INTERNATIONAL AUTUMN SCHOOL
ON FUNDAMENTAL AND ELECTRON CRYSTALLOGRAPHY

8-13 October 2017, Sofia, Bulgaria
SPACE GROUPS AND THEIR SYMMETRY RELATIONS
Space group $G$: The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $H \triangleleft G$: The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups $P_G$: The factor group of the space group $G$ with respect to the translation subgroup $T$: $P_G \cong G/H$
INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY
VOLUME A: SPACE-GROUP SYMMETRY

Extensive tabulations and illustrations of the 17 plane groups and of the 230 space groups

- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection conditions;
- symmetries of special projections;
HERMANN-MAUGUIN
SYMBOLISM
**Cmm2**

- Short Hermann-Mauguin symbol: **Cmm2**
- Schoenflies symbol: **C\textsubscript{2v}**
- Crystal class (point group): **mm2**
- Crystal system: Orthorhombic

**No. 35**

- Full Hermann-Mauguin symbol: **Cmm2**
- Patterson symmetry: **Cmmm**

**Number of space group**

**Full Hermann-Mauguin symbol**

**Patterson symmetry**
Hermann-Mauguin symbols for space groups

Orthorhombic

Bravais lattice

screw axis \(2_1//\hat{a}\)

glide plane \(n \perp \hat{a}\)

screw axis \(2_1//\hat{c}\)

glide plane \(a \perp \hat{c}\)

mirror plane \(m \perp \hat{b}\)
<table>
<thead>
<tr>
<th>crystal family</th>
<th>Lattice types</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$P$</td>
</tr>
<tr>
<td>triclinic</td>
<td><img src="image1" alt="Triclinic Lattice" /></td>
</tr>
<tr>
<td>monoclinic</td>
<td><img src="image2" alt="Monoclinic Lattice" /></td>
</tr>
<tr>
<td>orthorhombic</td>
<td><img src="image3" alt="Orthorhombic Lattice" /></td>
</tr>
<tr>
<td>tetragonal</td>
<td><img src="image4" alt="Tetragonal Lattice" /></td>
</tr>
<tr>
<td>hexagonal</td>
<td><img src="image5" alt="Hexagonal Lattice" /></td>
</tr>
<tr>
<td>cubic</td>
<td><img src="image6" alt="Cubic Lattice" /></td>
</tr>
</tbody>
</table>
Hermann-Mauguin symbols for space groups

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Symmetry direction (position in Hermann–Mauguin symbol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Primary</td>
</tr>
<tr>
<td>Triclinic</td>
<td>None</td>
</tr>
</tbody>
</table>
| Monoclinic*              | [010] (*unique axis b*)  
                          | [001] (*unique axis c*)  |             |
| Orthorhombic             | [100]       | [010]       | [001]       |
| Tetragonal               | [001]       | { [100] }   | { [110] }   |
|                          |             | { [010] }   |             |
|                          |             | { [110] }   |             |
| Hexagonal                | [001]       | { [100] }   | { [110] }   |
|                          |             | { [010] }   |             |
|                          |             | { [120] }   |             |
|                          |             | { [210] }   |             |
| Rhombohedral (hexagonal axes) | [001]      | { [100] }   |             |
|                          |             | { [010] }   |             |
|                          |             | { [110] }   |             |
| Rhombohedral (rhombohedral axes) | [111]   | { [110] }   |             |
|                          |             | { [011] }   |             |
|                          |             | { [101] }   |             |
| Cubic                    | { [100] }   | { [111] }   | { [110] [110] [011] [011] [011] [101] [101] |
SPACE-GROUP SYMMETRY OPERATIONS
Crystallographic symmetry operations

characteristics: fixed points of isometries \((W,w)X_f = X_f\) geometric elements

