12	B 20	AB 15	Reduction
Γ_E	3	$1+\tau$	$-\tau$	0	-1	Γ_2
Γ_I	3	$-\tau$	$1+\tau$	0	-1	Γ_3
Γ_E^2	9	$2+\tau$	$1-\tau$	0	1	
$\Gamma_E(g^2)$	3	$-\tau$	$1+\tau$	0	3	
$\Gamma_e = (\Gamma_E)_s^2$	6	1	1	0	2	$\Gamma_1 + \Gamma_5$
Γ_e^2	36	1	1	0	4	
$\Gamma_e(g^2)$	6	1	1	0	6	
$(\Gamma_e)_s^2$	21	1	1	0	5	$2\Gamma_1 + \Gamma_4 + 3\Gamma_5$
$\Gamma_f = \Gamma_E \times \Gamma_I$	9	-1	-1	0	1	$\Gamma_4 + \Gamma_5$
$(\Gamma_f)_s^2$	45	0	0	0	5	$2\Gamma_1 + \Gamma_2 + \Gamma_3 + 3\Gamma_4 + 5\Gamma_5$
$\Gamma_e \times \Gamma_f$	54	-1	-1	0	2	$\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 4\Gamma_4 + 5\Gamma_5$

carries a $(2+1)$-reducible representation $(\Gamma_1 \oplus \Gamma_5)$, the internal space an irreducible two-dimensional representation (Γ_7). The symmetrized square of the first is six-dimensional, and the product of first and second is also six-dimensional. The products of these two with the three-dimensional vector representation in physical space are both 18-dimensional. The first contains the identity representation three times, the other does not contain the identity representation. This implies that the piezoelectric tensor has three independent tensor elements, all belonging to p^e. The tensor p^f is zero.

1.10.4.5.2. *Elasticity tensor*

(See Section 1.3.3.2.) As an example of a fourth-rank tensor, we consider the elasticity tensor. The lowest-order elastic energy is a bilinear expression in e and f:

$$F = \int \mathrm{d}\mathbf{r} \left(\tfrac{1}{2} \sum_{ijkl} c^E_{ijkl} e_{ij} e_{kl} + \tfrac{1}{2} \sum_{ijkl} c^I_{ijkl} f_{ij} f_{kl} + \sum_{ijkl} c^{EI}_{ijkl} e_{ij} f_{kl} \right). \quad (1.10.4.18)$$

The elastic free energy is a scalar function. The integrand must be invariant under the operations of the symmetry group. When $\Gamma_E(K)$ is the vector representation of K in the physical space (*i.e.* the vectors in V_E transform according to this representation) and $\Gamma_I(K)$ the vector representation in V_I, the tensor e_{ij} transforms according to the symmetrized square of Γ_E and the tensor f_{ij} transforms according to the product $\Gamma_E \otimes \Gamma_I$. Let us call these representations Γ_e and Γ_f, respectively. This implies that the term that is bilinear in e transforms according to the symmetrized square of Γ_e, that the term bilinear in f transforms according to the symmetrized square of Γ_f, and that the mixed term transforms according to $\Gamma_e \otimes \Gamma_f$. The number of elastic constants follows from their transformation properties. If $d = 3$ and $n = 3 + p$, the number of constants c^E is 21, the number of constants c^I is $3p(3p+1)/2$ and the number of c^{IE} is $18p$. Therefore, without symmetry conditions, there are altogether $3(2+p)(7+3p)/2$ elastic constants. For arbitrary dimension d of the physical space and dimension n of the superspace this number is

$$\begin{aligned} &d(d+1)(d^2+d+2)/8 + pd(pd+1)/2 + d^2(d+1)p/2 \\ &\quad = d(2p+d+1)(2+d+d^2+2pd)/8. \end{aligned}$$

The number of independent elastic constants is the number of independent coefficients in F, and this is given by the number of invariants, *i.e.* the number of times the identity representation occurs as irreducible component of, respectively, the symmetrized square of Γ_e, the symmetrized square of Γ_f, and of $\Gamma_e \otimes \Gamma_f$. The first number is the number of elastic constants in classical theory. The other elastic constants involve the phason degrees of freedom, which exist for quasiperiodic structures. The theory of the generalized elasticity theory for quasiperiodic crystals has been given by Bak (1985), Lubensky *et al.* (1985), Socolar *et al.* (1986) and Ding *et al.* (1993).

