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1997 J. Phys.: Condens. Matter 9 3023

(http://iopscience.iop.org/0953-8984/9/14/016)

J. Phys.: Condens. Matter **9** (1997) 3023–3031. Printed in the UK PII: S0953-8984(97)78452-2

Symmetrical transformation of basic translation vectors in the supercell model of imperfect crystals and in the theory of special points of the Brillouin zone

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Received 8 October 1996

Abstract. The matrices of the symmetrical transformations for all the three-dimensional Bravais lattices are found. These matrices may be applied for the investigation of physical properties of single defects in crystals in the supercell model. The corresponding transformations of reciprocal lattices with a not more than 32-fold decrease of the Brillouin zone volume are used for the generation of special point sets for the approximative numerical integration over the Brillouin zone in cubic crystals with simple, face-centred and body-centred lattices.

1. Introduction

The supercell approach is widely used for the calculation of the energy levels of a crystal with a point defect in order to estimate the position of the local defect energy levels with respect to the energy band edges of the perfect crystal (a model of a crystal with a periodic defect or a supercell model of an imperfect crystal [1–6]). In this model the supercells obtained due to a symmetrical linear transformation of the basic vectors of a host lattice are favourable as this assures the largest possible distance between neighbouring defects for the fixed supercell volume [7].

Special points of the Brillouin zone are used in crystal calculations involving the averaging over the Brillouin zone of periodic functions of the wavevector. Many procedures for special point generation have been proposed [8–14]. The supercell method appears to be the most general and fruitful in practical applications [13, 14]. The symmetrical transformation of the basic vectors of the direct (and reciprocal) lattice is also favourable in the supercell method of special point generation as it gives as a rule the most efficient sets of special points.

In this paper both these aspects of application of the supercell method are considered. In section 2 the matrices of symmetrical transformation are generated for all the 14 three-dimensional Bravais lattices. In section 3 the main features of the procedure of special point generation by the supercell method are exposed. In section 4 are given the sets of special points for cubic crystals with simple (P), face-centred (F) and body-centred (I) lattices generated by the symmetrical increase of the unit cell volume up to 32-fold.

0953-8984/97/143023+09$19.50

2. The supercell method in the theory of imperfect crystals

The symmetry of the supercell model of a crystal with a point defect is studied in [7]. The general consideration is illustrated in detail by the examples of point defects of atomic and molecular types in the MgO crystal. The main point of the supercell model is the transition from the initial Bravais lattice to a 'rare' one consisting of supercells with the help of integer linear transformation of basic translation vectors of the initial lattice. This transformation is called symmetric if it does not change the symmetry of the lattice. The symmetric transformation is compatible with the change of lattice type in the limits of the same crystal system. As is pointed out in [7] the symmetrical transformation of basic translation vectors is the most efficient for the application of the supercell model when investigating physical properties of a single defect in a crystal.

Let $\boldsymbol{a}_i(\Gamma_1)$ ($i = 1, 2, 3$) be the basic translation vectors of the initial direct lattice of type Γ_1 and $\boldsymbol{A}_j(\Gamma_2)$ ($j = 1, 2, 3$) be the basic translation vectors of a new lattice of type Γ_2 with the same point symmetry but composed of supercells. Then

$$\boldsymbol{A}_j(\Gamma_2) = \sum_i l_{ji}(\Gamma_2\Gamma_1)\boldsymbol{a}_i(\Gamma_1) \qquad |\det l| = L \tag{1}$$

where $l_{ji}(\Gamma_2\Gamma_1)$ are integer elements of the matrix $l(\Gamma_2\Gamma_1)$ defining the transition from the lattice of type Γ_1 to the lattice of type Γ_2.

The vectors $\boldsymbol{A}_j(\Gamma_2)$ have well defined orientation with respect to point symmetry elements of the lattices which are the same for both lattices because of the symmetrical character of the transformation (1). Let us define the components of the vectors $\boldsymbol{A}_j(\Gamma_2)$ by the parameters s_k assuring their correct orientation relative to the lattice symmetry elements and the correct relations between their lengths (if there are any). Then three vector relations (1) give nine linear nonhomogeneous equations to determine nine matrix elements $l_{ij}(\Gamma_2\Gamma_1)$ as functions of the parameters s_k. The requirements that these matrix elements must be integers define the possible values of the parameters s_k giving the solution of the problem.

