18

Symmetry Properties of Tensors

In theories and experiments involving physical systems with high symmetry, one frequently encounters the question of how many independent terms are required by symmetry to specify a tensor of a given rank for each symmetry group. These questions have simple group theoretical answers [75]. This chapter deals with the symmetry properties of tensors, with particular attention given to those tensors of rank 2 and higher that arise in the physics of condensed matter concerning nonlinear optics and elasticity theory. In this analysis we consider the symmetry implied by the permutation group which gives the number of independent components in the case of no point group symmetry. We then consider the additional symmetry that is introduced by the presence of symmetry elements such as rotations, reflections and inversions. We explicitly discuss full rotational symmetry and several point group symmetries.

18.1 Introduction

We start by listing a few commonly occurring examples of tensors of rank 2, 3, and 4 that occur in condensed matter physics. Second rank symmetric tensors occur in the constitutive equations of Electromagnetic Theory, as for example in the linear equations relating the current density to the electric field intensity

$$\boldsymbol{J}^{(1)} = \overset{\leftrightarrow}{\sigma^e}^{(2)} \cdot \boldsymbol{E}\,, \tag{18.1}$$

where the electrical conductivity $\overset{\leftrightarrow}{\sigma^e}^{(2)}$ is a symmetric ($\sigma^e_{ij} = \sigma^e_{ji}$) second rank tensor. We use the superscript (2) to distinguish the second rank linear conductivity tensor from the nonlinear higher order tensor terms that depend on higher powers of the electric field $\boldsymbol{E}$ discussed below. A similar situation holds for the relation between the polarization and the electric field

$$\boldsymbol{P}^{(2)} = \overset{\leftrightarrow}{\alpha}^{(2)} \cdot \boldsymbol{E}\,, \tag{18.2}$$

where the polarizability $\overset{\leftrightarrow}{\alpha}^{(2)}$ is a symmetric second rank tensor, and where $\overset{\leftrightarrow}{\alpha}^{(2)} \equiv \overset{\leftrightarrow}{\chi}_E^{(2)}$ is often called the electrical susceptibility. A similar situation also holds for the relation between the magnetization and the magnetic field

$$\boldsymbol{M}^{(2)} = \overset{\leftrightarrow}{\chi}_H^{(2)} \cdot \boldsymbol{H}\,, \tag{18.3}$$

where the magnetic susceptibility $\overset{\leftrightarrow}{\chi}_H^{(2)}$ is also a symmetric second rank tensor. These relations all involve second rank symmetric tensors: $\overset{\leftrightarrow}{\sigma}^{(2)}$, $\overset{\leftrightarrow}{\alpha}^{(2)}$ and $\overset{\leftrightarrow}{\chi}_H^{(2)}$. Each second (3×3) rank tensor T_{ij} has nine components but because it is a symmetric tensor $T_{ij} = T_{ji}$ only six coefficients (rather than nine) are required to represent these symmetric second rank tensors. Thus, a symmetric second rank tensor, such as the polarizability tensor or the Raman tensor, has only six independent components. In this chapter we are concerned with the symmetry properties of these and other tensors under permutations and point group symmetry operations.

As an example of higher rank tensors, consider nonlinear optical phenomena, where the polarization in (18.2) is further expanded to higher order terms in $\boldsymbol{E}$ as

$$\boldsymbol{P} = \overset{\leftrightarrow}{\alpha}^{(2)} \cdot \boldsymbol{E} + \overset{\leftrightarrow}{\alpha}^{(3)} \cdot \boldsymbol{EE} + \overset{\leftrightarrow}{\alpha}^{(4)} \cdot \boldsymbol{EEE} + \cdots\,, \tag{18.4}$$

where we can consider the polarizability tensor $\overset{\leftrightarrow}{\alpha}$ to be field dependent

$$\overset{\leftrightarrow}{\alpha} = \overset{\leftrightarrow}{\alpha}^{(2)} + \overset{\leftrightarrow}{\alpha}^{(3)} \cdot \boldsymbol{E} + \overset{\leftrightarrow}{\alpha}^{(4)} \cdot \boldsymbol{EE} + \cdots\,, \tag{18.5}$$

because an increase in the magnitude of $\boldsymbol{E}$ will make the nonlinear terms in (18.4) and (18.5) more important. More will be said about the symmetry of the various $\overset{\leftrightarrow}{\alpha}^{(i)}$ tensors under permutations and point group operations in Sect. 18.3. Similar expansions can be made for (18.1) and (18.3).

As another example, consider the *piezoelectric* tensor which is a third rank tensor relating the polarization per unit volume $\boldsymbol{P}$ to the strain tensor, $\overset{\leftrightarrow}{e}$, where $\boldsymbol{P}$ is given by

$$\boldsymbol{P} = \overset{\leftrightarrow}{d}^{(3)} \cdot \overset{\leftrightarrow}{e}\,, \tag{18.6}$$

which can be rewritten to show the rank of each tensor explicitly

$$P_k = \sum_{i,j} d_{kij} \frac{u_i}{x_j}\,, \tag{18.7}$$

in which the vector u_i denotes the change in the length while x_j refers to the actual length. We note that there are 27 components in the tensor $\overset{\leftrightarrow}{d}^{(3)}$ without considering any symmetry of the system under permutation operations. A frequently used fourth rank tensor is the elastic constant tensor $\overleftrightarrow{C}^{(4)}$ defined by

$$\overleftrightarrow{\sigma}^{m} = \overleftrightarrow{C}^{(4)} \cdot \overleftrightarrow{e}\,, \tag{18.8}$$

where the second rank symmetric stress tensor $\overleftrightarrow{\sigma}^{m}$ and strain tensor $\overleftrightarrow{e}$ (i.e., the gradient of the displacement) are related through the fourth rank elastic constant tensor $\overleftrightarrow{C}^{(4)}$ (or C_{ijkl}), which neglecting permutation symmetry would have 81 components. More will be said about the elastic constant tensor below (see Sect. 18.6) where we will use $\overleftrightarrow{\sigma}^{m}$ to denote the mechanical stress tensor, but it should be noted that σ_{ij}^{e} is used to denote the linear electrical conductivity tensors (18.1). The superscripts m and e are used to distinguish σ_{ij}^{m} for the stress tensor from σ_{ij}^{e} for the electrical conductivity tensor.

These tensors and many more are discussed in a book by Nye [57]. The discussion of tensors which we give in this chapter is group theoretical, whereas Nye's book gives tables of the tensors which summarize many of the results which we can deduce from our group theoretical analysis.

In this chapter we use group theory to find the smallest number of independent coefficients for commonly occurring tensors in condensed matter physics, including permutation symmetry and point group symmetry. Let us now consider the total number of tensor components. As stated above $\overleftrightarrow{\alpha}^{(2)}$ has $3^2 = 9$ coefficients (six for the symmetric components, $\alpha_{ij} = \alpha_{ji}$). There are $3^3 = 27$ coefficients (10 symmetric) in $\overleftrightarrow{\alpha}^{(3)}$, $3^4 = 81$ coefficients (only 15 symmetric) in $\overleftrightarrow{\alpha}^{(4)}$, and $3^5 = 243$ coefficients (21 symmetric) in $\overleftrightarrow{\alpha}^{(5)}$, etc. We ask how many tensor components are independent? Which components are related to one another? How many independent experiments must be carried out to completely characterize these tensors? These are important questions that occur in many areas of condensed matter physics and materials science. We address these questions in this chapter.

In Sect. 18.2, we discuss the reduction in the number of independent coefficients arising from symmetries associated with the permutation of tensor indices while in Sect. 18.3 we discuss the corresponding reduction in the number of independent components of tensors obtained from point group symmetry (rotations, reflections and inversion). The number of independent coefficients for the case of complete isotropy (full rotational symmetry) is considered in Sect. 18.4, while lower point group symmetries are treated in Sect. 18.5. The independent coefficients of the elastic modulus tensor $\mathcal{C}_{ijkl}$ are discussed in Sect. 18.6. Since the number of independent symmetry elements can be found by considering the crystal symmetry group as a subgroup of the full rotation group without making contact to translational symmetry, point group symmetry is considered in finding the form of tensors in condensed matter systems.