As an example, we consider an icosahedral quasicrystal. The symmetry group 532 has five classes, which are given in Table 1.10.5.1. The vector representation is Γ_2. It has character $\chi(R) = 3, 1+\tau, -\tau, 0, -1$. The character of its symmetrized square is $6, 1, 1, 0, 2$. Then the character of the representation with which the elasticity tensor transforms is $21, 1, 1, 0, 5$. This representation contains the trivial representation twice. Therefore, there are two free parameters (c_{1111} and c_{1122}) in the elasticity tensor for the phonon degrees of freedom.

For the phason degrees of freedom, the displacements transform with the representation Γ_3. In this case, the phason elasticity tensor transforms with the symmetrized square of the product of Γ_2 and Γ_3. Its character is $45, 0, 0, 0, 5$. This representation contains the identity representation twice. This implies that this tensor also has two free parameters.

Finally, the coupling term transforms with the product of the symmetrized square of Γ_2, Γ_2 and Γ_3. This representation has character $54, -1, -1, 0, 2$ and consequently contains the identity representation once. In total, the number of independent elastic constants is five for icosahedral tensors. The fact that we have only used the rotation subgroup 532, instead of the full group $\bar{5}\bar{3}m$, does not change this number. The additional central inversion makes the irreducible representations either even or odd. The elasticity tensors should be even, and there are exactly as many even irreducible representations as odd ones. This is shown in Table 1.10.4.1 (*cf.* Table. 1.10.5.1 for the character table of the group 532).

1.10.4.5.3. *Electric field gradient tensor*

As an example, we consider a symmetric rank-two tensor, *e.g.* an electric field gradient tensor, in a system with superspace group symmetry $Pcmn(00\gamma)1s\bar{1}$. The Fourier transform of the tensor T_{ij} is nonzero only for multiples of the vector $\gamma\mathbf{c}^*$. The symmetry element consisting of a mirror operation M_y and a shift $\frac{1}{2}\mathbf{a}_{s4}$ in V_I then has

$$R_E\mathbf{k} = \mathbf{k}, \quad \mathbf{k}\cdot\mathbf{a}_E = 0, \quad R_I = +1, \quad \mathbf{k}_I \cdot \mathbf{a}_I = \pi.$$

Then equation (1.10.4.15) leads to the relation

$$\begin{aligned} \hat{T}(m\gamma\mathbf{c}^*) &= \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \\ &= (-1)^m \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

with solution

$$\hat{T} = \begin{pmatrix} a_{11} & 0 & a_{13} \\ 0 & a_{22} & 0 \\ a_{13} & 0 & a_{33} \end{pmatrix} \quad (m \text{ even}),$$

$$\hat{T} = \begin{pmatrix} 0 & a_{12} & 0 \\ a_{12} & 0 & a_{23} \\ 0 & a_{23} & 0 \end{pmatrix} \quad (m \text{ odd}).$$

This symmetry of the tensor can, for example, be checked by NMR (van Beest *et al.*, 1983).

1.10.4.6. *Determining the independent tensor elements*

In the previous sections some physical tensors have been studied, for which in a number of cases the number of the independent tensor elements has been determined. In this section the problem of determining the invariant tensor elements themselves will be addressed.