Let us demonstrate the procedure of finding the matrix of a symmetrical transformation (1) on the example of the rhombohedral crystal system where there is only one lattice type (R). The basic translation vectors of the initial lattice are the following:

$$\boldsymbol{a}_1 = (a, 0, c) \qquad \boldsymbol{a}_{2,3} = \left(-a/2, \pm a\sqrt{3}/2, c\right).$$

The basic translation vectors of the new lattice composed of supercells for symmetrical transformation (1) have the same form (the parameters a and c of the initial lattice are replaced with the parameters s_1a, s_2c)

$$\boldsymbol{A}_1 = (s_1a, 0, s_2c) \qquad \boldsymbol{A}_{2,3} = \left(-s_1a/2, \pm s_1a\sqrt{3}/2, s_2c\right).$$

Inserting them in (1) one obtains nine equations for nine elements of the matrix l. The solution of this system is

$$l_{ij} = \frac{s_2 + 2s_1}{3}\delta_{ij} + \frac{s_2 - s_1}{3}(1 - \delta_{ij}).$$

As the matrix elements l_{ij} must be integers let us assign $(s_2-s_1)/3 = n_2$ and $(s_2+2s_1)/3 = n_1 + n_2$. The matrix of the symmetrical transformation for a rhombohedral lattice with the corresponding value of L may be found in appendix A where the matrices of the symmetrical transformations for all three-dimensional crystal lattices are given. Let us explain the peculiarities of the consideration made for each of seven possible crystal systems.

In the triclinic crystal system an arbitrary matrix with integer elements defines a symmetrical transformation (any transformation seems to be symmetrical because of the low point symmetry of the lattice).

In the monoclinic crystal system there are two lattices, simple (P) and base-centred (A) each of which is defined by five parameters. Therefore the matrices of symmetrical transformations are determined by five integers.

In the hexagonal crystal system there is only one lattice type (P), but the basic translation vectors may be oriented in two different ways relative to the basic translation vectors of the initial lattice: either parallel to them or rotated through an angle of $\pi/6$ about the Z-axis. Therefore two types of symmetrical transformation are possible in this case (with two parameters for each).

In the orthorhombic crystal system the base-centred lattice merits special attention because of different possible settings. Let the initial base-centred lattice have the setting C. The transition to base-centred lattices with settings C and A (or B) gives different results (see appendix A). The change of setting for the transition to other types of lattice does not give new supercells.

In tetragonal crystal systems there are two types of Bravais lattice (P and I). All their symmetrical transformations may be obtained from the symmetrical transformations for orthorhombic lattices if one sets $n_1 = n_2$ and takes into account that base-centred and face-centred orthorhombic lattices become simple and body-centred tetragonal ones respectively.

The matrices of symmetrical transformations for all the types (P, F, I) of cubic lattices may be also obtained from the matrices of symmetrical transformations for orthorhombic lattices if one sets $n_1 = n_2 = n_3 = n$.

3. The supercell method of special point set generation

Let $\boldsymbol{B}_i(\tilde{\Gamma}_1)$ ($i = 1, 2, 3$) and $\boldsymbol{b}_j(\tilde{\Gamma}_2)$ ($j = 1, 2, 3$) be basic translation vectors of the reciprocal lattices corresponding to direct ones determined by basic translation vectors $\boldsymbol{a}_i(\Gamma_1)$ and $\boldsymbol{A}_j(\Gamma_2)$ respectively. The transformation (1) of the direct lattices is accompanied by the following transformation of reciprocal lattices:

$$\boldsymbol{b}_j(\tilde{\Gamma}_2) = \sum_i (l^{-1}(\Gamma_2\Gamma_1))_{ij}\boldsymbol{B}_i(\tilde{\Gamma}_1). \tag{2}$$

For the symmetrical transformation (1) the transformation (2) is also symmetrical as it does not change the point symmetry of the reciprocal lattice. The symmetrical transformation is compatible with the change of the reciprocal lattice type in the limits of the same crystal system too.

The vectors $\boldsymbol{b}_j$ defining the small Brillouin zone are very important in the theory of special points [13, 14]. Let $f(\boldsymbol{K})$ be the function with a point symmetry G to be integrated over the initial Brillouin zone where the wavevector $\boldsymbol{K}$ varies. Usually the point symmetry group G either coincides with the crystal class $\tilde{G}$ of the crystal (if $\tilde{G}$ contains the inversion I) or $G = \tilde{G} \times C_i$ (otherwise) [14]. The function $f(\boldsymbol{K})$ may be expanded in Fourier series over symmetrized plane waves $P_m(\boldsymbol{K})$