18.2 Independent Components of Tensors Under Permutation Group Symmetry

In this section we consider the effect of permutation symmetry on reducing the number of independent components of tensors. For example, second rank symmetric tensors occur frequently in condensed matter physics. In this case, the symmetry $\alpha_{ij} = \alpha_{ji}$ implied by the term symmetric tensor restricts the off-diagonal matrix elements to follow this additional permutation relation $ij = ji$, thereby reducing the number of allowed off-diagonal elements from six to three, since the symmetric combinations $(\alpha_{ij} + \alpha_{ji})/2$ are allowed and the combinations $(\alpha_{ij} - \alpha_{ji})/2$ vanish by symmetry. Furthermore, the three elements $(\alpha_{ij} - \alpha_{ji})/2$ constitute the three components of an antisymmetric second rank tensor, also called an axial vector; the angular momentum (listed in character tables as R_i) is an example of an antisymmetric second-rank tensor which has three components L_x, L_y, L_z.

Group theory is not needed to deal with the symmetry of a second-rank tensor because of its simplicity. As the rank of the tensor increases, group theory becomes increasingly helpful in the classification of symmetric tensors. Just for illustrative purposes, we now consider the case of the second-rank tensor from the point of view of permutation group symmetry. For this purpose we have listed in Table 18.1 the permutation groups which are needed to handle the tensors mentioned in Sect. 18.1. Referring to Table 18.1 (which is constructed from tables in Chap. 17), we see that a second rank symmetric tensor like the electrical conductivity tensor $\overleftrightarrow{\sigma}^e$ is represented in Table 18.1 by pp, which we can consider as the generic prototype of a second rank symmetric tensor. From the discussion of Chap. 17, we found that p^2 could have angular momentum states $L = 0$, 1, 2 with the indicated permutation group symmetries labeled "irreducible representations" in Table 18.1, and yielding a total number of states equal to the sum of $(2L + 1)$ to yield $1 + 3 + 5 = 9$. From the table, it is seen that the symmetric states (Γ_1^s) arise from the $L = 0$ and $L = 2$ entries, corresponding to 1+5=6 states. Thus we obtain six independent coefficients for a symmetric second rank tensor based on permutation symmetry alone. The number of independent coefficients for the second rank antisymmetric tensor (transforming Γ_1^a) is correspondingly equal to 3, and the antisymmetric contribution arises from the $L = 1$ state.

A third-rank symmetric tensor (such as $\overleftrightarrow{\alpha}^{(3)}$) is more interesting from a group theoretical standpoint. Here we need to consider permutations in Table 18.1 of the type p^3, so that p^3 can be considered as the appropriate basis function of the permutation group $P(3)$ for the permutation symmetry of $\overleftrightarrow{\alpha}^{(3)}$. Referring to (18.4), we note that the $\boldsymbol{EE}$ fields are clearly symmetric under interchange of $\boldsymbol{E} \leftrightarrow \boldsymbol{E}$; but since (18.5) defines the general nonlinear polarizability tensor $\overleftrightarrow{\alpha}$, then all terms in the expansion of $\overleftrightarrow{\alpha}$ must be symmetric under interchange of $\alpha_{ij} \to \alpha_{ji}$. From Table 18.1, we see that p^3 consists of $L = 0$, 1, 2, 3 angular momentum states. The entries for the p^3 configuration

Table 18.1. Transformation properties of various tensors under permutations[(a)]

tensor	configuration	state	irreducible representations	group
	SS	$L=0$	Γ_1^s	$P(2)$
	SD	$L=2$	$\Gamma_1^s+\Gamma_1^a$	$P(2)$
	DD	$L=0$	Γ_1^s	$P(2)$
$C_{(ij)(kl)}$	DD	$L=1$	Γ_1^a	$P(2)$
	DD	$L=2$	Γ_1^s	$P(2)$
	DD	$L=3$	Γ_1^a	$P(2)$
	DD	$L=4$	Γ_1^s	$P(2)$
	pS	$L=1$	$\Gamma_1^s+\Gamma_1^a$	$P(2)$
$d_{i(jk)}$	pD	$L=1$	$\Gamma_1^s+\Gamma_1^a$	$P(2)$
	pD	$L=2$	$\Gamma_1^s+\Gamma_1^a$	$P(2)$
	pD	$L=3$	$\Gamma_1^s+\Gamma_1^a$	$P(2)$
	p^2	$L=0$	Γ_1^s	$P(2)$
$\alpha^{(2)}$	p^2	$L=1$	Γ_1^a	$P(2)$
	p^2	$L=2$	Γ_1^s	$P(2)$
	p^3	$L=0$	Γ_1^a	$P(3)$
	p^3	$L=1$	$\Gamma_1^s+\Gamma_2$	$P(3)$
$\alpha^{(3)}$	p^3	$L=2$	Γ_2	$P(3)$
	p^3	$L=3$	Γ_1^s	$P(3)$
	p^4	$L=0$	$\Gamma_1^s+\Gamma_2$	$P(4)$
	p^4	$L=1$	$\Gamma_3+\Gamma_{3'}$	$P(4)$
$\alpha^{(4)}$	p^4	$L=2$	$\Gamma_1^s+\Gamma_2+\Gamma_3$	$P(4)$
	p^4	$L=3$	Γ_3	$P(4)$
	p^4	$L=4$	Γ_1^s	$P(4)$
	p^5	$L=0$	Γ_6	$P(5)$
	p^5	$L=1$	$\Gamma_1^s+\Gamma_4+\Gamma_5+\Gamma_{5'}$	$P(5)$
$\alpha^{(5)}$	p^5	$L=2$	$\Gamma_4+\Gamma_5+\Gamma_6$	$P(5)$
	p^5	$L=3$	$\Gamma_1^s+\Gamma_4+\Gamma_5$	$P(5)$
	p^5	$L=4$	Γ_4	$P(5)$
	p^5	$L=5$	Γ_1^s	$P(5)$
	p^6	$L=0$	$\Gamma_1^s+\Gamma_{5'''}+\Gamma_9$	$P(6)$
	p^6	$L=1$	$\Gamma_5+\Gamma_{5''}+\Gamma_{10}+\Gamma_{16}$	$P(6)$
	p^6	$L=2$	$\Gamma_1^s+\Gamma_5+2\Gamma_9+\Gamma_{16}$	$P(6)$
$\alpha^{(6)}$	p^6	$L=3$	$\Gamma_5+\Gamma_{5''}+\Gamma_9+\Gamma_{10}$	$P(6)$
	p^6	$L=4$	$\Gamma_1^s+\Gamma_5+\Gamma_9$	$P(6)$
	p^6	$L=5$	Γ_5	$P(6)$
	p^6	$L=6$	Γ_1^s	$P(6)$

[(a)] The irreducible representations associated with the designated permutation group, configuration and state are listed

Table 18.2. Number of independent components for various tensors for the listed group symmetries

			number of independent coefficients					
group	repr.[a]	angular momentum values[b]	$C_{(ij)(kl)}$	$d_{k(ij)}$	$\alpha^{(2)}$	$\alpha^{(3)}$	$\alpha^{(4)}$	$\alpha^{(5)}$
R_∞^c	$\Gamma_{\ell=0}$	$\ell = 0$	2	0	1	0	1	0
I_h	A_{1g}	$\ell = 0, 6, 10, \ldots$	2	0	1	0	1	0
O_h	A_{1g}	$\ell = 0, 4, 6, 8, 10, \ldots$	3	0	1	0	2	0
T_d	A_1	$\ell = 0, 3, 4, 6, 7, 8, 9, \ldots$	3	1	1	1	2	1
$D_{\infty h}$	A_{1g}	$\ell = 0, 2, 4, 6, \ldots$	5	1	2	0	3	0
$C_{\infty v}$	A_1	$\ell = 0, 1, 2, 3, 4, 5, \ldots$	5	4	2	2	3	3
D_{6h}	A_{1g}	$\ell = 0, 2, 4, 6, \ldots$	5	1	2	0	3	0
C_1	A_1	$\ell = 0, 1, 2, 3, 4, 5, \ldots$[d]	21	18	6	10	15	21

[a] The notation for the totally symmetric irreducible representation for each group is given

[b] The angular momentum states that contain the A_1 (or A_{1g}) irreducible representation for the various symmetry groups (see Table 18.1)