Consider an orthogonal transformation R acting on the vector space V. Its action on basis vectors is given by

$$\mathbf{e}'_i = \sum_j R_{ji}\mathbf{e}_j. \qquad (1.10.4.19)$$

If the basis is orthonormal, the matrix R_{ij} is orthogonal ($RR^T = E$). For a point group in superspace the action of R in V_E differs, in general, from that on V_I.

$$\mathbf{e}'_{Ei} = \sum_j R_{Eji}\mathbf{e}_{Ej}; \quad \mathbf{e}'_{Ii} = \sum_j R_{Iji}\mathbf{e}_{Ij}. \qquad (1.10.4.20)$$

The action of R on the tensor product space $V_1 \otimes V_2$, with V_i either V_E or V_I, is given by

$$\mathbf{e}'_{1i} \otimes \mathbf{e}'_{2j} = \sum_k \sum_l R^1_{ki}R^2_{lj}\mathbf{e}_{1k} \otimes \mathbf{e}_{2l}. \qquad (1.10.4.21)$$

If both R_i are orthogonal matrices, the tensor product is also orthogonal. For the symmetrized tensor square $(V \otimes V)_{\rm sym}$ the basis formed by $\mathbf{e}_i \otimes \mathbf{e}_i$ $(i = 1, \ldots)$ and $(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i)/\sqrt{2}$ $(i < j)$ is orthogonal.

A vector $\sum_{ij} c_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$ in the tensor product space is invariant if

$$RcR^T = c. \qquad (1.10.4.22)$$

A tensor as a (possibly symmetric or antisymmetric) bilinear function with coefficients $f_{ij} = f(\mathbf{e}_i, \mathbf{e}_j)$ is invariant if the matrix f_{ij} satisfies

$$R^T fR = f. \qquad (1.10.4.23)$$

For orthogonal bases the equations (1.10.4.22) and (1.10.4.23) are equivalent.

Which spaces have to be chosen for V_i depends on the physical tensor property. The algorithm for determining invariant tensors starts from the transformation of the basis vectors $\mathbf{e}_i$, from which the basis transformation in tensor space follows after due orthogonalization in the case of (anti)symmetric tensors. This procedure can be continued to obtain higher-rank tensors. For orthogonal bases the invariant subspace is spanned by vectors corresponding to the independent tensor elements. We give a number of examples below.

Table 1.10.4.2. *Sign change of $\partial_i E_j$ under the generators A, B, C*

	A	B	C
11	+	+	+
12	−	−	+
13	−	+	−
21	−	−	+
22	+	+	+
23	+	−	−
31	−	+	−
32	+	−	−
33	+	+	+
41	−	+	−
42	+	−	−
43	+	+	+

1.10.4.6.1. *Metric tensor for an octagonal three-dimensional quasicrystal*

From the Fourier module for an octagonal quasicrystal in 3D the generators of the point group can be expressed as 5D integer matrices. They are

$$A = 8(8^3) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B = m_z(1) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

and

$$C = m(m) = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

and span an integer representation of the point group $8/mmm(8^31mm)$. Solution of the three simultaneous equations $S^T gS = g$ is equivalent with the determination of the subspace of the 15D symmetric tensor space that is invariant under the point group. The space has as basis the elements e_{ij} with $i \leq j$. The solution is given by

$$g = \begin{pmatrix} g_{11} & g_{12} & 0 & -g_{12} & 0 \\ g_{12} & g_{11} & g_{12} & 0 & 0 \\ 0 & g_{12} & g_{11} & g_{12} & 0 \\ -g_{12} & 0 & g_{12} & g_{11} & 0 \\ 0 & 0 & 0 & 0 & g_{55} \end{pmatrix}.$$

If $\mathbf{e}_i \otimes \mathbf{e}_j$ is denoted by ij, the solution follows because 55 is left invariant by A, B and C, whereas the orbits of 11 and 12 are $11 \to 22 \to 33 \to 44 \to 11$ and $12 \to 23 \to 34 \to -14 \to 12$, respectively.

1.10.4.6.2. *EFG tensor for Pcmn*

The electric field gradient tensor transforms as the product of a reciprocal vector and a vector. In Cartesian coordinates the transformation properties are the same. The point group for the basic structure of many IC phases of the family of A_2BX_4 compounds is mmm, and the point group for the modulated phase is the 4D group $mmm(11\bar{1})$, with generators

$$A = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The tensor elements $\partial_i E_j$ being indicated by *ij*, the transformation under the generators gives a factor ± 1 as shown in Table 1.10.4.2.