Types of isometries preserve handedness

identity: the whole space fixed

translation \(t\): no fixed point \(\tilde{x} = x + t\)

rotation: one line fixed rotation axis \(\phi = k \times 360^\circ / N\)

screw rotation: no fixed point screw axis screw vector
Types of isometries

donot
preserve handedness

roto-inversion: centre of roto-inversion fixed
roto-inversion axis

inversion: centre of inversion fixed

development of
reflection/mirror plane

reflection: plane fixed
reflection/mirror plane

glide reflection: no fixed point
glide plane glide vector
Matrix formalism

\[
\begin{pmatrix}
\tilde{x} \\
\tilde{y} \\
\tilde{z}
\end{pmatrix}
= 
\begin{pmatrix}
W_{11} & W_{12} & W_{13} \\
W_{21} & W_{22} & W_{23} \\
W_{31} & W_{32} & W_{33}
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
+ 
\begin{pmatrix}
w_1 \\
w_2 \\
w_3
\end{pmatrix}
\]

linear/matrix part  
translation column part

\[
\tilde{x} = W \ x + w
\]

\[
\tilde{x} = (W, w) x \quad \text{or} \quad \tilde{x} = \{W \mid w\} x
\]

matrix-column pair  
Seitz symbol
Space group $Cmm2$ (No. 35)

How are the symmetry operations represented in ITA?

Symmetry operations
For $(0,0,0)+$ set
(1) 1
(2) 2 $0,0,z$
(3) $m x,0,z$
(4) $m 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set
(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) 2 $\frac{1}{2},\frac{1}{2},z$
(3) $a x,\frac{1}{2},z$
(4) $b \frac{1}{4},y,z$

General Position
Coordinates
$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$

8 $f$ 1
(1) $x,y,z$
(2) $\bar{x},\bar{y},z$
(3) $x,\bar{y},z$
(4) $\bar{x},y,z$
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X=\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under $(W,w)$ of $G$

-presentation of infinite image points $\tilde{X}$ under the action of $(W,w)$ of $G$

(ii) short-hand notation of the matrix-column pairs $(W,w)$ of the symmetry operations of $G$

-presentation of infinite symmetry operations of $G$

$(W,w) = (I,t_n)(W,w_0), \ 0 \leq w_{i0} < 1$
Space Groups: infinite order

Coset decomposition $G:T_G$

$(I,0)$ $(W_2,w_2)$ ... $(W_m,w_m)$ ... $(W_i,w_i)$

$(I,t_1)$ $(W_2,w_2+t_1)$ ... $(W_m,w_m+t_1)$ ... $(W_i,w_i+t_1)$

$(I,t_2)$ $(W_2,w_2+t_2)$ ... $(W_m,w_m+t_2)$ ... $(W_i,w_i+t_2)$

... ... ... ... ... ...

$(I,t_j)$ $(W_2,w_2+t_j)$ ... $(W_m,w_m+t_j)$ ... $(W_i,w_i+t_j)$

... ... ... ... ... ...

Factor group $G/T_G$

isomorphic to the point group $P_G$ of $G$

Point group $P_G = \{I, W_2, W_3, \ldots, W_i\}$
Coset decomposition $P2_1/c:T$

**Point group?**

- (1) $x,y,z$
- (2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$
- (3) $\bar{x},\bar{y},\bar{z}$
- (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

<table>
<thead>
<tr>
<th>(I,0)</th>
<th>(2,0 $\frac{1}{2}$ $\frac{1}{2}$)</th>
<th>($\bar{I}$,0)</th>
<th>(m,0 $\frac{1}{2}$ $\frac{1}{2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(l,t₁)</td>
<td>(2,0 $\frac{1}{2}$ $\frac{1}{2}$ +t₁)</td>
<td>($\bar{l}$,t₁)</td>
<td>(m,0 $\frac{1}{2}$ $\frac{1}{2}$ +t₁)</td>
</tr>
<tr>
<td>(l,t₂)</td>
<td>(2,0 $\frac{1}{2}$ $\frac{1}{2}$ +t₂)</td>
<td>($\bar{l}$,t₂)</td>
<td>(m,0 $\frac{1}{2}$ $\frac{1}{2}$ +t₂)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>(l,tₖ)</td>
<td>(2,0 $\frac{1}{2}$ $\frac{1}{2}$ +tₖ)</td>
<td>($\bar{l}$,tₖ)</td>
<td>(m,0 $\frac{1}{2}$ $\frac{1}{2}$ +tₖ)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

**Inversion centers**

$(\bar{l},pqr): \bar{l}$ at $p/2,q/2,r/2$

**2/ₚ Screw axes**

$(2,u \frac{1}{2}+v \frac{1}{2} +w)$

- $(2,0 \frac{1}{2}+v \frac{1}{2})$
- $(2,u \frac{1}{2} \frac{1}{2} +w)$
Space group $P2_1/c$ (No. 14)