[c] The full rotational symmetry group is denoted by R_∞

[d] For this lowest point group symmetry, the A_1 representation occurs $2\ell + 1$ times. For the other groups in this table, there is only one occurrence of A_1 for each listed ℓ value. However, for higher ℓ values, multiple occurrences of A_1 may arise (e.g., in O_h symmetry, the $\ell = 12$ state has two A_{1g} modes)

in Table 18.1 come from Table 17.4 which contains a variety of configurations of the permutation group $P(3)$ that can be constructed from three electrons (or more generally from three interchangeable vectors). The total number of states in the p^3 configuration is found by multiplying the degeneracy $(2L+1)$ of each angular momentum state along with the corresponding number of irreducible representations occurring for each of the $L = 0, 1, 2, 3$ multiplets and then summing all of these products to get

$$(1)(1) + 3(1 + 2) + 5(2) + 7(1) = 27$$

which includes all 3^3 combinations. Of this total, the number of symmetric combinations that go with Γ_1^s is only $3(1) + 7(1) = 10$. Similarly Table 18.1 shows that there is only one antisymmetric combination (for $L = 0$). Of interest is the large number of combinations that are neither symmetric nor antisymmetric: $3(2) + 5(2) = 16$ for $\overset{\leftrightarrow}{\alpha}^{(3)}$ for the $P(3)$ permutation group. Thus, Table 18.1 shows that on the basis of permutation symmetry, there are only ten independent coefficients for $\overset{\leftrightarrow}{\alpha}^{(3)}$, assuming no additional point group symmetry. This result is summarized in Table 18.2.

As the next example, consider $\overset{\leftrightarrow}{\alpha}^{(4)}$ which is a fourth rank tensor that couples $\boldsymbol{P}$ and $\boldsymbol{EEE}$ symmetrically. The generic tensor for this case is p^4 in Table 18.1 (taken from Table 17.6 for $P(4)$ for four electrons) with $3^4 = 81$

coefficients neglecting permutational and point group symmetries, which is also obtained from the entries in Table 18.1 for p^4 as follows:

$$(1)(1+2)+(3)(3+3)+5(1+2+3)+7(3)+9(1)=81\,.$$

Of these, $1+5+9=15$ are symmetric (transforms as Γ_1^s) and this entry is included in Table 18.2. There are no antisymmetric combinations (i.e., there is no Γ_1^a for p^4 in $P(4)$).

Another commonly occurring tensor in solid state physics is the elastic modulus tensor $\mathcal{C}_{ijkl} = C_{(ij)(kl)}$ which relates two symmetric tensors $\overleftrightarrow{\sigma}^m$ and $\overleftrightarrow{e}$, each having six independent components, and thus leading to $6\times 6 = 36$ components for the product. But $C_{(ij)(kl)}$ is further symmetric under interchange of $ij \leftrightarrow kl$, reducing the 30 off-diagonal components of the 6×6 matrix into 15 symmetric and 15 antisymmetric combinations, in addition to the six diagonal symmetric components. This gives a total of 21 independent symmetric coefficients, as is explained in standard condensed matter physics texts. From a group theoretical standpoint, the (ij) and (kl) are each treated as p^2 units which form total angular momentum states of $L=0$ (labeled S in Table 18.1) and $L=2$ (labeled D). Under the permutation group $P(2)$, we can make one SS combination ($L=0$), one symmetric and one antisymmetric SD combination ($L=$2), and finally DD combinations can be made with $L=0$, 1, 2, 3, 4. Adding up the total number of combinations that can be made from $C_{(ij)(kl)}$ we get

$$(1)(1)+5(1+1)+1(1)+3(1)+5(1)+7(1)+9(1)=36\,,$$

in agreement with the simple argument given above. Of these, 21 are symmetric (i.e., go with Γ_1^s) while 15 are antisymmetric (i.e., go with Γ_1^a), and the number 21 appears in Table 18.2. If we had instead used p^4 in Table 18.1 as the basis function for the permutation of the elastic tensor $\mathcal{C}_{ijkl}$, we would have neglected the symmetric interchange of the stress and strain tensors $(ij) \leftrightarrow (kl)$.

The final tensor that we will consider is the piezoelectric tensor $d_{i(jk)}$ formed as the symmetric direct product of a vector and a symmetric second rank tensor ($3\times 6 = 18$ components). The symmetries are calculated following the pS and pD combinations, using the concepts discussed for the transformation properties of the $\overleftrightarrow{\alpha}^{(2)}$ and $C_{(ij)(kl)}$ tensors. This discussion yields 18 independent coefficients for $d_{i(jk)}$ under permutation symmetry.

In summary, each second rank symmetric tensor is composed of irreducible representations $L=0$ and $L=2$ of the full rotation group, the third rank symmetric tensor from $L=1$ and $L=3$, the fourth rank symmetric tensor from $L=0$, $L=2$ and $L=4$, the elastic tensor from $L=0$, $2L=2$ and $L=4$, and the piezoelectric tensor from $2L=1$, $L=2$ and $L=3$. We use these results to now incorporate the various rotational symmetries to further reduce the number of independent coefficients for each symmetry group.

18.3 Independent Components of Tensors: Point Symmetry Groups

In this section we discuss a very general group theoretical result for tensor components arising from point group symmetry operations such as rotations, reflections and inversions. These symmetry operations further reduce the number of independent coefficients that need to be introduced for the various tensors in crystals having various point group symmetries.

Let us consider a relation between a tensor of arbitrary rank $J_{ij\ldots}$ and another tensor $F_{i'j'}\ldots$ also of arbitrary rank and arbitrary form where the two tensors in general will be of different ranks.

$$J_{ij\ldots} = \sum_{i'j'\ldots} \{t_{ij\ldots,i'j'\ldots}\} F_{i'j'\ldots} \,. \tag{18.9}$$

What we have in mind in (18.9) are relations such as are given in (18.1) to (18.8), where $J_{ij\ldots}$ appears as either a simple vector or as a second rank symmetrical tensor. Likewise $F_{i'j'\ldots}$ denotes either a simple vector, the product of two vectors, the product of three vectors, or a symmetric second rank tensor etc.

Theorem. *The number of independent non-zero tensor components $t_{ij\ldots,i'j'\ldots}$ allowed by point group symmetry in (18.9) is determined by finding the irreducible representations contained in both $\{\Gamma_{J_{ij\ldots}}\} = \sum \alpha_i \Gamma_i$ and $\{\Gamma_{F_{i'}F_{j'}\ldots}\} = \sum \beta_j \Gamma_j$.*

Proof. Only coefficients $t_{ij\ldots,i'j'\ldots}$ coupling $\{\boldsymbol{J}\}_{\Gamma_i}$ and $\{\boldsymbol{F}\}_{\Gamma_j}$ that correspond to the same partner of the same irreducible representation contained in both Γ_i and Γ_j can be nonzero, since $\overleftrightarrow{t}$ must be invariant under the symmetry operations of the group. Thus the number of independent matrix elements in the tensor $t_{ij\ldots i'j'\ldots}$ is the number of times the scalar representation Γ_1^+ occurs in the decomposition of the direct product

$$\{\Gamma_{\boldsymbol{J}}\} \otimes \{\Gamma_{\boldsymbol{F}\ldots}\} = \sum_i \alpha_i \Gamma_i \otimes \sum_j \beta_j \Gamma_j = \sum_k \gamma_k \Gamma_k \,, \tag{18.10}$$

thus completing the proof. □

The only nonvanishing couplings between $\{\boldsymbol{J}\}_{\Gamma_i}$ and $\{\boldsymbol{F}\}_{\Gamma_j}$ are between partners transforming according to the same irreducible representation because only these lead to matrix elements that are invariant under the symmetry operations of the group. We therefore transform (18.9) to make use of the symmetrized form

$$\{\boldsymbol{J}\}_{\Gamma_i} = t_{\Gamma_1^+} \, \{\boldsymbol{F}\}_{\Gamma_i} \,, \tag{18.11}$$

where the $\{\boldsymbol{J}\}_{\Gamma_i}$ and $\{\boldsymbol{F}\}_{\Gamma_i}$ correspond to the same partners of the same irreducible representation and $t_{\Gamma_1^+}$ transforms as a scalar which has Γ_1^+ symmetry.

In most cases of interest, permutation symmetry requirements on the products $\{\boldsymbol{F}\}_{\Gamma_i}$ further limit the number of independent matrix elements of a tensor matrix, as discussed below (Sect. 18.4).

Application of this theorem is given for the maximum amount of rotational symmetry (the full rotation group) in Sect. 18.4 and for specific point group symmetries in Sect. 18.5 and Sect. 18.6.