From this, it follows that the four independent tensor elements are $\partial_1 E_1$, $\partial_2 E_2$, $\partial_3 E_3$ and the phason part $\partial_4 E_3$.

1.10.4.6.3. *Elasticity tensor for a two-dimensional octagonal quasicrystal*

The point group of the standard octagonal tiling is generated by the 2D orthogonal matrices

$$A = \begin{pmatrix} \sqrt{1/2} & -\sqrt{1/2} \\ \sqrt{1/2} & \sqrt{1/2} \end{pmatrix}, \quad B = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

In the tensor space one has the following transformations of the basis vectors; they are denoted by *ij* for $\mathbf{e}_i \otimes \mathbf{e}_j$:

$$\begin{aligned} 11 &\rightarrow \tfrac{1}{2}(11 + 12 + 21 + 22) \\ 12 &\rightarrow \tfrac{1}{2}(-11 + 12 - 21 + 22) \\ 21 &\rightarrow \tfrac{1}{2}(-11 - 12 + 21 + 22) \\ 22 &\rightarrow \tfrac{1}{2}(11 - 12 - 21 + 22). \end{aligned}$$

In the space spanned by $a = 11$, $b = \sqrt{1/2}(12 + 21)$ and $c = 22$, the eightfold rotation is represented by the matrix

$$S_E = \begin{pmatrix} \frac{1}{2} & -\sqrt{1/2} & \frac{1}{2} \\ \sqrt{1/2} & 0 & -\sqrt{1/2} \\ \frac{1}{2} & \sqrt{1/2} & \frac{1}{2} \end{pmatrix}.$$

In the six-dimensional space with basis aa, $\sqrt{1/2}(ab + ba)$, $\sqrt{1/2}(ac + ca)$, bb, $\sqrt{1/2}(bc + cb)$ and cc, the rotation gives the transformation

$$\begin{pmatrix} \frac{1}{4} & \frac{1}{2} & \sqrt{2}/4 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \sqrt{2}/4 & 0 & \frac{1}{2} & -\sqrt{1/2} & 0 & \sqrt{2}/4 \\ \frac{1}{2} & 0 & -\sqrt{1/2} & 0 & 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{4} & -\frac{1}{2} & \sqrt{2}/4 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{4} \end{pmatrix}.$$

The vector $\mathbf{v}$ such that $\mathbf{S} \cdot \mathbf{v} = \mathbf{v}$ then is of the form

$$\mathbf{v} = (v_1, 0, (v_1 - v_4)\sqrt{2}, v_4, 0, v_1)^T.$$

This vector is also invariant under the mirror B. This means that there are two independent phonon elastic constants c^E_{1111} and c^E_{1212}, whereas the other tensor elements satisfy the relations

$$c^E_{1112} = c^E_{1222} = 0, \quad c^E_{2222} = c^E_{1111},$$
$$c^E_{1122} = (c^E_{1111} + c^E_{1212})\sqrt{1/2}.$$

The internal component of the eightfold rotation is A^3, that of the mirror B is B itself. The phason strain tensor transforms with the tensor product of external and internal components. This implies that the basis vectors, denoted by *ij* ($i = 1, 2$; $j = 3, 4$), transform under the eightfold rotation according to

$$\begin{aligned} 13 &\rightarrow (-13 + 14 - 23 + 24)/2 \\ 14 &\rightarrow (-13 - 14 - 23 - 24)/2 \\ 23 &\rightarrow (13 - 14 - 23 + 24)/2 \\ 24 &\rightarrow (13 + 14 - 23 - 24)/2. \end{aligned}$$

