

distinction. Thus, the longitudinal chain translation, favored at higher temperatures, can be frozen into the lattice as a distribution of static displacements. A small number of chain-end link defects, moreover, will guarantee that the lamellar interface will not, on average, deviate from a planar geometry.

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Crystallography, Geometry and Physics in Higher Dimensions. X. Super Point Groups in Five-Dimensional Space for the Di-Incommensurate Structures

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Abstract

This paper, the third of a series devoted to crystallography in five-dimensional space E^5 , deals with the di-incommensurate structures. Physical considerations on the vectors of modulation have enabled the definition and listing of the di-incommensurate point symmetry operations, the di-incommensurate point symmetry groups and the di-incommensurate crystal families of the space E^5 .

Introduction

A crystal lattice is said to be di-incommensurate (DI for short) if the vectors describing the main and

satellite reflections may be labelled with five Miller indices as follows:

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m_1\mathbf{q}_1^* + m_2\mathbf{q}_2^* \quad (1)$$

where h, k, l, m_1 and m_2 are integers and

$$\begin{aligned} \mathbf{q}_1^* &= \alpha_1\mathbf{a}^* + \beta_1\mathbf{b}^* + \gamma_1\mathbf{c}^* \\ \mathbf{q}_2^* &= \alpha_2\mathbf{a}^* + \beta_2\mathbf{b}^* + \gamma_2\mathbf{c}^*. \end{aligned} \quad (2)$$

One at least of the three entries, α_1, β_1 and γ_1 , is irrational, and also for the entries α_2, β_2 and γ_2 . Then we can describe a reciprocal lattice in a (3+2)-

dimensional space as follows:

$$\begin{aligned} \mathbf{b}_1 &= \mathbf{a}^* & \mathbf{b}_4 &= \mathbf{q}_1^* + \mathbf{d}_1 \\ \mathbf{b}_2 &= \mathbf{b}^* & \mathbf{b}_5 &= \mathbf{q}_2^* + \mathbf{d}_2. \\ \mathbf{b}_3 &= \mathbf{c}^* \end{aligned} \quad (3)$$

The vectors \mathbf{d}_1 and \mathbf{d}_2 are unit orthogonal vectors, orthogonal to the physical space $(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)$. Moreover, the projection of the reciprocal superlattice onto the reciprocal physical space is the pattern of diffraction experimentally observed, *i.e.* the vector \mathbf{H} . Consequently, the basis vectors of the direct lattice are

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - (\alpha_1 \mathbf{d}_1 + \alpha_2 \mathbf{d}_2) & \mathbf{a}_4 &= \mathbf{d}_1 \\ \mathbf{a}_2 &= \mathbf{b} - (\beta_1 \mathbf{d}_1 + \beta_2 \mathbf{d}_2) & \mathbf{a}_5 &= \mathbf{d}_2. \\ \mathbf{a}_3 &= \mathbf{c} - (\gamma_1 \mathbf{d}_1 + \gamma_2 \mathbf{d}_2) \end{aligned}$$

They define the dual basis of the basis

$$(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_5).$$

A di-incommensurate point symmetry operation (DIPSO for short) is a PSO which leaves the DI phase invariant; this phase is a crystal in the superspace E^5 with $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5)$ as a cell.

I. Different types of di-incommensurate point symmetry operations of E^5

The different types of DIPSOs can be obtained by studying all possible distributions of irrational entries occurring in (2) (Phan, 1989). The result is the nine kinds listed in Table 1. We have written the irrational entries only; the others are either rational or zero. The first kind corresponding to

$$\mathbf{q}_1^* = \alpha_1 \mathbf{a}^*, \quad \mathbf{q}_2^* = \alpha_2 \mathbf{a}^*$$

can be explained as follows.