18.4 Independent Components of Tensors Under Full Rotational Symmetry

The highest point group symmetry is the full isotropy provided by the full rotation group R_∞. In Sect. 18.3 we showed that the number of independent coefficients in a tensor $t_{ij\ldots i'j'\ldots}$ in (18.9) coupling two tensors is the number of times the direct product in (18.10) contains Γ_1^s. For full rotational symmetry we use in the fully symmetric irreducible representation $L = 0$. Thus we must look for the occurrence of $L = 0$ in Table 18.1.

Referring to Table 18.1, we find $\Gamma_{L=0}$ and that for the second rank tensor, we have Γ_1 contained once, giving only a single independent coefficient $\{\Gamma_{\boldsymbol{j}}\} \otimes \{\Gamma_{\boldsymbol{t}}\}$. Consequently, group theory tells us that the one independent coefficient is $\alpha_{11} = \alpha_{22} = \alpha_{33}$ while the off-diagonal terms vanish $\alpha_{12} = \alpha_{23} = \alpha_{31} = 0$ for a symmetric second rank tensor in a medium with full rotational symmetry. This result for the number of independent components is given in Table 18.2.

Likewise Table 18.1 shows that there are no independent coefficients for $\overset{\leftrightarrow}{\alpha}^{(3)}$ in full rotational symmetry. Group theory thus tells us that this tensor vanishes by symmetry for the case of full rotational symmetry. This analysis further tells us that we cannot have any non-vanishing tensors of odd rank given by (18.4).

With regard to the fourth rank tensor, $\overset{\leftrightarrow}{\alpha}^{(4)}$, Table 18.1 shows that we can have only one independent coefficient for full rotational symmetry. In contrast, the $C_{(ij)(kl)}$ fourth rank tensor contains two independent coefficients in full rotational symmetry and the components of $d_{i(jk)}$ all vanish by symmetry.

This completes the discussion for the form of the various tensors in Table 18.2 under full rotational symmetry. Also listed in the table are the number of independent coefficients for several point group symmetries, including I_h, O_h, T_d, $D_{\infty h}$, $C_{\infty v}$, D_{6h}, and C_1. These results can be derived by considering these groups as subgroups of the full rotational group, and going from higher to lower symmetry. Some illustrative examples of the various point group symmetries are given in the following sections.

18.5 Tensors in Nonlinear Optics

In this section we consider polarizability tensors arising in nonlinear optics, including symmetric second rank, third rank and fourth rank tensors, such as those appearing in (18.5). We now consider these tensors for groups with symmetries lower than the full rotational group thereby filling in entries in Table 18.2.

18.5.1 Cubic Symmetry: O_h

The character table for group O_h is shown in Table 10.2 using solid state physics notation together with basis functions for each irreducible representation. We first consider the transformation properties of the linear response tensor $\overset{\leftrightarrow}{\alpha}^{(2)}$ and the nonlinear polarizability tensors $\overset{\leftrightarrow}{\alpha}^{(3)}$ and $\overset{\leftrightarrow}{\alpha}^{(4)}$ (see (18.5)). Consider for example the second rank tensor $\overset{\leftrightarrow}{\alpha}^{(2)}$ defined by

$$\boldsymbol{P} = \overset{\leftrightarrow}{\alpha}^{(2)} \cdot \boldsymbol{E} \tag{18.12}$$

in linear response theory. Both $\boldsymbol{P}$ and $\boldsymbol{E}$ transform as Γ_{15}^- (or Γ_{15} in Table 10.2), which gives for the direct product:

$$\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{E}} = \Gamma_{15}^- \otimes \Gamma_{15}^- = \Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{15}^+ + \Gamma_{25}^+ \,, \tag{18.13}$$

in which we use a notation which explicitly displays the irreducible representations that are even (+) or odd (−) under inversion, as can immediately be identified from the basis functions given in Table 10.2. But since the symmetry elements in Γ_{15}^+ are represented by a 3×3 matrix for the angular momentum R_{ij}, this 3×3 matrix is antisymmetric under interchange of $i \leftrightarrow j$ so that $R_{ij} = -R_{ji}$ and we have

$$\Gamma_{\overset{\leftrightarrow}{\alpha}}^{(s)} = \Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+ \,, \quad \Gamma_{\overset{\leftrightarrow}{\alpha}}^{(a)} = \Gamma_{15}^+ \tag{18.14}$$

showing the symmetries of the six partners for the second rank symmetric tensor, and the three partners for the second rank antisymmetric tensor. These results can also be obtained starting from the full rotation group, considering the decomposition of the $L = 0$ and $L = 2$ states for the symmetric partners and the $L = 1$ states for the antisymmetric partners.

Since Γ_1^+ is contained only once in the direct product $\Gamma_{15}^- \otimes \Gamma_{15}^-$ in cubic O_h symmetry (18.13), there is only one independent tensor component for $\overset{\leftrightarrow}{\alpha}^{(2)}$ and we can write $\overset{\leftrightarrow}{\alpha}^{(2)} = \alpha^0 \overset{\leftrightarrow}{1}$, where $\overset{\leftrightarrow}{1}$ is the unit tensor and α^0 is a constant. As a consequence of this general result, the electrical conductivity in cubic symmetry (O_h or T_d) is independent of the direction of the fields relative to the crystal axes and only one experiment is required to measure the polarizability or the conductivity of an unoriented cubic crystal.

In non-linear optics the lowest order non-linear term is $\overset{\leftrightarrow}{\alpha}^{(2)} \cdot \boldsymbol{EE}$ in (18.4) where $\overset{\leftrightarrow}{\alpha}^{(2)}$ is a third rank tensor. Since $(\boldsymbol{EE})$ is symmetric under interchange, then $(\boldsymbol{EE})$ transforms as

$$\Gamma_{\boldsymbol{EE}}^{(s)} = \Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+ \,, \tag{18.15}$$

where we have thrown out the Γ_{15}^+ term because it is antisymmetric under interchange of $E_iE_j \longrightarrow E_jE_i$. Thus, we obtain the irreducible representations contained in the direct product:

$$\begin{aligned}\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{EE}}^{(s)} &= \Gamma_{15}^- \otimes \{\Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+\} \\ &= (\Gamma_2^- + 2\Gamma_{15}^- + \Gamma_{25}^-)^{(s)} \\ &\quad +(\Gamma_{12}^- + \Gamma_{15}^- + \Gamma_{25}^-)\end{aligned} \tag{18.16}$$

yielding 18 partners, ten of which are symmetric, in agreement with the general result in Table 18.1. Of particular significance is the fact that none of the ten symmetric irreducible representations have Γ_1^+ symmetry. Thus there are no nonvanishing tensor components for a third rank tensor (such as $\overset{\leftrightarrow}{\alpha}^{(3)}$) in O_h symmetry, a result which could also be obtained by going from full rotational symmetry to O_h symmetry. The ten symmetric partners are found from Table 18.1 and includes angular momentum states $L = 1$ (corresponding to Γ_{15}^-) and $L = 3$ (corresponding to $\Gamma_2^- + \Gamma_{15}^- + \Gamma_{25}^-$) and the decomposition of these angular momentum states in full rotational symmetry yields the irreducible representations of group O_h as shown in Table 5.6 in Chap. 5.

We will now use the symmetric partners of the third rank tensor to discuss the fourth rank tensors. The next order term in (18.4) for the nonlinear response to a strong optical beam (e.g., multiple photon generation) is the fourth rank tensor $\overset{\leftrightarrow}{\alpha}^{(4)}$ defined by

$$\boldsymbol{P}^{(3)} = \overset{\leftrightarrow}{\alpha}^{(4)} \cdot \boldsymbol{EEE} \,. \tag{18.17}$$

If we consider the product $\boldsymbol{EEE}$ to arise from the symmetric combination for a third rank tensor (see (18.16)), then

$$\Gamma_{\boldsymbol{EEE}}^{(s)} = \Gamma_2^- + 2\Gamma_{15}^- + \Gamma_{25}^- \tag{18.18}$$

in cubic O_h symmetry, and

$$\begin{aligned}\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{EEE}}^{(s)} &= \Gamma_{15}^- \otimes \{\Gamma_2^- + 2\Gamma_{15}^- + \Gamma_{25}^-\} \\ &= 2\Gamma_1^+ + \Gamma_2^+ + 3\Gamma_{12}^+ + 3\Gamma_{15}^+ + 4\Gamma_{25}^+ \,.\end{aligned} \tag{18.19}$$

Referring to Table 18.1 we see that the symmetric partners for p^4 correspond to $L = 0$ (giving Γ_1^+), $L = 2$ (giving $\Gamma_{12}^+ + \Gamma_{25}^+$) and $L = 4$ (giving $\Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{15}^+ + \Gamma_{25}^+$) yielding the 15 symmetric partners

$$(2\Gamma_1^+ + 2\Gamma_{12}^+ + \Gamma_{15}^+ + 2\Gamma_{25}^+)^{(s)} \,,$$

showing which irreducible representations of (18.19) correspond to symmetric tensors. Since Γ_1^+ is contained twice among the 15 symmetric partners in cubic O_h symmetry, the symmetric fourth rank tensor $\overset{\leftrightarrow}{\alpha}^{(4)}$ has two independent coefficients that would need to be determined by experiments.