$$f(\boldsymbol{K}) = \sum_m f_m P_m(\boldsymbol{K}) \tag{3}$$

$$P_m(\boldsymbol{K}) = \frac{1}{n_G}\sum_{g\epsilon G}\exp(\mathrm{i}\boldsymbol{K}\cdot g\boldsymbol{a_m}) \tag{4}$$

where $\boldsymbol{a_m} = \sum_{i=1}^{3} m_i \boldsymbol{a}_i$ is some translation vector of the direct lattice, the integer $m = 0, 1, 2, \ldots$ numerates the stars of vectors $g\boldsymbol{a_m}(g\epsilon G)$ in order of increasing length. The functions $P_m(\boldsymbol{K})$ have the properties [9]

$$\frac{1}{V_{BZ}} \int_{BZ} P_m(\boldsymbol{K})\,\mathrm{d}\boldsymbol{K} = \delta_{m0} \qquad m = 0, 1, 2, \ldots . \tag{5}$$

Let $\bar{m}$ be a subset of m corresponding to the stars of vectors $g\boldsymbol{A_m}(g\epsilon G)$. As it is proved in [13] and [14], for symmetrical transformation (1) L points in the initial Brillouin zone (related to the initial basic translation vectors $\boldsymbol{a}_i$)

$$\boldsymbol{K}_l^{(k)} = \boldsymbol{k} + \sum_j q_{tj} \boldsymbol{b}_j \tag{6}$$

where q_{tj} are integers and $\boldsymbol{k}$ is an arbitrary vector in the small Brillouin zone (related to the basic translation vectors $\boldsymbol{A}_j$), satisfy the relation

$$\sum_{t=1}^{L} P_m(\boldsymbol{K}_t^{(\boldsymbol{k})}) = L \sum_{\bar{m}} P_{\bar{m}}(\boldsymbol{k}) \delta_{m\bar{m}} \tag{7}$$

or

$$\sum_{s=1}^{N} w_s P_m(\boldsymbol{K}_s^{(\boldsymbol{k})}) = \sum_{\bar{m}} P_{\bar{m}}(\boldsymbol{k}) \delta_{m\bar{m}}. \tag{8}$$

In the latter relation s numbers the different irreducible wavevector $\boldsymbol{K}$ stars which contain the points (6) and $w_s = L_s/L$ (L_s is the number of points (6) belonging to the sth star, $\sum_{s=1}^{N} L_s = L$). The points $\boldsymbol{K}_s^{(\boldsymbol{k})}$ are usually chosen in the irreducible part of the Brillouin zone.

Relations (3), (5) and (8) give the following formula of the approximative numerical integration:

$$\frac{1}{V_{BZ}} \int_{BZ} f(\boldsymbol{K})\,\mathrm{d}\boldsymbol{K} \approx \sum_{s=1}^{N} w_s f(\boldsymbol{K}_s^{(\boldsymbol{k})}). \tag{9}$$

Let $M = s_0$ be the number denoting the set of vectors $g\boldsymbol{A_m}$ with the smallest (nonzero) lengths. If $f(\boldsymbol{K})$ is some linear combination of $P_m(\boldsymbol{K})$ with $m < M$, then the formula (9) appears to be exact. The number M characterizes the accuracy of the numerical integration formula. The special choice of $\boldsymbol{k}$ can either increase the accuracy M, or change the number N of points $\boldsymbol{K}_s^{(\boldsymbol{k})}$ (or both) [13, 14].

To generate the set of points $\boldsymbol{K}_s^{(\boldsymbol{k})}$ for any of 14 Bravais lattices it is sufficient to find the inverse of the corresponding matrix from appendix A, to pick out according to (6) L points in the Brillouin zone related to basic translation vectors $\boldsymbol{a}_i$ and to distribute them over stars. The distribution of these points over stars depends on the symmetry group G of the function $f(\boldsymbol{K})$ and cannot be made in general form. In the next section the special point sets are generated for cubic lattices.

4. Special point sets for cubic crystals

The sets of special points for numerical integration over the Brillouin zone of cubic crystals are given in tables 1–3. They are obtained by symmetrically increasing the unit cells of cubic lattices for $L \leqslant 32$. The tables contain the sets (6) with $\boldsymbol{k} = \boldsymbol{0}$ and some efficient sets with $\boldsymbol{k} \neq \boldsymbol{0}$. Some sets were found earlier in [8–14]. The types of lattice (TL) composed of supercells are indicated in the second columns. The symbols of the matrices $Q = l^{-1}$ (2)

Table 1. Special points of the Brillouin zone for the simple cubic lattice generated by the symmetrical transformation: $\boldsymbol{B}_1 = (2\pi/a)(1,0,0)$, $\boldsymbol{B}_2 = (2\pi/a)(0,1,0)$, $\boldsymbol{B}_3 = (2\pi/a)(0,0,1)$; $\boldsymbol{K}_s = \alpha_1\boldsymbol{B}_1 + \alpha_2\boldsymbol{B}_2 + \alpha_3\boldsymbol{B}_3 \equiv (\alpha_1, \alpha_2, \alpha_3)$.