Legendre

**Matrix-column presentation**

**Geometric interpretation**

### Generators selected

1. $t(1,0,0)$
2. $t(0,1,0)$
3. $t(0,0,1)$
4. $t(1,0,0)$

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$e$</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $x,y,z$</td>
</tr>
<tr>
<td>(2) $\bar{x} , y + \frac{1}{2} , z + \frac{1}{2}$</td>
</tr>
<tr>
<td>(3) $\bar{x} , y , z$</td>
</tr>
<tr>
<td>(4) $x , y + \frac{1}{2} , z + \frac{1}{2}$</td>
</tr>
</tbody>
</table>

### Symmetry operations

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(2) $2(0,\frac{1}{2},0)$</td>
<td>$0,y,\frac{1}{2}$</td>
<td>(3) $\bar{1}$</td>
</tr>
</tbody>
</table>
SPACE-GROUP DIAGRAMS
Diagrams of symmetry elements

three different settings

diagram of general position points

permutations of \(a, b, c\)

Diagram of general position points
ORIGINS AND ASYMMETRIC UNITS
Space group $Cmm2$ (No. 35): left-hand page ITA

$Cmm2$

No. 35

$C_{2v}$

$Cmm2$

$mm2$

Orthorhombic

Patterson symmetry $Cmmm$

Origin statement

The site symmetry of the origin is stated, if different from the identity.
A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any.

Origin on $mm2$

Space groups with two origins

For each of the two origins the location relative to the other origin is also given.
Example: Different origins for \( P_{nmm} \)

\[ P_{nmm} \quad D_{2h}^2 \quad mmm \quad \text{Orthorhombic} \]

No. 48

\( P 2/n 2/n 2/n \)

**ORIGIN CHOICE 1**

\( P^{2}_{n} 2^{2} 2^{2}_{n} \)

Origin at \( 222 \), at \( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \) from \( \bar{1} \)

**ORIGIN CHOICE 2**

\( P^{2}_{2} 2^{2} 2^{2}_{n} \)

Origin at \( \bar{1} \) at \( nnn \), at \( -\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4} \) from \( 222 \)
An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled.
Example: Asymmetric units for the space group P121

Number of vertices: 8
0, 1, 1/2
1, 1, 0
1, 0, 0
0, 0, 1/2
1, 0, 1/2
0, 0, 0
0, 1, 0
1, 1, 1/2

Number of facets: 6
x >= 0
x < 0
y >= 0
y < 0
z >= 0 [x <= 1/2]
z <= 1/2 [x <= 1/2]

[Guide to notation]
GENERAL AND SPECIAL WYCKOFF POSITIONS SITE-SYMMETRY
A group action of a group $\mathcal{G}$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair $(g, \omega)$ an object $\omega' = g(\omega)$ of $\Omega$ such that the following hold:

(i) applying two group elements $g$ and $g'$ consecutively has the same effect as applying the product $g'g$, i.e. $g'(g(\omega)) = (g'g)(\omega)$

(ii) applying the identity element $e$ of $\mathcal{G}$ has no effect on $\omega$, i.e. $e(\omega) = \omega$ for all $\omega$ in $\Omega$.

The set $\omega^g := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of $\omega$ is called the orbit of $\omega$ under $\mathcal{G}$.

The set $S_g(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object $\omega$ is a subgroup of $\mathcal{G}$ called the stabilizer of $\omega$ in $\mathcal{G}$.

Often, two objects $\omega$ and $\omega'$ are regarded as equivalent if there is a group element moving $\omega$ to $\omega'$.

Via this equivalence relation, the action of $\mathcal{G}$ partitions the objects in $\Omega$ into equivalence classes.
General and special Wyckoff positions

Orbit of a point $X_0$ under $G$: $G(X_0) = \{(W,w) \cdot X_0 : (W,w) \in G\}$

Site-symmetry group $S_0 = \{(W,w)\}$ of a point $X_0$

$(W,w) \cdot X_0 = X_0$

\[
\begin{pmatrix}
  a & b & c \\
  d & e & f \\
  g & h & i
\end{pmatrix}
\begin{pmatrix}
  w \\
  w \\
  w
\end{pmatrix}
\begin{pmatrix}
  x_0 \\
  y_0 \\
  z_0
\end{pmatrix}
= 
\begin{pmatrix}
  x_0 \\
  y_0 \\
  z_0
\end{pmatrix}
\]