As α_1 and α_2 are the only irrational entries, the vector \mathbf{H} can be written

$$\mathbf{H} = h\mathbf{a}^* + k'\mathbf{b}^* + l'\mathbf{c}^* + m_1(\alpha_1 \mathbf{a}^*) + m_2(\alpha_2 \mathbf{a}^*)$$

where

$$\begin{aligned} k' &= k + m_1\beta_1 + m_2\beta_2 \\ l' &= l + m_1\gamma_1 + m_2\gamma_2. \end{aligned}$$

Thus, the basis vectors of the direct lattice are the following:

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1 \mathbf{d}_1 - \alpha_2 \mathbf{d}_2 & \mathbf{a}_4 &= \mathbf{d}_1 \\ \mathbf{a}_2 &= \mathbf{b} & \mathbf{a}_5 &= \mathbf{d}_2. \\ \mathbf{a}_3 &= \mathbf{c} \end{aligned}$$

We notice that vectors \mathbf{a}_2 and \mathbf{a}_3 are the only ones which do not depend on modulation vectors \mathbf{d}_1 and \mathbf{d}_2 , so that a DIPSO can be regarded as a commutative product of two PSOs. The first one acts without

Table 1. Irrational entries of the vectors \mathbf{q}_1^* and \mathbf{q}_2^*

In the first column (second column) the irrational entries of the vector \mathbf{q}_1^* (vector \mathbf{q}_2^*) are given. In the third column, the number of the different kinds are indicated. All unwritten entries are either rational or zero.

| $\mathbf{q}_1^* = \alpha_1 \mathbf{a}^* + \beta_1 \mathbf{b}^* + \gamma_1 \mathbf{c}^*$ | $\mathbf{q}_2^* = \alpha_2 \mathbf{a}^* + \beta_2 \mathbf{b}^* + \gamma_2 \mathbf{c}^*$ | |
|---|---|---|
| α_1 | α_2 | 1 |
| α_1 | β_2 (or γ_2) | 2 |
| α_1 | α_2, β_2 (or γ_2) | 3 |
| α_1 | β_2, γ_2 | 4 |
| α_1 | $\alpha_2, \beta_2, \gamma_2$ | 5 |
| α_1, β_1 | α_2, β_2 | 6 |
| α_1, β_1 | α_2, γ_2 | 7 |
| α_1, β_1 | $\alpha_2, \beta_2, \gamma_2$ | 8 |
| $\alpha_1, \beta_1, \gamma_1$ | $\alpha_2, \beta_2, \gamma_2$ | 9 |

restriction on \mathbf{a}_2 and \mathbf{a}_3 , and leaves each of vectors $\mathbf{a}_1, \mathbf{a}_4, \mathbf{a}_5$ invariant. The second one maps either each element of the set $(\mathbf{a}_1, \mathbf{a}_4, \mathbf{a}_5)$ on itself or on its opposite and leaves \mathbf{a}_2 and \mathbf{a}_3 invariant. With respect to basis $(\mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_1, \mathbf{a}_4, \mathbf{a}_5)$, the matrices of these PSOs are the matrices no. 1 where A is the matrix of a general PSO of space E^2 and ε equals +1 or -1.

$$\begin{aligned} & \left(\begin{array}{c|ccc} A & 0 & 0 & 0 \\ \hline & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array} \right) \times \left(\begin{array}{c|ccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & \varepsilon & 0 & 0 \\ \hline 0 & 0 & 0 & \varepsilon & 0 \\ \hline 0 & 0 & 0 & 0 & \varepsilon \end{array} \right) \\ & = \left(\begin{array}{c|ccc} A & 0 & 0 & 0 \\ \hline & 0 & 0 & 0 \\ \hline 0 & 0 & \varepsilon & 0 & 0 \\ \hline 0 & 0 & 0 & \varepsilon & 0 \\ \hline 0 & 0 & 0 & 0 & \varepsilon \end{array} \right) \end{aligned}$$

Matrix no. 1 of a DIPSO of the first type. A is the matrix of a general PSO of space E^2 and $\varepsilon = +1$ or $\varepsilon = -1$.

Now, we study the second kind corresponding to irrational entries α_1 and β_2 . Two types of DIPSOs appear corresponding to entries α_1 and β_2 either different or equal. These two kinds are respectively named 2 and 2^a in Table 2.