L	TL	$l^{(-1)}$	M	Special points $\boldsymbol{K}_s$ {weights w_s}
2	F	$\frac{1}{2}Q_2$	2	$(0,0,0)\ \{\frac{1}{2}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{2}\}$
4	I	$\frac{1}{2}Q_3$	3	$(0,0,0)\ \{\frac{1}{4}\}\ (\frac{1}{2},\frac{1}{2},0)\ \{\frac{3}{4}\}$
			4	$(\frac{1}{4},0,0)\ \{\frac{1}{4}\}\ [(\frac{1}{2},0,\frac{1}{4})\ \{\frac{1}{4}\}\ (\frac{1}{2},\frac{1}{4},0)\ \{\frac{1}{4}\}]\ (\frac{1}{2},\frac{1}{2},\frac{1}{4})\ \{\frac{1}{4}\}$
8	P	$\frac{1}{2}Q_1$	4	$(0,0,0)\ \{\frac{1}{8}\}\ (\frac{1}{2},0,0)\ \{\frac{3}{8}\}\ (\frac{1}{2},\frac{1}{2},0)\ \{\frac{3}{8}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{8}\}$
			15 (19)	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})\ \{\frac{1}{8}\}\ (\frac{3}{8},\frac{1}{8},\frac{1}{8})\ \{\frac{3}{8}\}\ (\frac{3}{8},\frac{3}{8},\frac{1}{8})\ \{\frac{3}{8}\}\ (\frac{3}{8},\frac{3}{8},\frac{3}{8})\ \{\frac{1}{8}\}$
16	F	$\frac{1}{4}Q_2$	7	$(0,0,0)\ \{\frac{1}{16}\}\ (\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \{\frac{1}{2}\}\ (\frac{1}{2},0,0)\ \{\frac{3}{16}\}\ (\frac{1}{2},\frac{1}{2},0)\ \{\frac{3}{16}\}\ (1,1,1)\ \{\frac{1}{16}\}$
27	P	$\frac{1}{3}Q_1$	9	$(0,0,0)\ \{\frac{1}{27}\}\ (\frac{1}{3},0,0)\ \{\frac{2}{9}\}\ (\frac{1}{3},\frac{1}{3},0)\ \{\frac{4}{9}\}\ (\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \{\frac{8}{27}\}$
32	I	$\frac{1}{4}Q_3$	12	$(0,0,0)\ \{\frac{1}{32}\}\ (\frac{1}{4},\frac{1}{4},0)\ \{\frac{3}{8}\}\ (\frac{1}{2},0,0)\ \{\frac{3}{32}\}\ (\frac{1}{2},\frac{1}{4},\frac{1}{4})\ \{\frac{3}{8}\}\ (\frac{1}{2},\frac{1}{2},0)\ \{\frac{3}{32}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{32}\}$

Table 2. Special points of the Brillouin zone for the face-centred cubic lattice generated by the symmetrical transformation: $\boldsymbol{B}_1 = (2\pi/a)(-1,1,1)$, $\boldsymbol{B}_2 = (2\pi/a)(1,-1,1)$, $\boldsymbol{B}_3 = (2\pi/a)(1,1,-1)$; $\boldsymbol{K}_s = \alpha_1\boldsymbol{B}_1 + \alpha_2\boldsymbol{B}_2 + \alpha_3\boldsymbol{B}_3 \equiv (\alpha_1, \alpha_2, \alpha_3)$.