The symmetrized tensor square of this matrix gives the transformation in the space of phason–phason elasticity tensors, the direct product of the transformations in the 3D phonon strain space and the 4D phason strain space gives the transformation in the space of phonon–-phason elasticity tensors. The first matrix is given by

$$\frac{1}{16}\begin{pmatrix} 1 & \sqrt{2} & -\sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & -\sqrt{2} & 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & 2 & 0 & \sqrt{2} & 0 & -2 & -\sqrt{2} & 0 & \sqrt{2} \\ \sqrt{2} & 2 & 0 & 0 & \sqrt{2} & 0 & 0 & -\sqrt{2} & -2 & -\sqrt{2} \\ -\sqrt{2} & 0 & 0 & 2 & \sqrt{2} & -2 & 0 & \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & -\sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 0 & 0 & -2 & \sqrt{2} & 2 & 0 & \sqrt{2} & 0 & -\sqrt{2} \\ \sqrt{2} & -2 & 0 & 0 & \sqrt{2} & 0 & 0 & -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & \sqrt{2} & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & -2 & 0 & \sqrt{2} & 0 & 2 & -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & \sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & \sqrt{2} & 1 & -\sqrt{2} & 1 \end{pmatrix}.$$

Vectors invariant under this operation and the transformation corresponding to the mirror B correspond to invariant elasticity tensors. For the transformation B, all tensor elements with an odd number of indices 1 or 3 are zero. In the space of phason–phason tensors the general invariant vector is

$$(x_1, 0, 0, -x_6 + (x_5 - x_1)\sqrt{2}, x_5, x_6, 0, x_5, 0, x_1).$$

There are three independent elastic constants, $x_1 = c_{1313}$, $x_5 = c_{1414}$ and $x_6 = c_{1423}$. For the phonon–phason elastic constants the corresponding invariant vector is

$$(x, 0, 0, x, 0, x/\sqrt{2}, -x/\sqrt{2}, 0, -x, 0, 0, -x).$$

The independent elastic constant is $x = c_{1113} = c_{1124} = c_{1214}\sqrt{2} = -c_{1223}\sqrt{2} = -c_{2213} = -c_{2224}$.

1.10.4.6.4. *Piezoelectric tensor for a three-dimensional octagonal quasicrystal*

A quasicrystal with octagonal point group $8/mmm(8^3 1mm)$ will not show a piezoelectric effect because the point group contains the central inversion. We consider here the point group $8mm(8^3mm)$ which is a subgroup without central inversion. It is generated by the matrices

$$A = \begin{pmatrix} \alpha & -\alpha & 0 & 0 & 0 \\ \alpha & \alpha & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\alpha & -\alpha \\ 0 & 0 & 0 & \alpha & -\alpha \end{pmatrix},$$

$$B = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Here $\alpha = \sqrt{2}/2$. There are two components for the strain, a phonon component e and a phason component f. The phonon strain tensors form a 6D space, the phason strain tensors also a 6D space. The phonon strain space transforms with the symmetrized square of the physical parts of the operations, the phason strain space with the product of physical and internal parts. For the eightfold rotation the corresponding matrices are

$$S_e = \begin{pmatrix} \frac{1}{2} & -\alpha & 0 & \frac{1}{2} & 0 & 0 \\ \alpha & 0 & 0 & -\alpha & 0 & 0 \\ 0 & 0 & \alpha & 0 & -\alpha & 0 \\ \frac{1}{2} & \alpha & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \alpha & 0 & \alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$S_f = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\alpha & -\alpha \\ 0 & 0 & 0 & 0 & \alpha & -\alpha \end{pmatrix}.$$

The action on the space of piezoelectric tensors is given, for the phonon and the phason part, by taking the product of these matrices with the physical part A_E. The invariant vectors under these matrices give the invariant tensors. If the second generator is taken into account, which requires that the number of indices 1 or 4 is even, this results in the independent tensor elements

$$x_3 = c_{113}, \quad x_{16} = c_{322}, \quad x_{18} = c_{333}$$

with relation $c_{223} = c_{113}$, whereas all other elements are zero for the coupling between the electric field and phonon strain. There is no nontrivial invariant vector in the second case. Therefore, all tensor elements for the coupling between the electric field and phason strain are zero.