Then, kinds nos. 3, 4 and 6 only give two types of DIPSOs which are particular kinds of the first one. Let us consider kind no. 3 for instance, *i.e.* α_1, α_2 and β_2 are the irrational entries. The basis vectors of the lattice are the following:

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1 \mathbf{d}_1 - \alpha_2 \mathbf{d}_2 & \mathbf{a}_4 &= \mathbf{d}_1 \\ \mathbf{a}_2 &= \mathbf{b} - \beta_2 \mathbf{d}_2 & \mathbf{a}_5 &= \mathbf{d}_2. \\ \mathbf{a}_3 &= \mathbf{c} \end{aligned}$$

With respect to basis $(\mathbf{a}_3, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_4, \mathbf{a}_5)$, the matrix of the corresponding DIPSO is matrix no. 2. It is easy to verify that it is a particular kind of matrix no. 1 where A' is matrix no. 3.

Table 2. *Different types of DIPSOs*

| No. | Irrational parameters | Lattice basis | Basis with respect to the matrix is written | Matrix of a DIPSO compatible with the lattice |
|----------------|---|---|---|---|
| 1 | $q_1 = \alpha_1 a^*$ $q_2^* = \alpha_2 a^*$ | $a_1 = a - \alpha_1 d_1 - \alpha_2 d_2$ $a_2 = b$ $a_3 = c$ $a_4 = d_1$ $a_5 = d_2$ | $(a_2, a_3, a_1, a_4, a_5)$ | $\begin{pmatrix} A & & 0 & 0 & 0 \\ \hline 0 & 0 & & \varepsilon & 0 \\ 0 & 0 & & 0 & \varepsilon \\ 0 & 0 & & 0 & 0 & \varepsilon \end{pmatrix}$ |
| 2 | $q_1^* = \alpha_1 a^*$ $q_2^* = \beta_2 b^*$ | $a_1 = a - \alpha_1 d_1$ $a_2 = b - \beta_2 d_2$ $a_3 = c$ $a_4 = d_1$ $a_5 = d_2$ | $(a_3, a_1, a_4, a_2, a_5)$ | $\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_3 \end{pmatrix}$ |
| 2 ^u | $q_1^* = k a^*$ $q_2^* = k b^*$ | $a_1 = a - k d_1$ $a_2 = b - k d_2$ $a_3 = c$ $a_4 = d_1$ $a_5 = d_2$ | $(a_3, a_1, a_2, a_4, a_5)$ | $\begin{pmatrix} \varepsilon & & 0 & 0 & & 0 & 0 \\ \hline 0 & & 0 & 0 & & 0 & 0 \\ 0 & & A & & 0 & 0 \\ \hline 0 & & 0 & 0 & & 0 & 0 \\ 0 & & 0 & 0 & & A \end{pmatrix}$ |

Table 3. *DIPSOs*

There are 18 types of DIPSOs, *i.e.*:

1; $\bar{1}$; m ; 2; $\bar{1}_4$; $\bar{1}_5$; 3; 4; 6; $\bar{3}$; $\bar{4}$; $\bar{6}$; 33; 44; 66; $\bar{3}\bar{3}$; $\bar{4}\bar{4}$; $\bar{6}\bar{6}$.

$\bar{4}_{xy}^{+1} = 4_{xy}^{+1} \bar{1}_5 = 4_{xy}^{-1} \bar{1}_{z, tu}$
 $\bar{3}_{1z}^1 \bar{3}_{1u}^1 = 3_{1z}^1 \bar{3}_{1u}^1 \bar{1}_5 = 6_{1z}^1 \bar{6}_{1u}^1 m$ (Weigel *et al.*, 1990).