18.5.2 Tetrahedral Symmetry: T_d

The group T_d has half the number of symmetry operations of the group O_h, has slightly different classes from group O, and lacks inversion symmetry. Since $\Gamma_2^-(O_h) \to \Gamma_1(T_d)$, the corresponding relations to (18.16) shows that there exists one nonvanishing tensor component in T_d symmetry for a third rank tensor $\overset{\leftrightarrow}{\alpha}^{(3)}$. This means that zinc-blende structures such as (GaAs and InSb) can have nonvanishing nonlinear optical terms in $\overset{\leftrightarrow}{\alpha}^{(3)}$ because in T_d symmetry, the symmetric partners of the direct product transform as

$$(\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{EE}}^{(s)})^{(s)} = \Gamma_1 + 2\Gamma_{25} + \Gamma_{15} \tag{18.20}$$

and the Γ_1 representation is contained once (see Table 18.2).

18.5.3 Hexagonal Symmetry: D_{6h}

The character table for D_{6h} (hexagonal symmetry) is shown in Table A.21. In this subsection we will use the notation found in this character table. Vector forces in hexagonal symmetry decompose into two irreducible representations

$$\Gamma_{\text{vector}} = A_{2u} + E_{1u} \,. \tag{18.21}$$

Thus the second rank conductivity tensor requires consideration of

$$\begin{aligned}\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{E}} &= (A_{2u} + E_{1u}) \otimes (A_{2u} + E_{1u}) \\ &= 2A_{1g} + A_{2g} + 2E_{1g} + E_{2g} \\ &= (2A_{1g} + E_{1g} + E_{2g})^{(s)} + (A_{2g} + E_{1g})^{(a)} \,. \end{aligned} \tag{18.22}$$

Equation (18.22) indicates that there are two independent components for a symmetric second rank tensor such as the conductivity tensor. Hence, one must measure both in-plane and out-of-plane conductivity components to determine the conductivity tensor, which is as expected because of the equivalence of transport in the in-plane directions and along the c-axis. The symmetric tensor components (six partners) of (18.22) are

$$\Gamma_{\boldsymbol{EE}}^{(s)} = 2A_{1g} + E_{1g} + E_{2g} \tag{18.23}$$

and the antisymmetric components (three partners) are $(A_{2g} + E_{1g})$. Hence for the symmetric third rank tensor we can write

$$\begin{aligned}\Gamma_{\boldsymbol{P}} \otimes \Gamma_{\boldsymbol{EE}}^{(s)} &= (A_{2u} + E_{1u}) \otimes (2A_{1g} + E_{1g} + E_{2g}) \\ &= (A_{1u} + A_{2u} + B_{1u} + B_{2u} + 2E_{1u} + E_{2u})^{(s)} \\ &\quad +(2A_{2u} + 4E_{1u} + E_{2u})^{(a)} \end{aligned} \tag{18.24}$$

and there are thus no nonvanishing third rank tensor components in hexagonal D_{6h} symmetry because of parity considerations. For the fourth rank tensor we have

$$\begin{aligned}\Gamma_{\boldsymbol{P}} \otimes \Gamma^{(s)}_{\boldsymbol{EEE}} &= (A_{2u} + E_{1u}) \otimes (A_{1u} + A_{2u} + B_{1u} + B_{2u} + 2E_{1u} + 2E_{2u}) \\ &= (3A_{1g} + B_{1g} + B_{2g} + 2E_{1g} + 3E_{2g})^{(s)} \\ &\quad +(3A_{2g} + 2B_{1g} + 2B_{2g} + 4E_{1g} + 3E_{2g})^{(a)}\end{aligned} \tag{18.25}$$

and there are three independent tensor components. This result could also be obtained by going from full rotational symmetry ($L = 0$, $L = 2$, and $L = 4$), yielding the identical result

$$[A_{1g} + (A_{1g} + E_{1g} + E_{2g}) + (A_{1g} + B_{1g} + B_{2g} + E_{1g} + 2E_{2g})]^{(s)} .$$

The results for D_{6h} and $D_{\infty h}$ (see Table 18.2) show great similarity in behavior between all the tensors that are enumerated in this table, and these similarities stem from the angular momentum states to which they relate (see Table 5.6).

In lowering the symmetry from D_{6h} to D_{3h} which has no inversion symmetry, we get $\Gamma_i^{\pm}(D_{6h}) \to \Gamma_i(D_{3h})$ for the various irreducible representations. The only difference between the tensor properties in D_{6h} and D_{3d} symmetries involves odd rank tensors. Referring to (18.24) we can see that for D_{3h} there is a nonvanishing third rank tensor component and once again piezoelectric phenomena are symmetry allowed.

18.6 Elastic Modulus Tensor

The elastic modulus tensor represents a special case of a fourth rank tensor (see (18.8)). The elastic energy is written as

$$W = \frac{1}{2}\mathcal{C}_{ijkl} e_{ij} e_{kl} , \tag{18.26}$$

where W transforms as a scalar, the e_{ij} strain tensors transform as second rank symmetric tensors, and the $\mathcal{C}_{ijkl}$ matrices transform as a fourth rank tensor formed by the direct product of two symmetric second rank tensors. The symmetry of $\mathcal{C}_{ijkl}$ with regard to permutations was considered in Sect. 18.2. With regard to point group symmetry, we have the result following (18.10) that the maximum number of independent components of the $\mathcal{C}_{ijkl}$ tensor is the number of times the totally symmetric representation A_{1g} is contained in the direct product of the symmetric part of $\Gamma_{e_{ij}} \otimes \Gamma_{e_{kl}}$. In this section we provide a review of the conventions used to describe the $\mathcal{C}_{ijkl}$ tensor and then give results for a few crystal symmetries.

To make a connection between the elastic constants as discussed from the group theory perspective and in conventional solid state physics books, we introduce a contracted notation for the stress tensor and the strain tensor [57]:

$$\begin{aligned}
\sigma_1^m &= \sigma_{11}^m & \varepsilon_1 &= e_{11} \\
\sigma_2^m &= \sigma_{22}^m & \varepsilon_2 &= e_{22} \\
\sigma_3^m &= \sigma_{33}^m & \varepsilon_3 &= e_{33} \\
\sigma_4^m &= (\sigma_{23}^m + \sigma_{32}^m)/2 & \varepsilon_4 &= (e_{23} + e_{32}) \\
\sigma_5^m &= (\sigma_{13}^m + \sigma_{31}^m)/2 & \varepsilon_5 &= (e_{13} + e_{31}) \\
\sigma_6^m &= (\sigma_{12}^m + \sigma_{21}^m)/2 & \varepsilon_6 &= (e_{12} + e_{21})\,.
\end{aligned} \tag{18.27}$$

Since both the stress and strain tensors are symmetric, then $\mathcal{C}_{ijkl}$ can have no more than 36 components. We further note from (18.26) that the $\mathcal{C}_{ijkl}$ are symmetric under the interchange of $ij \leftrightarrow kl$, thereby reducing the number of independent components to 21 for a crystal with no symmetry operations beyond translational symmetry of the lattice. Crystals with non-trivial symmetry operations such as rotations, reflections and inversions will have fewer than 21 independent coefficients. Using the notation of (18.27) for the stress and strain tensors, the stress–strain relations can be written as

$$\begin{bmatrix} \sigma_1^m \\ \sigma_2^m \\ \sigma_3^m \\ \sigma_4^m \\ \sigma_5^m \\ \sigma_6^m \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}, \tag{18.28}$$

where the contracted C_{ij} matrix is symmetric, with the 21 independent coefficients containing 15 off-diagonal components and six diagonal components. In the most compact form, we write

$$\sigma_i^m = C_{ij}\varepsilon_j\,, \quad i, j = 1, \ldots 6\,, \tag{18.29}$$

where the C_{ij} components are normally used in the description of the mechanical properties of solids. The introduction of additional symmetry operations reduces the number of independent components from the maximum of 21 for a monoclinic crystal group C_1 with no symmetry to a much smaller number (e.g., two for the full rotational group R_∞). We consider here the case of full rotational symmetry, icosahedral symmetry, cubic symmetry, full axial symmetry, and hexagonal symmetry.