L	TL	$l^{(-1)}$	M	Special points $\boldsymbol{K}_s$ {weights w_s}
4	P	$\frac{1}{2}Q_3$	2	$(0,0,0)\ \{\frac{1}{4}\}\ (0,\frac{1}{2},\frac{1}{2})\ \{\frac{3}{4}\}$
			2	$(\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \{1\}$
			2	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{1\}$
8	F	$\frac{1}{2}Q_1$	4	$(0,0,0)\ \{\frac{1}{8}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{2}\}\ (0,\frac{1}{2},\frac{1}{2})\ \{\frac{3}{8}\}$
			4	$(0,\frac{1}{4},\frac{1}{4})\ \{\frac{1}{4}\}\ (\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \{\frac{1}{2}\}\ (\frac{\bar{1}}{4},\frac{1}{4},\frac{1}{2})\ \{\frac{1}{4}\}$
			8 (10)	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \{\frac{1}{4}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{4})\ \{\frac{3}{4}\}$
16	I	$\frac{1}{4}Q_4$	6 (7)	$(0,0,0)\ \{\frac{1}{16}\}\ (\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \{\frac{3}{4}\}\ (0,\frac{1}{2},\frac{1}{2})\ \{\frac{3}{16}\}$
			6 (7)	$(0,\frac{1}{4},\frac{1}{4})\ \{\frac{3}{8}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{4}\}\ (\frac{\bar{1}}{4},\frac{1}{4},\frac{1}{2})\ \{\frac{3}{8}\}$
27	F	$\frac{1}{3}Q_1$	10	$(0,0,0)\ \{\frac{1}{27}\}\ (\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \{\frac{8}{27}\}\ (0,\frac{1}{3},\frac{1}{3})\ \{\frac{2}{9}\}\ (\frac{1}{3},\frac{1}{3},\frac{2}{3})\ \{\frac{4}{9}\}$
32	P	$\frac{1}{4}Q_3$	8	$(0,0,0)\ \{\frac{1}{32}\}\ (0,\frac{1}{4},\frac{1}{4})\ \{\frac{3}{16}\}\ (\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \{\frac{3}{8}\}\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \{\frac{1}{8}\}\ (0,\frac{1}{2},\frac{1}{2})\ \{\frac{3}{32}\}\ (\frac{1}{4},\frac{1}{2},\frac{3}{4})\ \{\frac{3}{16}\}$

of transformation of basic vectors of reciprocal lattices are given in the third column. The matrices Q_i themselves are given in appendix B.

The system of symmetrized plane waves $P_m(\boldsymbol{K})$ depends on the crystal class. Therefore the number M which characterizes the efficiency of the set of special points may be different for different crystal classes [14]. In tables 1–3 the numbers M are given for crystal classes T_d, O, O_h and T, T_h (in parentheses). Besides, in table 1 for $L = 4$ two special points $(1/2, 0, 1/4)$ and $(1/2, 1/4, 0)$ are related to different stars in crystal classes T, T_h and each of them is a special point with the weight 1/4; in crystal classes T_d, O, O_h they are related to the same star and this three-special-point set contains only one of these points with the weight 1/2.

Appendix A. Matrices of the symmetrical transformations of three-dimensional Bravais lattices

A.1. The triclinic crystal system

(i) $l(\mathrm{P}, \mathrm{P})$ is an arbitrary integer matrix.

Table 3. Special points of the Brillouin zone for the body-centred cubic lattice generated by the symmetrical transformation: $\boldsymbol{B}_1 = (2\pi/a)(0, 1, 1)$, $\boldsymbol{B}_2 = (2\pi/a)(1, 0, 1)$, $\boldsymbol{B}_3 = (2\pi/a)(1, 1, 0)$; $\boldsymbol{K}_s = \alpha_1\boldsymbol{B}_1 + \alpha_2\boldsymbol{B}_2 + \alpha_3\boldsymbol{B}_3 \equiv (\alpha_1, \alpha_2, \alpha_3)$.