| | | |
|---|---|--|
| Type no. 1 | Type no. 2 | Type no. 2 ^u |
| $\begin{pmatrix} A & & 0 & 0 & 0 \\ \hline 0 & 0 & & \varepsilon & 0 \\ 0 & 0 & & 0 & \varepsilon \\ 0 & 0 & & 0 & 0 & \varepsilon \end{pmatrix}$ | $\begin{pmatrix} \varepsilon_1 & & 0 & 0 & & 0 & 0 \\ \hline 0 & & \varepsilon_2 & 0 & & 0 & 0 \\ 0 & & 0 & \varepsilon_2 & & 0 & 0 \\ \hline 0 & & 0 & 0 & & \varepsilon_3 & 0 \\ 0 & & 0 & 0 & & 0 & \varepsilon_3 \end{pmatrix}$ | $\begin{pmatrix} \varepsilon & & 0 & 0 & & 0 & 0 \\ \hline 0 & & 0 & 0 & & 0 & 0 \\ 0 & & A & & 0 & 0 \\ \hline 0 & & 0 & 0 & & 0 & 0 \\ 0 & & 0 & 0 & & A \end{pmatrix}$ |
| 1; $\bar{1}_5$ $m_x; m_y; m_{x,y}$ $m_{2x,y}; m_{x-2y}$ $\bar{1}_{z, tu}$ $\bar{1}_{x,z,t,u}; \bar{1}_{x,z,t,u}; \bar{1}_{x=y,z,t,u}$ | 1; $\bar{1}_5$ m_x $\bar{1}_{x,y,z}; \bar{1}_{x,t,u}$ | 1; $\bar{1}_5$ m_x $\bar{1}_{x,y,t}; \bar{1}_{x,z,u}; \bar{1}_{x,y+z,t+u}$ $\bar{1}_{x,y,z,t-u}; \bar{1}_{x,2y-z,2t-u}$ $\bar{1}_{x,y-2z,t-2u}$ $\bar{1}_{x,z,t,u}$ |
| $\bar{1}_{2x-1,y,z,t,u}; \bar{1}_{x-2y,z,t,u}$ 2_{xy} $3_{xy}^{+1}, 4_{xy}^{+1}, 6_{xy}^{+1}$ $3_{xy}^{-1}, 4_{xy}^{-1}, 6_{xy}^{-1}$ | $\bar{1}_{x,z,t,u}$ $2_{xy}; 2_{tu}$ | $3_{1z}^1, 3_{1u}^1; 4_{1z}^1; 4_{1u}^1; 6_{1z}^1, 6_{1u}^1$ $3_{1z}^1, 3_{1u}^1; 4_{1z}^1, 4_{1u}^1; 6_{1z}^1, 6_{1u}^1$ $3_{1z}^{-1}, 3_{1u}^{-1}; 4_{1z}^{-1}, 4_{1u}^{-1}; 6_{1z}^{-1}, 6_{1u}^{-1}$ $3_{1z}^{-1}, 3_{1u}^{-1}; 4_{1z}^{-1}, 4_{1u}^{-1}; 6_{1z}^{-1}, 6_{1u}^{-1}$ |

$$\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & 0 & 0 \\ 0 & 0 & \varepsilon & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & 0 & \varepsilon \end{pmatrix}$$

Matrix no. 2 of a DIPSO of the third type. $\varepsilon_1 = +1$ or $\varepsilon_1 = -1$ and $\varepsilon = +1$ or $\varepsilon = -1$.

$$A' = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon \end{pmatrix}$$

Matrix no. 3. ε_1 (and ε) equal to +1 or -1.

Table 4. *47 DIPSGs of E⁵*

| Type no. 1 | Type no. 2 | Type no. 2 ^u |
|--|--|----------------------------------|
| 2, $m, m; m \perp \bar{1}$ | $\bar{1}_4, \bar{1}, \bar{1};$ | $33^*; m \perp 33^*$ |
| $2, \bar{1}_4, \bar{1}_4; \bar{1} \perp 2, m, m$ | $2/m;$ | $33^*, 2; m \perp 33^*, 2$ |
| $3; \bar{3}; 3, m$ | $2 \perp 2; m \perp 2 \perp 2$ | $44^*; m \perp 44^*$ |
| $3, \bar{1}_4; \bar{3}, m$ | | $44^*, 2; m \perp 44^*, 2$ |
| $4; \bar{4}; 4, m, n$ | | $66^*; m \perp 66^*$ |
| $\bar{4}, m, \bar{1}_4; 4, \bar{1}_4, \bar{1}_4$ | | $2, 66^*, 2; m \perp 2, 66^*, 2$ |
| $4 \perp \bar{1}; \bar{1} \perp 4, m, m$ | | |
| $6; 6; 6, m, m$ | | |
| $(3, m) \perp \bar{1}; 6, \bar{1}_4, \bar{1}_4$ | | |
| $6 \perp \bar{1}; \bar{1} \perp 6, m, m$ | | |
| | $2; \bar{1} \perp 2$ | |
| | 1; $\bar{1}; \bar{1}; \bar{1}_4; m; \bar{1} \perp m$ | |