Fiber reinforced composites represent an interesting application of these symmetry forms. If the fibers are oriented in three-dimensional space in the six directions prescribed by icosahedral symmetry, then isotropy of the elastic modulus tensor will be obtained. In the corresponding two dimensional situation, if the fibers are oriented at 60° intervals, then isotropy is obtained in the plane. It is standard practice in the field of fiber composites to use fiber composite sheets stacked at 60° angular intervals to obtain "quasiplanar isotropy".

18.6.1 Full Rotational Symmetry: 3D Isotropy

The highest overall symmetry for an elastic medium is the full rotation group which corresponds to "jellium". For the case of full rotational symmetry, the rules for the addition of angular momentum tell us that a general second rank tensor transforms according to the representations that can be written as a sum of symmetric and an antisymmetric part

$$\Gamma = \Gamma^{(s)} + \Gamma^{(a)}\,, \tag{18.30}$$

where the symmetric components for full rotational symmetry transform as the irreducible representations

$$\Gamma^{(s)} = \Gamma_{\ell=0} + \Gamma_{\ell=2} \tag{18.31}$$

and the antisymmetric components transform as

$$\Gamma^{(a)} = \Gamma_{\ell=1}\,, \tag{18.32}$$

in which the irreducible representations of the full rotation group are denoted by their total angular momentum values ℓ, which are symmetric (antisymmetric) if ℓ is even (odd). Since the stress tensor $\boldsymbol{\nabla} \cdot \boldsymbol{F} \equiv \overset{\leftrightarrow}{\sigma}{}^{m}$ and the strain tensor $\overset{\leftrightarrow}{e}$ are *symmetric* second rank tensors, both σ_α^m and e_{ij} transform according to $(\Gamma_{\ell=0}+\Gamma_{\ell=2})$ in full rotational symmetry, where σ_α^m denotes a force in the x direction applied to a plane whose normal is in the α direction.

The fourth rank symmetric $\mathcal{C}_{ijkl}$ tensor of (18.26) transforms according to the symmetric part of the direct product of two second rank symmetric tensors $\Gamma^{(s)}_{\overset{\leftrightarrow}{e}} \otimes \Gamma^{(s)}_{\overset{\leftrightarrow}{e}}$ yielding

$$\begin{aligned}(\Gamma_{\ell=0} + \Gamma_{\ell=2}) \otimes (\Gamma_{\ell=0} + \Gamma_{\ell=2}) = {} & (2\Gamma_{\ell=0} + 2\Gamma_{\ell=2} + \Gamma_{\ell=4})^{(s)} \\ & +(\Gamma_{\ell=1} + \Gamma_{\ell=2} + \Gamma_{\ell=3})^{(a)}\,,\end{aligned} \tag{18.33}$$

in which the direct product has been broken up into the 21 partners that transform as symmetric irreducible representations (s) and the 15 partners for the antisymmetric irreducible representations (a). In the case of no crystal symmetry e_{ij} is specified by six constants and the $\mathcal{C}_{ijkl}$ tensor by 21 constants because $\mathcal{C}_{ijkl}$ is symmetrical under the interchange of $ij \leftrightarrow kl$. Since all the symmetry groups of interest are subgroups of the full rotation group, the procedure of going from higher to lower symmetry can be used to determine the irreducible representations for less symmetric groups that correspond to the stress and strain tensors and to the elastic tensor $\mathcal{C}_{ijkl}$.

As stated in Sect. 18.3 and in Sect. 18.4, the number of times the totally symmetric representation (e.g., $\Gamma_{\ell=0}$ for the full rotational group) is contained in the irreducible representations of a general matrix of arbitrary rank determines the minimum number of independent nonvanishing constants needed to specify that matrix. In the case of full rotational symmetry, (18.33) shows that the totally symmetric representation ($\Gamma_{\ell=0}$) is contained only twice in the direct product of the irreducible representations for two second rank symmetric tensors, indicating that only two independent nonvanishing constants are needed to describe the 21 constants of the $\mathcal{C}_{ijkl}$ tensor in full rotational symmetry, a result that is well known in elasticity theory for isotropic media and is discussed above (see Sect. 18.4).

We denote the two independent non-vanishing constants needed to specify the $\mathcal{C}_{ijkl}$ tensor by C_0 for $\Gamma_{\ell=0}$ and by C_2 for $\Gamma_{\ell=2}$ symmetry. We then use these two constants to relate symmetrized stresses and strains labeled by the irreducible representations $\Gamma_{\ell=0}$ and $\Gamma_{\ell=2}$ in the full rotation group. The symmetrized stress–strain equations are first written in full rotational symmetry, using basis functions for the partners of the pertinent irreducible representations (one for $\ell = 0$ and five for the $\ell = 2$ partners):

$$\begin{aligned}
(X_x + Y_y + Z_z) &= C_0(e_{xx} + e_{yy} + e_{zz}) && \text{for} \quad \ell = 0, m = 0 \\
(X_x - Y_y + iY_x + iX_y) &= C_2(e_{xx} - e_{yy} + ie_{xy} + ie_{yx}) && \text{for} \quad \ell = 2, m = 2 \\
(Z_x + X_z + iY_z + iZ_y) &= C_2(e_{zx} + e_{xz} + ie_{yz} + ie_{zy}) && \text{for} \quad \ell = 2, m = 1 \\
(Z_z - \frac{1}{2}(X_x + Y_y)) &= C_2(e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})) && \text{for} \quad \ell = 2, m = 0 \\
(Z_x + X_z - iY_z - iZ_y) &= C_2(e_{zx} + e_{xz} - ie_{yz} - ie_{zy}) && \text{for} \quad \ell = 2, m = -1 \\
(X_x - Y_y - iY_x - iX_y) &= C_2(e_{xx} - e_{yy} - ie_{xy} - ie_{yx}) && \text{for} \quad \ell = 2, m = -2
\end{aligned} \tag{18.34}$$

in which X, Y and Z are the Cartesian components of the stress tensor $\overleftrightarrow{\sigma}^m$ and the subscripts denote the shear directions. Since the basis functions in full rotational symmetry are specified by angular momentum states, the quantum numbers ℓ and m are used to denote the irreducible representations and their partners.

From the first, second, fourth and sixth relations in (18.34) we solve for X_x in terms of the strains, yielding

$$X_x = \left(\frac{C_0}{3} + \frac{2C_2}{3}\right) e_{xx} + \left(\frac{C_0}{3} - \frac{C_2}{3}\right) (e_{yy} + e_{zz}) \,. \tag{18.35}$$

Likewise five additional relations are then written down for the other five stress components in (18.34).