L	TL	$l^{(-1)}$	M	Special points $\boldsymbol{K}_s$ {weights w_s}
2	P	$\frac{1}{2}Q_2$	2	$(0, 0, 0)\ \{\frac{1}{2}\}\ (\frac{\bar{1}}{2}, \frac{1}{2}, \frac{1}{2})\ \{\frac{1}{2}\}$
			2	$(\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{4})\ \{1\}$
			2	$(0, 0, \frac{1}{2})\ \{1\}$
			2	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\ \{1\}$
			3	$(\frac{\bar{1}}{12}, \frac{1}{4}, \frac{1}{4})\ \{1\}$
4	F	$\frac{1}{4}Q_5$	3	$(0, 0, 0)\ \{\frac{1}{4}\}\ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{2}\}\ (\frac{\bar{1}}{2}, \frac{1}{2}, \frac{1}{2})\ \{\frac{1}{4}\}$
			3	$(\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{2}\}\ (0, 0, \frac{1}{2})\ \{\frac{1}{2}\}$
			6	$(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})\ \{\frac{1}{2}\}\ (\frac{3}{8}, \frac{3}{8}, \frac{3}{8})\ \{\frac{1}{2}\}$
8	I	$\frac{1}{2}Q_1$	5	$(0, 0, 0)\ \{\frac{1}{8}\}\ (0, 0, \frac{1}{2})\ \{\frac{3}{4}\}\ (\frac{\bar{1}}{2}, \frac{1}{2}, \frac{1}{2})\ \{\frac{1}{8}\}$
			5	$(\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{3}{4}\}\ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{4}\}$
			6	$(0, 0, \frac{1}{4})\ \{\frac{1}{4}\}\ (0, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{2}\}\ (\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{2})\ \{\frac{1}{4}\}$
16	P	$\frac{1}{4}Q_2$	6	$(0, 0, 0)\ \{\frac{1}{16}\}\ (\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{3}{8}\}\ (0, 0, \frac{1}{2})\ \{\frac{3}{8}\}\ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{8}\}\ (\frac{\bar{1}}{2}, \frac{1}{2}, \frac{1}{2})\ \{\frac{1}{16}\}$
			6	$(\frac{\bar{1}}{8}, \frac{1}{8}, \frac{1}{8})\ \{\frac{1}{8}\}\ (\frac{\bar{1}}{8}, \frac{1}{8}, \frac{3}{8})\ \{\frac{1}{2}\}\ (\frac{5}{8}, \frac{3}{8}, \frac{3}{8})\ \{\frac{1}{8}\}\ (\frac{3}{8}, \frac{1}{8}, \frac{1}{8})\ \{\frac{1}{4}\}$
27	I	$\frac{1}{3}Q_1$	10 (11)	$(0, 0, 0)\ \{\frac{1}{27}\}\ (0, 0, \frac{1}{3})\ \{\frac{4}{9}\}\ (\frac{\bar{1}}{3}, \frac{1}{3}, \frac{1}{3})\ \{\frac{2}{9}\}\ (0, \frac{1}{3}, \frac{1}{3})\ \{\frac{8}{27}\}$
32	F	$\frac{1}{8}Q_5$	12	$(0, 0, 0)\ \{\frac{1}{32}\}\ (\frac{1}{8}, \frac{1}{8}, \frac{1}{8})\ \{\frac{1}{4}\}\ (\frac{\bar{1}}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{3}{16}\}\ (0, 0, \frac{1}{2})\ \{\frac{3}{16}\}\ (\frac{\bar{1}}{8}, \frac{3}{8}, \frac{3}{8})\ \{\frac{1}{4}\}\ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\ \{\frac{1}{16}\}\ (\frac{\bar{1}}{2}, \frac{1}{2}, \frac{1}{2})\ \{\frac{1}{32}\}$

A.2. *The monoclinic crystal system*

$$\text{(i)}\ l(\mathrm{P,P}) = \begin{pmatrix} n_1 & n_5 & 0 \\ n_4 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix} \qquad L = (n_1n_2 - n_4n_5)n_3 \tag{A1}$$

$$\text{(ii)}\ l(\mathrm{A,P}) = \begin{pmatrix} n_1 & n_5 & 0 \\ n_4 & n_2 & -n_3 \\ n_4 & n_2 & n_3 \end{pmatrix} \qquad L = 2(n_1n_2 - n_4n_5)n_3$$

$$\text{(iii)}\ l(\mathrm{P,A}) = \begin{pmatrix} n_1 & n_4 & n_4 \\ n_5 & n_2 & n_2 \\ 0 & -n_3 & n_3 \end{pmatrix} \qquad L = 2(n_1n_2 - n_4n_5)n_3$$

$$\text{(iv)}\ l(\mathrm{A,A}) = \begin{pmatrix} n_1 & n_5 & n_5 \\ n_4 & n_2+n_3 & n_2-n_3 \\ n_4 & n_2-n_3 & n_2+n_3 \end{pmatrix} \qquad L = 4(n_1n_2 - n_4n_5)n_3.$$

A.3. *The hexagonal crystal system*

$$\text{(i)}\ l^{(1)}(\mathrm{P,P}) = \begin{pmatrix} n_1 & 0 & 0 \\ 0 & n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix} \qquad L = n_1^2n_2 \tag{A2}$$

$$\text{(ii)}\ l^{(2)}(\mathrm{P,P}) = \begin{pmatrix} n_1 & -n_1 & 0 \\ n_1 & 2n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix} \qquad L = 3n_1^2n_2.$$

A.4. The rhombohedral crystal system

$$\text{(i) } l(\mathrm{R},\mathrm{R}) = \begin{pmatrix} n_1+n_2 & n_2 & n_2 \\ n_2 & 2n_1+n_2 & n_2 \\ n_2 & n_2 & n_1+n_2 \end{pmatrix} \qquad L = n_1^2(n_1+3n_2).$$

