International Tables for Crystallography (2006). Vol. D, Section 1.10.4.5.3, pp. 252–253.

Table 1.10.4.1. *Characters of the point group* $10mm(10^3mm)$ *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:

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

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

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

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 $S^T g S = g$ 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 $i \le j$. 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

references