Multiplicity: $|P|/|S_0|$

General position $X_0$

$S = \{(1,0)\} \approx 1$

Multiplicity: $|P|$

Special position $X_0$

$S > 1 = \{(1,0), ...,\}$

Multiplicity: $|P|/|S_0|$

Site-symmetry groups: oriented symbols
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under $(W,w)$ of $G$

-presentation of infinite image points $\tilde{X}$ under the action of $(W,w)$ of $G$

(ii) short-hand notation of the matrix-column pairs $(W,w)$ of the symmetry operations of $G$

-presentation of infinite symmetry operations of $G$

$(W,w) = (I,t_n)(W,w_0), \ 0 \leq w_{i0} < 1$
**General Position of Space groups**

As coordinate triplets of an image point $\tilde{X}$ of the original point $X=\begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under $(W,w)$ of $G$:

<table>
<thead>
<tr>
<th>$(l,0)X$</th>
<th>$(W_2,w_2)X$</th>
<th>...</th>
<th>$(W_m,w_m)X$</th>
<th>...</th>
<th>$(W_i,w_i)X$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(l,t_1)X$</td>
<td>$(W_2,w_2+t_1)X$</td>
<td>...</td>
<td>$(W_m,w_m+t_1)X$</td>
<td>...</td>
<td>$(W_i,w_i+t_1)X$</td>
</tr>
<tr>
<td>$(l,t_2)X$</td>
<td>$(W_2,w_2+t_2)X$</td>
<td>...</td>
<td>$(W_m,w_m+t_2)X$</td>
<td>...</td>
<td>$(W_i,w_i+t_2)X$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$(l,t_j)X$</td>
<td>$(W_2,w_2+t_j)X$</td>
<td>...</td>
<td>$(W_m,w_m+t_j)X$</td>
<td>...</td>
<td>$(W_i,w_i+t_j)X$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

**General position**
Example: Calculation of the Site-symmetry groups

Group P-1

S = {(W, w), (W, w) X_o = X_o}

\[
\begin{pmatrix}
-1 & 0 & 1/2 \\
-1 & 0 & -1/2 \\
-1 & 0 & 0 \\
0 & 1/2 & 0 \\
0 & -1/2 & 0 \\
0 & 0 & 1/2 \\
\end{pmatrix}
\]

\[
S_f = \{ (1,0), (-1,101) X_f = X_f \}
\]

\[
S_f \cong \{ 1, -1 \} \quad \text{isomorphic}
\]
EXERCISES

General and special Wyckoff positions of P4mm

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>g</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>g</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

(1) $x, y, z$
(2) $\bar{x}, \bar{y}, z$
(3) $\bar{y}, x, z$
(4) $y, \bar{x}, z$
(5) $x, \bar{y}, z$
(6) $\bar{x}, y, z$
(7) $\bar{y}, \bar{x}, z$
(8) $y, x, z$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $4^+ 0,0,z$
(4) $4^- 0,0,z$
(5) $m x,0,z$
(6) $m 0,y,z$
(7) $m x,\bar{x},z$
(8) $m x,x,z$
MAXIMAL SUBGROUPS OF SPACE GROUPS

I. MAXIMAL TRANSLATIONENGLEICHE SUBGROUPS
Subgroups: Some basic results (summary)

Subgroup $H \triangleleft G$

1. $H=\{e,h_1,h_2,\ldots,h_k\} \subset G$
2. $H$ satisfies the group axioms of $G$

Proper subgroups $H \triangleleft G$, and

trivial subgroup: $\{e\}, G$

Index of the subgroup $H$ in $G$: $[i]=|G|/|H|$

(order of $G$)/(order of $H$)

Maximal subgroup $H$ of $G$

NO subgroup $Z$ exists such that:

$H \triangleleft Z \triangleleft G$
Coset decomposition $G:H$

**Group-subgroup pair** $H < G$

- **left coset decomposition**
  \[ G = H + g_2 H + \ldots + g_m H, \quad g_i \notin H, \quad m = \text{index of } H \text{ in } G \]

- **right coset decomposition**
  \[ G = H + H g_2 + \ldots + H g_m, \quad g_i \notin H \quad m = \text{index of } H \text{ in } G \]

**Normal subgroups**

\[ H g_i = g_i H, \text{ for all } g_i = 1, \ldots, [i] \]
Subgroups of Space groups