A.5. The orthorhombic crystal system

(i) $l(\mathrm{P},\mathrm{P})$ coincides with (A1)

$$\text{(ii) } l(\mathrm{C},\mathrm{P}) = \begin{pmatrix} n_1 & -n_2 & 0 \\ n_1 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix} \qquad L = 2n_1n_2n_3$$

$$\text{(iii) } l(\mathrm{F},\mathrm{P}) = \begin{pmatrix} 0 & n_2 & n_3 \\ n_1 & 0 & n_3 \\ n_1 & n_2 & 0 \end{pmatrix} \qquad L = 2n_1n_2n_3$$

$$\text{(iv) } l(\mathrm{I},\mathrm{P}) = \begin{pmatrix} -n_1 & n_2 & n_3 \\ n_1 & -n_2 & n_3 \\ n_1 & n_2 & -n_3 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(v) } l(\mathrm{P},\mathrm{C}) = \begin{pmatrix} n_1 & n_1 & 0 \\ -n_2 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix} \qquad L = 2n_1n_2n_3$$

$$\text{(vi) } l(\mathrm{C},\mathrm{C}) = \begin{pmatrix} n_1 & n_2 & 0 \\ n_2 & n_1 & 0 \\ 0 & 0 & n_3 \end{pmatrix} \qquad L = (n_1^2-n_2^2)n_3$$

$$\text{(vii) } l(\mathrm{A},\mathrm{C}) = \begin{pmatrix} n_1 & n_1 & 0 \\ -n_2 & n_2 & -n_3 \\ -n_2 & n_2 & n_3 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(viii) } l(\mathrm{F},\mathrm{C}) = \begin{pmatrix} -n_2 & -n_2 & n_3 \\ n_1 & n_1 & n_3 \\ n_1-n_2 & n_1+n_2 & 0 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(ix) } l(\mathrm{I},\mathrm{C}) = \begin{pmatrix} -n_1 & -n_2 & n_3 \\ n_1 & n_2 & n_3 \\ n_2 & n_1 & -n_3 \end{pmatrix} \qquad L = 2(n_1^2-n_2^2)n_3$$

$$\text{(x) } l(\mathrm{P},\mathrm{F}) = \begin{pmatrix} -n_1 & n_1 & n_1 \\ n_2 & -n_2 & n_2 \\ n_3 & n_3 & -n_3 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(xi) } l(\mathrm{C},\mathrm{F}) = \begin{pmatrix} -n_1 & n_1 & n_2 \\ -n_2 & n_2 & n_1 \\ n_3 & n_3 & -n_3 \end{pmatrix} \qquad L = 2(n_1^2-n_2^2)n_3$$

$$\text{(xii) } l(\mathrm{F},\mathrm{F}) = \frac{1}{2}\begin{pmatrix} n_2+n_3 & -n_2+n_3 & n_2-n_3 \\ -n_1+n_3 & n_1+n_3 & n_1-n_3 \\ -n_1+n_2 & n_1-n_2 & n_1+n_2 \end{pmatrix} \qquad L = n_1n_2n_3;$$

n_1, n_2, n_3 are of the same parity.

$$\text{(xiii) } l(\mathrm{I},\mathrm{F}) = \begin{pmatrix} n_1+n_2+n_3 & -n_3 & -n_2 \\ -n_3 & n_1+n_2+n_3 & -n_1 \\ -n_2 & -n_1 & n_1+n_2+n_3 \end{pmatrix}$$

$$L = 2[(n_1+n_2+n_3)(n_1n_2+n_2n_3+n_3n_1) - n_1n_2n_3]$$

$$\text{(xiv) } l(\mathrm{P}, \mathrm{I}) = \begin{pmatrix} 0 & n_1 & n_1 \\ n_2 & 0 & n_2 \\ n_3 & n_3 & 0 \end{pmatrix} \qquad L = 2n_1n_2n_3$$

$$\text{(xv) } l(\mathrm{C}, \mathrm{I}) = \begin{pmatrix} -n_2 & n_1 & n_1 - n_2 \\ n_2 & n_1 & n_1 + n_2 \\ n_3 & n_3 & 0 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(xvi) } l(\mathrm{F}, \mathrm{I}) = \begin{pmatrix} n_2 + n_3 & n_3 & n_2 \\ n_3 & n_1 + n_3 & n_1 \\ n_2 & n_1 & n_1 + n_2 \end{pmatrix} \qquad L = 4n_1n_2n_3$$

$$\text{(xvii) } l(\mathrm{I}, \mathrm{I}) = \frac{1}{2}\begin{pmatrix} n_2 + n_3 & -n_1 + n_3 & -n_1 + n_2 \\ -n_2 + n_3 & n_1 + n_3 & n_1 - n_2 \\ n_2 - n_3 & n_1 - n_3 & n_1 + n_2 \end{pmatrix} \qquad L = n_1n_2n_3;$$

n_1, n_2, n_3 are of the same parity.