$$Y_y = \left(\frac{C_0}{3} + \frac{2C_2}{3}\right) e_{yy} + \left(\frac{C_0}{3} - \frac{C_2}{3}\right) (e_{zz} + e_{xx}) \,, \tag{18.36}$$

$$Z_z = \left(\frac{C_0}{3} + \frac{2C_2}{3}\right) e_{zz} + \left(\frac{C_0}{3} - \frac{C_2}{3}\right) (e_{xx} + e_{yy}) \,, \tag{18.37}$$

$$Z_y + Y_z = C_2\,(e_{zy} + e_{yz}) \,, \tag{18.38}$$

$$Y_x + X_y = C_2\,(e_{yx} + e_{xy}) \,, \tag{18.39}$$

$$Z_x + X_z = C_2\,(e_{zx} + e_{xz})\ . \tag{18.40}$$

In the notation that is commonly used in elasticity theory, we write the stress–strain relations as

$$\sigma_i^m = \sum_{j=1,6} C_{ij}\varepsilon_j\ , \tag{18.41}$$

where the six components of the symmetric stress and strain tensors are written in accordance with (18.27) as

$$\begin{array}{lcl}
\sigma_1^m = X_x & & \\
\sigma_2^m = Y_y & & \varepsilon_1 = e_{xx} \\
\sigma_3^m = Z_z & & \varepsilon_2 = e_{yy} \\
\sigma_4^m = \frac{1}{2}(Y_z + Z_y) & \text{and} & \varepsilon_3 = e_{zz} \\
\sigma_5^m = \frac{1}{2}(Z_x + X_z) & & \varepsilon_4 = (e_{yz} + e_{zy}) \\
 & & \varepsilon_5 = (e_{zx} + e_{xz}) \\
\sigma_6^m = \frac{1}{2}(X_y + Y_x) & & \varepsilon_6 = (e_{xy} + e_{yx})
\end{array} \tag{18.42}$$

and C_{ij} is the 6×6 elastic modulus matrix. In this notation the 21 partners that transform as $(2\Gamma_{\ell=0} + 2\Gamma_{\ell=2} + \Gamma_{\ell=4})$ in (18.33) correspond to the symmetric coefficients of C_{ij}. From the six relations for the six stress components (given explicitly by (18.35) through (18.40)), the relations between the C_0 and C_2 and the C_{ij} coefficients follow:

$$\begin{aligned}
C_{11} &= \frac{1}{3}(C_0 + 2C_2) = C_{22} = C_{33} \\
C_{12} &= \frac{1}{3}(C_0 - C_2) = C_{13} = C_{23} \\
C_{44} &= \frac{1}{2}C_2 = C_{55} = C_{66} \\
C_{ij} &= C_{ji}
\end{aligned} \tag{18.43}$$

from which we construct the C_{ij} matrix for a 3D isotropic medium. Note that the elastic modulus tensor for full rotational symmetry only two independent constants C_{11} and C_{12}

$$C_{ij} = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
 & C_{11} & C_{12} & 0 & 0 & 0 \\
 & & C_{11} & 0 & 0 & 0 \\
 & & & \frac{1}{2}(C_{11} - C_{12}) & 0 & 0 \\
 & & & & \frac{1}{2}(C_{11} - C_{12}) & 0 \\
 & & & & & \frac{1}{2}(C_{11} - C_{12})
\end{bmatrix} . \tag{18.44}$$

18.6.2 Icosahedral Symmetry

Any subgroup of the full rotation group for which the fivefold $\Gamma_{\ell=2}$ level degeneracy is not lifted will leave the form of the C_{ij} matrix invariant. The icosahedral group with inversion symmetry I_h, which is a subgroup of the full rotation group, and the icosahedral group without inversion I, which is a subgroup of both the full rotation group and the group I_h, are two examples of groups which preserve the fivefold degenerate level of the full rotation group and hence retain the form of the C_{ij} matrix given by (18.44). This result follows from at least two related arguments. The first argument relates to the compatibility relations between the full rotation group and the I_h group for which the basis functions follow the compatibility relations

$$\Gamma_{\ell=0} \longrightarrow (A_g)_{I_h} \quad \text{and} \quad \Gamma_{\ell=2} \longrightarrow (H_g)_{I_h} \, . \tag{18.45}$$

Thus, for the icosahedral group, we have for a symmetric second rank tensor:

$$\Gamma^{(s)}_{\overleftrightarrow{e}} = (A_g)_{I_h} + (H_g)_{I_h} \, . \tag{18.46}$$

From (18.46) we see that with respect to second rank tensors no lifting of degeneracy occurs in going from full rotational symmetry to I_h symmetry from which it follows that the number of nonvanishing independent constants in the C_{ij} matrix remains at 2 for I_h (and I) symmetry.

The same conclusion follows from the fact that the basis functions for $\Gamma_{\ell=0}$ and $\Gamma_{\ell=2}$ for the full rotation group can also be used as basis functions for the A_g and H_g irreducible representations of I_h. Therefore the same stress–strain relations are obtained in I_h symmetry as are given in (18.34) for full rotational symmetry. It therefore follows that the form of the C_{ij} matrix will also be the same for either group I_h or full rotational symmetry, thereby completing the proof.

Clearly, the direct product $\Gamma^{(s)}_{\overleftrightarrow{e}} \otimes \Gamma^{(s)}_{\overleftrightarrow{e}}$ given by (18.33) is not invariant as the symmetry is reduced from full rotational symmetry to I_h symmetry since the ninefold representation $\Gamma_{\ell=4}$ in (18.33) splits into the irreducible representations $(G_g + H_g)$ in going to the lower symmetry group I_h. But this is not of importance to the linear stress–strain equations which are invariant to this particular lowering of symmetry. However, when nonlinear effects are taken into account, and perturbations from (18.26) are needed to specify the nonlinear stress–strain relations, different mechanical behavior would be expected to occur in I_h symmetry in comparison to the full rotation group.

18.6.3 Cubic Symmetry

It should be noted that all symmetry groups forming Bravais lattices in condensed matter physics have too few symmetry operations to preserve the fivefold degeneracy of the $\ell = 2$ level of the full rotation group. For example, the Bravais lattice with the highest symmetry is the cubic group O_h.

The $\ell = 2$ irreducible representation in full rotational symmetry corresponds to a reducible representation of group O_h which splits into a threefold and a twofold level (the T_{2g} and E_g levels), so that in this case we will see below, three elastic constants are needed to specify the 6×6 matrix for C_{ij} in cubic O_h symmetry.

Since e_{ij} (where $i, j = x, y, z$) is a symmetric second rank tensor, the irreducible representations for e_{ij} in cubic symmetry are found as

$$\Gamma^{(s)}_{\overleftrightarrow{e}} = \Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+ . \tag{18.47}$$

From the direct product we obtain

$$\begin{aligned} \Gamma^{(s)}_{\overleftrightarrow{e}} \otimes \Gamma^{(s)}_{\overleftrightarrow{e}} &= (\Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+) \otimes (\Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+) \\ &= 3\Gamma_1^+ + \Gamma_2^+ + 4\Gamma_{12}^+ + 3\Gamma_{15}^+ + 5\Gamma_{25}^+ , \end{aligned} \tag{18.48}$$

which has 21 symmetric partners $(3\Gamma_1^+ + 3\Gamma_{12}^+ + \Gamma_{15}^+ + 3\Gamma_{25}^+)$ and 15 antisymmetric partners $(\Gamma_2^+ + \Gamma_{12}^+ + 2\Gamma_{15}^+ + 2\Gamma_{25}^+)$ and three independent C_{ij} coefficients. These results could also be obtained by going from higher (full rotational R_∞) symmetry to lower (O_h) symmetry using the cubic field splittings of the angular momenta shown in Table 5.6.

Forming basis functions for the irreducible representations of the stress and strain tensors in cubic O_h symmetry, we can then write the symmetrized elastic constant equations as

$$\begin{array}{rcll} (X_x + Y_y + Z_z) &=& C_{\Gamma_1^+}(e_{xx} + e_{yy} + e_{zz}) & \text{for} \quad \Gamma_1^+ \\ (X_x + \omega Y_y + \omega^2 Z_z) &=& C_{\Gamma_{12}^+}(e_{xx} + \omega e_{yy} + \omega^2 e_{zz}) & \text{for} \quad \Gamma_{12}^+ \\ (X_x + \omega^2 Y_y + \omega Z_z) &=& C_{\Gamma_{12}^+}(e_{xx} + \omega^2 e_{yy} + \omega e_{zz}) & \text{for} \quad \Gamma_{12}^{+*} \\ (Y_z + Z_y) &=& C_{\Gamma_{25}^+}(e_{yz}) & \text{for} \quad \Gamma_{25x}^+ \\ (Z_x + X_z) &=& C_{\Gamma_{25}^+}(e_{xz}) & \text{for} \quad \Gamma_{25y}^+ \\ (X_y + Y_x) &=& C_{\Gamma_{25}^+}(e_{xy}) & \text{for} \quad \Gamma_{25z}^+ . \end{array} \tag{18.49}$$

As in Sect. 18.6.1, we now solve for X_x, Y_y and Z_z in terms of e_{xx}, e_{yy} and e_{zz} to connect the three symmetry-based elastic constants $C^+_{\Gamma_1}$, $C^+_{\Gamma_{12}}$ and $C^+_{\Gamma_{25}}$ and the C_{11}, C_{12} and C_{44} in Nye's book (and other solid state physics books)

$$\begin{aligned} C_{11} &= (C^+_{\Gamma_1} + 2C^+_{\Gamma_{12}})/3 \\ C_{12} &= (C_{\Gamma_1} - C^+_{\Gamma_{12}})/3 \\ C_{44} &= C^+_{\Gamma_{25}}/2 , \end{aligned} \tag{18.50}$$

yielding an elastic tensor for cubic symmetry O_h in the form

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{bmatrix} . \tag{18.51}$$

18.6.4 Other Symmetry Groups

We briefly sketch results for C_{ijkl} for several groups of lower symmetry.