Coset decomposition $G:T_G$

<table>
<thead>
<tr>
<th>$(I,0)$</th>
<th>$(W_2,w_2)$</th>
<th>...</th>
<th>$(W_m,w_m)$</th>
<th>...</th>
<th>$(W_i,w_i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(I,t_1)$</td>
<td>$(W_2,w_2+t_1)$</td>
<td>...</td>
<td>$(W_m,w_m+t_1)$</td>
<td>...</td>
<td>$(W_i,w_i+t_1)$</td>
</tr>
<tr>
<td>$(I,t_2)$</td>
<td>$(W_2,w_2+t_2)$</td>
<td>...</td>
<td>$(W_m,w_m+t_2)$</td>
<td>...</td>
<td>$(W_i,w_i+t_2)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$(I,t_j)$</td>
<td>$(W_2,w_2+t_j)$</td>
<td>...</td>
<td>$(W_m,w_m+t_j)$</td>
<td>...</td>
<td>$(W_i,w_i+t_j)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Factor group $G/T_G$

isomorphic to the point group $P_G$ of $G$

Point group $P_G = \{ I, W_2, W_3, \ldots, W_i \}$
**Example: P1 2/m1**

**Factor group G/T_G ≈ P_G**

**Coset decomposition G:T_G**

\[ P_G = \{ 1, 2, \bar{1}, m \} \]

<table>
<thead>
<tr>
<th>T_G</th>
<th>T_G 2</th>
<th>T_G \bar{1}</th>
<th>T_G m</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,0)</td>
<td>(2,0)</td>
<td>(\bar{1},0)</td>
<td>(m,0)</td>
</tr>
<tr>
<td>(1,t_1)</td>
<td>(2,t_1)</td>
<td>(\bar{1}, t_1)</td>
<td>(m, t_1)</td>
</tr>
<tr>
<td>(1,t_2)</td>
<td>(2,t_2)</td>
<td>(\bar{1}, t_2)</td>
<td>(m,t_2)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>(1,t_j)</td>
<td>(2,t_j)</td>
<td>(\bar{1}, t_j)</td>
<td>(m, t_j)</td>
</tr>
</tbody>
</table>

...                     ...          ...         ...         ...

|                      | ...          | ...        | ...         | ...
| -1                   | n_1          | ...        | ...         | ...
|                      |              | -1         | n_2          |
|                      |              |            | -1          | n_3          |
| \bar{1}             |              |            |              | \bar{1} at n_1/2 |
|                      |              |            |              | \bar{1} at n_2/2 |
|                      |              |            |              | \bar{1} at n_3/2 |

inversion centres (\(\bar{1}, t\)):
Translation engleche subgroups $H < G$: \[
\begin{align*}
T_H &= T_G \\
P_H &< P_G
\end{align*}
\]

Subgroups of space groups

Example: $P12/m1$

Coset decomposition

$t$-subgroups: $H_1 = T_G \cup T_G2$  
$H_2 = T_G \cup T_G \bar{1}$  
$H_3 = T_G \cup T_G m$

$P121$
Example: P12/m1

Translationengleiche subgroups $H < G$:

$P\bar{1} = T_G \cup T_G \bar{1}$

$P121 = T_G \cup T_G 2$
Example: \( \text{P12}/\text{m1} \)

Subgroup diagram of point group \( 2/m \)

Translationengleiche subgroups of space group \( P2/m \)

\[ \text{H}<\text{G} : \]

\( \begin{align*}
\bar{I} & \quad 2/m \\
2 & \quad I \\
I & \quad m
\end{align*} \]

\[ \text{index} \]

\[ [1] \]

\[ [2] \]

\[ [4] \]
Construct the diagram of the $t$-subgroups of $P4mm$ using the ‘analogy’ with the subgroup diagram of $4mm$.
\( P4mm \) \hspace{1cm} \( C_{4v} \) \hspace{1cm} \( 4mm \) \hspace{1cm} Tetragonal

No. 99 \hspace{1cm} \( P4mm \)

Patterson symmetry \( P4/mmm \)

Origin on \( 4mm \)

Asymmetric unit 
\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry operations

(1) 1  
(2) 2 0,0,z  
(3) 4 0,0,z  
(4) 4 0,0,z  
(5) m x,0,z  
(6) m 0,y,z  
(7) m x,\bar{x},z  
(8) m x,x,z