A.6. The tetragonal crystal system

(i) $l^{(1)}(\mathrm{P}, \mathrm{P})$ coincides with (A.2)

$$\text{(ii) } l^{(2)}(\mathrm{P}, \mathrm{P}) = \begin{pmatrix} n_1 & -n_1 & 0 \\ n_1 & n_1 & 0 \\ 0 & 0 & n_2 \end{pmatrix} \qquad L = 2n_1^2n_2$$

$$\text{(iii) } l^{(1)}(\mathrm{I}, \mathrm{P}) = \begin{pmatrix} 0 & n_1 & n_2 \\ n_1 & 0 & n_2 \\ n_1 & n_1 & 0 \end{pmatrix} \qquad L = 2n_1^2n_2$$

$$\text{(iv) } l^{(2)}(\mathrm{I}, \mathrm{P}) = \begin{pmatrix} -n_1 & n_1 & n_2 \\ n_1 & -n_1 & n_2 \\ n_1 & n_1 & -n_2 \end{pmatrix} \qquad L = 4n_1^2n_2$$

$$\text{(v) } l^{(1)}(\mathrm{P}, \mathrm{I}) = \begin{pmatrix} 0 & n_1 & n_1 \\ n_1 & 0 & n_1 \\ n_2 & n_2 & 0 \end{pmatrix} \qquad L = 2n_1^2n_2$$

$$\text{(vi) } l^{(2)}(\mathrm{P}, \mathrm{I}) = \begin{pmatrix} -n_1 & n_1 & 0 \\ n_1 & n_1 & 2n_1 \\ n_2 & n_2 & 0 \end{pmatrix} \qquad L = 4n_1^2n_2$$

$$\text{(vii) } l^{(1)}(\mathrm{I}, \mathrm{I}) = \begin{pmatrix} n_1 + n_2 & n_2 & n_1 \\ n_2 & n_1 + n_2 & n_1 \\ n_1 & n_1 & 2n_1 \end{pmatrix} \qquad L = 4n_1^2n_2$$

$$\text{(viii) } l^{(2)}(\mathrm{I}, \mathrm{I}) = \frac{1}{2}\begin{pmatrix} n_1 + n_2 & -n_1 + n_2 & 0 \\ -n_1 + n_2 & n_1 + n_2 & 0 \\ n_1 - n_2 & n_1 - n_2 & 2n_1 \end{pmatrix} \qquad L = n_1^2n_2;$$

n_1, n_2 are of the same parity.

A.7. The cubic crystal system

$$\text{(i) } l(\mathrm{P}, \mathrm{P}) = l(\mathrm{F}, \mathrm{F}) = l(\mathrm{I}, \mathrm{I}) = \begin{pmatrix} n & 0 & 0 \\ 0 & n & 0 \\ 0 & 0 & n \end{pmatrix} \qquad L = n^3$$

$$\text{(ii) } l(\mathrm{F}, \mathrm{P}) = l(\mathrm{P}, \mathrm{I}) = \begin{pmatrix} 0 & n & n \\ n & 0 & n \\ n & n & 0 \end{pmatrix} \qquad L = 2n^3$$

(iii) $l(\mathrm{I}, \mathrm{P}) = l(\mathrm{P}, \mathrm{F}) = \begin{pmatrix} -n & n & n \\ n & -n & n \\ n & n & -n \end{pmatrix} \qquad L = 4n^3$

(iv) $l(\mathrm{I}, \mathrm{F}) = \begin{pmatrix} 3n & -n & -n \\ -n & 3n & -n \\ -n & -n & 3n \end{pmatrix} \qquad L = 16n^3$

(v) $l(\mathrm{F}, \mathrm{I}) = \begin{pmatrix} 2n & n & n \\ n & 2n & n \\ n & n & 2n \end{pmatrix} \qquad L = 4n^3.$

Appendix B. Matrices Q_i

$$Q_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad Q_2 = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \qquad Q_3 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$Q_4 = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} \qquad Q_5 = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

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