Table 5. *Di-incommensurate crystal families of E⁵*

The first column gives the name of crystal families of E^5 and their no. in the classification of Plesken (1981). The second column gives the WPV symbol of the holohedry of each family and the third one the WPV symbols of PSGs, subgroups of this holohedry. The last column gives the number of DIPSGs of each family. Thus, we obtain another classification of the 47 DIPSGs, family by family.

| Number and name of the family | WPV symbol of the holohedry | WPV symbol of the other DIPSGs | Number of DIPSGs |
|--|-----------------------------|--|------------------|
| I Decaclinic | $\bar{1}$ | 1 | 2 |
| II Right hyperprism based on hexaclinic | $m \perp \bar{1}_4$ | $m; \bar{1}_4$ | 3 |
| III Orthogonal triclinic (XYZ) parallelogram (TU) | $\bar{1} \perp 2$ | 2; $\bar{1}$ | 3 |
| IV Orthogonal triclinic (XYZ) rectangle (TU) | $\bar{1} \perp 2, m, m$ | 2, $m, m; 2, \bar{1}_4, \bar{1}_4; \bar{1} \perp m$ | 4 |
| V Right hyperprism based on di-orthogonal parallelograms | $m \perp 2 \perp 2$ | $2 \perp 2; 2/m; \bar{1}_4, \bar{1}, \bar{1}$ | 4 |
| VI Orthogonal triclinic (XYZ) square (TU) | $\bar{1} \perp 4, m, m$ | $\bar{1} \perp 4; 4, m, m; 4; \bar{4}; 4, \bar{1}_4, \bar{1}_4; \bar{4}, m, \bar{1}_4$ | 7 |
| VII Orthogonal triclinic (XYZ) hexagon (TU) | $\bar{1} \perp 6, m, m$ | 6, $\bar{1}_4, \bar{1}_4; \bar{1} \perp 6; 6, m, m; 6; \bar{6}$ 3, $\bar{1}_4; 1 \perp 3, m; 1 \perp 3; 3, m; 3; \bar{3}$ | 12 |
| XII Right hyperprism based on di-diclinic squares (YZ)(TU) | $m \perp 44^*$ | 44* | 2 |
| XIII Right hyperprism based on di-diclinic hexagons (YZ)(TU) | $m \perp 66^*$ | 66*; 33*; $m \perp 33^*$ | 4 |
| XVI Right hyperprism based on di-monoclinic squares (YZ)(TU) | $m \perp 44^*, 2$ | 44*, 2 | 2 |
| XVII Right hyperprism based on di-monoclinic hexagons (YZ)(TU) | $m \perp 66^*, 2$ | 33*, 2; 66*2; $m \perp 33^*, 2$ | 4 |

Finally, kinds nos. 5, 7, 8 and 9 only give two types of DIPSOs: the PSO identity and its opposite. As an example, we can easily verify this property on kind no. 7. The basis vectors are the following:

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1 \mathbf{d}_1 - \alpha_2 \mathbf{d}_2 & \mathbf{a}_4 &= \mathbf{d}_1 \\ \mathbf{a}_2 &= \mathbf{b} - \beta_1 \mathbf{d}_1 & \mathbf{a}_5 &= \mathbf{d}_2 \\ \mathbf{a}_3 &= \mathbf{c} - \gamma_2 \mathbf{d}_2 \end{aligned}$$

and consequently all vectors must be unchanged or must be mapped on their opposite through a DIPSO.

As a conclusion, only three types of DIPSOs appear. They are listed in Table 2. Then, all the crystallographic DIPSOs of E^5 , corresponding to each of the previous three types, are explicitly described in Table 3. We can see that among the 38 types of crystallographic PSOs of E^5 (Weigel, Phan & Veysseyre 1990) only 18 types are DIPSOs.

II. Di-incommensurate point symmetry groups of E^5

(1) A point symmetry group (PSG) of E^5 is said to be a DIPSG if it is composed of PSOs belonging to one and only one type of DIPSO listed in Table 3.

Let us consider two PSGs of E^5 :

(i) the first example has the WPV symbol $m \perp \bar{1}_4$. This is the holohedry of the crystal family named right hyperprism based on hexaclinic (YZTU) (Veysseyre, Phan & Weigel 1991).