One simple method for finding the irreducible representations for lower symmetry groups is to make use of the compatibility relations between the full rotation group and the lower symmetry groups. For example, for group $D_{\infty h}$ (see character Table A.34) we have

$$\begin{aligned} \Gamma_{\ell=0} &\longrightarrow A_{1g} \\ \Gamma_{\ell=1} &\longrightarrow A_{2u} + E_{1u} \\ \Gamma_{\ell=2} &\longrightarrow A_{1g} + E_{1g} + E_{2g} \\ \Gamma_{\ell=3} &\longrightarrow A_{2u} + E_{1u} + E_{2u} + E_{3u} \\ \Gamma_{\ell=4} &\longrightarrow A_{1g} + E_{1g} + E_{2g} + E_{3g} + E_{4g} . \end{aligned} \tag{18.52}$$

Since the symmetric second rank tensor e_{ij} transforms according to the sum $\Gamma_{\ell=0}+\Gamma_{\ell=2}$, then we look for the irreducible representations contained therein. For $D_{\infty h}$ symmetry we would then obtain

$$\Gamma^{(s)}_{\overset{\leftrightarrow}{e}} = A_{1g} + (A_{1g} + E_{1g} + E_{2g}) = 2A_{1g} + E_{1g} + E_{2g} , \tag{18.53}$$

and a similar procedure would be used for other low symmetry groups.

From the symmetric terms in (18.33) and (18.52), we find that the $\mathcal{C}_{ijkl}$ tensor transforms according to $2\Gamma_{\ell=0}+2\Gamma_{\ell=2}+\Gamma_{\ell=4}$ which for $D_{\infty h}$ symmetry becomes

$$\begin{aligned} \Gamma_{C_{ijkl}} &= (2A_{1g}) + (2A_{1g} + 2E_{1g} + 2E_{2g}) + (A_{1g} + E_{1g} + E_{2g} + E_{3g} + E_{4g}) \\ &= 5A_{1g} + 3E_{1g} + 3E_{2g} + E_{3g} + E_{4g} . \end{aligned} \tag{18.54}$$

The same result as in (18.54) can be obtained by taking the direct product of $(A_{1g} + E_{1g} + E_{2g}) \otimes (A_{1g} + E_{1g} + E_{2g})$ which comes from $\Gamma_{\ell=2} \otimes \Gamma_{\ell=2}$ and retaining only the symmetric terms. From (18.54), we see that there are only five independent elastic constants remain for $D_{\infty h}$ symmetry.

To find the form of the elasticity matrix C_{ij} we go through the process of finding the (6×6) stress=strain relations for $\ell = 0, m = 0$ and

$\ell = 2, m = 2, 1, 0, -1, -2$ and then relate symmetry coefficients to obtain the C_{ij} coefficients and the relation between these to obtain the C_{ij} matrix for full axial $D_{\infty h}$ symmetry:

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & \frac{1}{2}(C_{11} - C_{12}) \end{bmatrix} . \tag{18.55}$$

The symmetric combination of irreducible representations for the group D_{6h} is

$$\Gamma^{(s)}_{\overleftrightarrow{e}} = 2A_{1g} + E_{1g} + E_{2g} \, , \tag{18.56}$$

which is isomorphic to $D_{\infty h}$. Using (18.33) and the irreducible representations contained in the angular momentum states $\ell = 0$, $\ell = 2$, and $\ell = 4$ in D_{6h} symmetry, we get

$$\begin{aligned} \Gamma_{\ell=0} &\rightarrow A_{1g} \\ \Gamma_{\ell=1} &\rightarrow A_{2u} + E_{1u} \\ \Gamma_{\ell=2} &\rightarrow A_{1g} + E_{1g} + E_{2g} \\ \Gamma_{\ell=3} &\rightarrow A_{2u} + B_{1u} + B_{2u} + E_{1u} + E_{2u} \\ \Gamma_{\ell=4} &\rightarrow A_{1g} + B_{1g} + B_{2g} + E_{1g} + 2E_{2g} \, , \end{aligned} \tag{18.57}$$

which gives

$$\Gamma_{C_{(ij)(kl)}} = 5A_{1g} + B_{1g} + B_{2g} + 3E_{1g} + 4E_{2g} \tag{18.58}$$

yielding five independent C_{ij} coefficients.

A similar analysis to that for the group $D_{\infty h}$, yields for D_{6h} the same form of C_{ij} as for $D_{\infty h}$ given by (18.55). As we go to lower symmetry more independent coefficients are needed.

For D_{2h} group symmetry which is the case of symmetry with respect to three mutually orthogonal planes (called *orthotropy* in the engineering mechanics literature), there remain nine independent components of C_{ij}. The C_{ij} tensor in this case assumes the form

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix} . \tag{18.59}$$

The lowest nontrivial symmetry group for consideration of the elastic tensor is group C_{2h} with a single symmetry plane. In this case C_{ij} has 13 independent components and assumes the form

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ & C_{22} & C_{23} & 0 & 0 & C_{26} \\ & & C_{33} & 0 & 0 & C_{36} \\ & & & C_{44} & C_{45} & 0 \\ & & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix} . \qquad (18.60)$$

Selected Problems

18.1. Consider the third rank tensor $d_{i(jk)}$ in (18.6) and (18.7).

(a) Show from Table 18.1 that there are exactly 18 independent coefficients after taking permutational symmetry into account.
(b) Find the number of independent coefficients for full rotational symmetry.
(c) Find the number of independent coefficients for O_h and T_d symmetries.
(d) Finally find the number of independent coefficients for D_{4h} symmetry.

18.2. Suppose that stress is applied to FCC aluminum Al in the (100) direction, and suppose that the effect of the resulting strain is to lower the symmetry of aluminum from cubic O_h symmetry to tetragonal D_{4h} symmetry. The situation outlined here arises in the fabrication of superlattices using the molecular beam epitaxy technique.

(a) How many independent elastic constants are there in the stressed aluminum Al?
(b) What is the new symmetrized form of the stress–strain relations (see (18.34))?
(c) What is the form of the C_{ijkl} tensor for D_{4h} symmetry (see (18.44))?

18.3. (a) Assume that the material in Problem 18.2 is a nonlinear elastic material and the stress–strain relation is of the form

$$\sigma_{ij}^{m} = C_{ijkl}^{(2)} \varepsilon_{kl} + C_{ijklmn}^{(3)} \varepsilon_{kl} \varepsilon_{mn} + \cdots$$

Consider the symmetry of the nonlinear tensor coefficient $C_{ijklmn}^{(3)}$ explicitly. How many independent constants are there in $C_{ijklmn}^{(3)}$ assuming that the point group symmetry is C_1 (i.e., no rotational symmetry elements other than the identity operation), but taking into account permutation symmetry?

(b) How many independent constants are there when taking into account both permutation and crystal (O_h) symmetry? (*Note:* To do this problem, you may have to make a new entry to Table 18.1.)

18.4. Suppose that we prepare a quantum well using as the constituents GaAs and $GaAs_{1-x}P_x$. In bulk form GaAs and similar III–V compounds have T_d symmetry. The lattice mismatch introduces lattice strain and lowers the symmetry. Denote by $\hat{z}$ the direction normal to the layer. Find the number of independent coefficients in the polarizability tensor, including $\overleftrightarrow{\alpha}^{(2)}$, $\overleftrightarrow{\alpha}^{(3)}$, and $\overleftrightarrow{\alpha}^{(4)}$, for

(i) $\hat{z} \parallel (100)$
(ii) $\hat{z} \parallel (111)$
(iii) $\hat{z} \parallel (110)$

Using these results, how can infrared and Raman spectroscopy be used to distinguish between the crystalline orientation of the quantum well?