1.10.4.6.5. *Elasticity tensor for an icosahedral quasicrystal*

The point group of an icosahedral quasicrystal is $532(5^2 32)$ with generators having components

$$A_E = \begin{pmatrix} 1 & \tau & -1-\tau \\ \tau & 1+\tau & 1 \\ 1+\tau & -1 & \tau \end{pmatrix} /2,$$

$$B_E = \begin{pmatrix} -\tau & 1+\tau & -1 \\ 1+\tau & 1 & \tau \\ 1 & -\tau & -1-\tau \end{pmatrix} /2$$

in physical space and components

$$A_I = \begin{pmatrix} -1 & \tau & -1-\tau \\ -\tau & \tau^{-1} & 1 \\ 1+\tau & 1 & -\tau \end{pmatrix} /2, \quad B_I = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

in internal space (see Table 1.10.5.2). The phonon and phason strain tensors form a 6D, respectively 9D, vector space, in which the point group acts with matrices

$$S_e = \frac{1}{4} \begin{pmatrix} 1 & \tau\sqrt{2} & -\varphi\sqrt{2} & 1-\tau & -\sqrt{2} & 2+\tau \\ \tau\sqrt{2} & 2 & 0 & \sqrt{2} & -2 & -\varphi\sqrt{2} \\ \varphi\sqrt{2} & 0 & -2 & -\tau\sqrt{2} & 2 & -\sqrt{2} \\ 1-\tau & \sqrt{2} & \tau\sqrt{2} & 2+\tau & \varphi\sqrt{2} & 1 \\ \sqrt{2} & 2 & 2 & -\varphi\sqrt{2} & 0 & \tau\sqrt{2} \\ 2+\tau & -\varphi\sqrt{2} & \sqrt{2} & 1 & -\tau\sqrt{2} & 1-\tau \end{pmatrix},$$

$$S_f = \frac{1}{4} \begin{pmatrix} -\tau & \varphi & -1 & \tau-1 & 1 & -\tau & 1 & -2-\tau & \varphi \\ \varphi & 1 & \tau & 1 & \tau & 1-\tau & -2-\tau & -\varphi & -1 \\ 1 & -\tau & -\varphi & \tau & \tau-1 & -1 & -\varphi & 1 & 2+\tau \\ \tau-1 & 1 & -\tau & -1 & 2+\tau & -\varphi & -\tau & \varphi & -1 \\ 1 & \tau & 1-\tau & 2+\tau & \varphi & 1 & \varphi & 1 & \tau \\ \tau & \tau-1 & -1 & \varphi & -1 & -2-\tau & 1 & -\tau & -\varphi \\ -1 & 2+\tau & -\varphi & \tau & -\varphi & 1 & \tau-1 & 1 & -\tau \\ 2+\tau & \varphi & 1 & -\varphi & -1 & -\tau & 1 & \tau & 1-\tau \\ \varphi & -1 & -2-\tau & -1 & \tau & \varphi & \tau & \tau-1 & -1 \end{pmatrix}$$

and

$$T_e = \frac{1}{4} \begin{pmatrix} 1 & -\tau\sqrt{2} & \varphi\sqrt{2} & 1-\tau & -\sqrt{2} & 2+\tau \\ \tau\sqrt{2} & -2 & 0 & \sqrt{2} & -2 & -\varphi\sqrt{2} \\ -\varphi\sqrt{2} & 0 & -2 & \tau\sqrt{2} & -2 & \sqrt{2} \\ 1-\tau & -\sqrt{2} & -\tau\sqrt{2} & 2+\tau & \varphi\sqrt{2} & 1 \\ -\sqrt{2} & 2 & 2 & \varphi\sqrt{2} & 0 & -\tau\sqrt{2} \\ 2+\tau & \varphi\sqrt{2} & -\sqrt{2} & 1 & -\tau\sqrt{2} & 1-\tau \end{pmatrix},$$

$$T_f = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & -\tau & 0 & 0 & \varphi \\ 1 & 0 & 0 & -\tau & 0 & 0 & \varphi & 0 & 0 \\ 0 & -1 & 0 & 0 & \tau & 0 & 0 & -\varphi & 0 \\ 0 & 0 & \tau & 0 & 0 & -\varphi & 0 & 0 & -1 \\ \tau & 0 & 0 & -\varphi & 0 & 0 & -1 & 0 & 0 \\ 0 & -\tau & 0 & 0 & \varphi & 0 & 0 & 1 & 0 \\ 0 & 0 & -\varphi & 0 & 0 & -1 & 0 & 0 & \tau \\ -\varphi & 0 & 0 & -1 & 0 & 0 & \tau & 0 & 0 \\ 0 & \varphi & 0 & 0 & 1 & 0 & 0 & -\tau & 0 \end{pmatrix}.$$