The PSOs of this group of order 4 are

$$1; m_x; \bar{1}_{yztu}; \bar{1}_5.$$

As these PSOs belong to type no. 2^a, the PSG $m \perp \bar{1}_4$ is a DIPSG.

(ii) The second example is the PSG $2, \bar{1}, \bar{1}$, of order 4, belonging to the crystal family orthogonal parallelogram (XY) orthorhombic (ZTU) (Veysseyre *et al.*, 1991). Its elements are

$$1, 2_{zt}, \bar{1}_{xyz}, \bar{1}_{xyt}.$$

They do not belong to the same type of DIPSOs. Therefore, the PSG $2, \bar{1}, \bar{1}$, is not a DIPSG.

(2) The 47 DIPSGs of E^5 .

Now, we establish the list of all PSGs of E^5 generated by the DIPSOs of the same type. For instance, the DIPSOs of type no. 2 generate the following twelve PSGs and only these:

$$\begin{aligned} &1; \bar{1}; m; \bar{1}; \bar{1}_4; \bar{1}_4, \bar{1}, \bar{1}; m \perp \bar{1}_4 \\ &2; 2/m; \bar{1} \perp 2; 2 \perp 2; m \perp 2 \perp 2. \end{aligned}$$

The exhaustive list of the DIPSGs of E^5 is given in Table 4. These PSGs are classified type by type and we find:

- 23 DIPSGs of type no. 1 and only of this type
- 4 DIPSGs of type no. 2 and only of this type
- 12 DIPSGs of type no. 2^a and only of this type
- 2 PSGs belong to both types no. 1 and no. 2
- 6 PSGs belong to three types nos. 1, 2 and 2^a.

The total is 47 DIPSGs.

III. Di-incommensurate crystal families of E^5

(1) As previously, a crystal family of E^5 is said to be di-incommensurate if it is only composed of DIPSGs. For instance, family no. V: right hyperprism based on di-orthogonal parallelograms (YZ)(TU)

has the holohedry $m\bar{1}2\bar{1}2$. (Veyssyre *et al.*, 1991). The subgroups of this holohedry are the following:

$$2\bar{1}2; 2/m; \bar{1}_4, \bar{1}, \bar{1}; \bar{1}\bar{1}2; m\bar{1}\bar{1}_4; \\ \bar{1}; 2; \bar{1}_4; m; \bar{1}; 1.$$

All these PSGs are DIPSGs of E^5 . Therefore this family is a DI crystal family.

(2) The eleven DI crystal families of E^5 .

In space E^5 , eleven crystal families are DI families. In Table 5, we give their names, together with the WPV symbols of their holohedries and of their PSGs.

Concluding remarks

The study of the different possibilities for the entries of the modulation vectors to be either rational or not enables us to define the DIPSOs, then the DIPSGs and the DI crystal families.

de Wolff, Janssen & Janner (1981) published a list of Bravais classes of the crystal families of E^3

necessary for the study of incommensurate phases of internal dimensions equal to 1, 2 or 3 and they proposed a notation for these Bravais classes.

In a previous paper, we established a connection between the two approaches and the two notations for the mono-incommensurate structures (Grebille, Weigel, Veyssyre & Phan 1990).

In a forthcoming paper, the same work will be developed for the di-incommensurate structures and some physical examples studied.

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Phase Determination for Membrane Diffraction by Anomalous Dispersion

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Abstract

The phase problem of membrane diffraction is usually solved by the swelling method; however, this method does not always resolve the phases unambiguously. An alternative method of phase determination using anomalous dispersion is illustrated by the multiple-wavelength diffraction of membranes containing gramicidin ion channels. The anomalously scattering atoms are thallium ions bound to the channel. The result determines the location of the ion-binding sites in the gramicidin channel and the electron-density

profile of the membrane. The applicability and limitation of the anomalous-dispersion method are discussed.

Introduction

Membrane scattering has been used to determine the structures of membranes and to reveal structural properties of molecules embedded in membranes, such as cholesterol (*e.g.* Franks & Lieb, 1979), rhodopsin (*e.g.* Yeager, 1975) and ion channels (*e.g.* Olah, Huang, Liu & Wu, 1991). When membranes are in the smectic liquid-crystalline form, the resolution of membrane diffraction is usually limited to a few ångströms. Nevertheless, if heavy atoms in the system are bound to a few well defined sites, it is

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