This implies that the phonon elasticity tensors form a 21D space, the phason elasticity tensors a 45D space and the phonon–phason coupling a 54D space. The invariant vectors under these orthogonal transformations correspond to invariant elastic tensors. Their coordinates are the elastic constants. For the given presentation of the point group, these are given in Table 1.10.4.3. The tensor elements are expressed in parameters x and y where there are two independent tensor elements. The tensor elements that are not given are zero or equal to that given by the permutation symmetry. If bases for the phonon and phason strain are introduced by

$$[1] = 11, [2] = 12, [3] = 13, [4] = 22, [5] = 23, [6] = 33$$

for the phonon part and

$$[1] = 14, [2] = 15, [3] = 16, [4] = 24, [5] = 25, [6] = 26,$$
$$[7] = 34, [8] = 35, [9] = 36$$

for the phason part, the elastic tensors may be given in matrix form as

$$c^{ee} = \begin{pmatrix} x+y & 0 & 0 & x & 0 & x \\ 0 & y & 0 & 0 & 0 & 0 \\ 0 & 0 & y & 0 & 0 & 0 \\ x & 0 & 0 & x+y & 0 & x \\ 0 & 0 & 0 & 0 & y & 0 \\ x & 0 & 0 & x & 0 & x+y \end{pmatrix},$$

$$c^{ff} = \begin{pmatrix} z & \tau^2 u & -\tau u & -\tau u & \tau u & -\tau u & -u & 0 & \tau u \\ \tau^2 u & z-2\tau u & u & \tau u & u & 0 & 0 & \tau^2 u & \tau u \\ -\tau u & u & z & -\tau u & 0 & -\tau^2 u & \tau u & \tau u & \tau u \\ -\tau u & \tau u & -\tau u & z & \tau u & u & -\tau^2 u & \tau u & 0 \\ \tau u & u & 0 & \tau u & z & -\tau^2 u & \tau u & -\tau u & -\tau u \\ -\tau u & 0 & -\tau^2 u & u & -\tau^2 u & z-2\tau u & 0 & -\tau u & u \\ -u & 0 & \tau u & -\tau^2 u & \tau u & 0 & z-2\tau u & -u & -\tau^2 u \\ 0 & \tau^2 u & \tau u & \tau u & -\tau u & -\tau u & -u & z & -\tau u \\ \tau u & \tau u & \tau u & 0 & -\tau u & u & -\tau^2 u & -\tau u & z \end{pmatrix},$$

$$c^{ef} = \begin{pmatrix} -v & -\tau v & -\tau^2 v & -\tau^3 v & \tau v & -\tau^2 v & v & -\tau v & -\tau^{-1} v \\ -\tau^3 v & \tau v & -\tau^2 v & \tau^2 v & v & \tau v & 0 & 0 & 0 \\ v & -\tau v & -\tau^{-1} v & 0 & 0 & 0 & -\tau v & -\tau^2 v & -\tau^3 v \\ \tau^{-1} v & v & \tau v & -\tau^2 v & v & -\tau v & -\tau^2 v & -\tau^3 v & \tau v \\ 0 & 0 & 0 & -\tau^2 v & \tau^3 v & \tau v & \tau v & -\tau^{-1} v & v \\ -\tau v & -\tau^2 v & -\tau^3 v & \tau v & -\tau^{-1} v & v & -\tau v & \tau^2 v & v \end{pmatrix}.$$

The parameters x, y, z, u, v are the five independent elastic constants.

1.10.5. Tables

In this section are presented the irreducible representations of point groups of quasiperiodic structures up to rank six that do not occur as three-dimensional crystallographic point groups.