Generators selected

(1); \( t(1,0,0); t(0,1,0); t(0,0,1); \) (2); (3); (5)

Positions

Multiplicity, Coordinates

Wyckoff letter, Site symmetry

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) ( x,y,z )</td>
</tr>
<tr>
<td></td>
<td>(5) ( x,\bar{y},z )</td>
</tr>
</tbody>
</table>
Subgroup diagram of point group 4mm

Translationengleiche subgroups of space group $P4mm$
Problem 2.3.1

SOLUTION

\[ P = (a-b, a+b, c) \]

\[ a' = a - b \]

\[ b' = a + b \]
Remark 1. Due to the convention to choose the basis vectors parallel to the rotation axes, \( C \)-centered cells appear although the translation lattice has not changed. If the retained twofold axes are diagonal, the conventional basis vectors \( \mathbf{a}', \mathbf{b}', \mathbf{c}' \) of the subgroup are \( \mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{c} \) with respect to the basis vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) of \( P4mm \). Referred to \( \mathbf{a}', \mathbf{b}', \mathbf{c}' \) the cell is \( C \)-centered.
Example: P4mm

Maximal subgroups of space groups

\[ \begin{array}{l}
\text{I Maximal translationengleiche subgroups} \\
[2] P411 (75, P4) \quad 1; 2; 3; 4 \\
[2] P21m (35, Cmm2) \quad 1; 2; 7; 8 \\
[2] P2m1 (25, Pmm2) \quad 1; 2; 5; 6 \\
\end{array} \]

\[ \begin{array}{l}
\text{II Maximal klassengleiche subgroups} \\
\bullet \text{ Enlarged unit cell} \\
[2] c' = 2c \\
P4_{4mc} (105) \quad (2; 5; 3 + (0,0,1)) \quad a, b, 2c \\
P4_{4cc} (103) \quad (2; 3; 5 + (0,0,1)) \quad a, b, 2c \\
P4_{4cm} (101) \quad (2; (3; 5) + (0,0,1)) \quad a, b, 2c \\
P4_{4mm} (99) \quad (2; 3; 5) \quad a, b, 2c \\
\bullet \text{ Series of maximal isomorphic subgroups} \\
[p] c' = pc \\
P4_{4mm} (99) \quad (2; 3; 5) \quad a, b, pc \\
p > 1 \\
no conjugate subgroups \\
\[p^2\] a' = pa, b' = pb \\
P4_{4mm} (99) \quad (2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (0, 2v, 0)) \quad pa, pb, c \quad u, v, 0 \\
p > 2; 0 \leq u < p; 0 \leq v < p \\
p^2 \text{ conjugate subgroups for the prime } p
\end{array} \]
DATA ITAI: Maximal Subgroups

Transformation matrix: \((P,p)\)

- **group G**: \(\{e, g_2, g_3, ..., g_i, ..., g_{n-1}, g_n\}\)
- **subgroup H < G (non-conventional)**: \(\{e, g_2, g_3, ..., g_i, ..., g_{n-1}, g_n\}\)
- **subgroup H < G**: \(\{e, h_2, h_3, ..., h_m\}\)

Subgroup specification: HM symbol, \([i]\), \((P,p)\)
MAXIMAL SUBGROUPS OF SPACE GROUPS

II. MAXIMAL KLASSENGLEICHE SUBGROUPS
Klassengleiche subgroups $H < G$:

Example: $P1$

$t = u a + v b + w c$

Coset decomposition

$T_e = \{ t(u=2n,v,w) \}$

$T_e t_a$

\[
\begin{array}{ll}
(T_e, (l,0)) & (l,t_a) \\
(T_e, (l,t_1)) & (l,t_1 + t_a) \\
(T_e, (l,t_2)) & (l,t_2 + t_a) \\
\vdots & \vdots \\
(T_e, (l,t_j)) & (l,t_j + t_a) \\
\vdots & \vdots \\
\end{array}
\]

Subgroups of space groups

\[
\begin{align*}
T_H & < T_G \\
P_H & = P_G
\end{align*}
\]

isomorphic $k$-subgroups:

$P1(2a, b, c)$
Klassengleiche subgroups $H < G$:

Example: $P1$  

$T_e = \{ t(u=2n,v,w) \}$

Coset decomposition

$P1 = T_e + T_e t_a$

Isomorphic $k$-subgroup:

$P1(2a,b,c)$

Series of isomorphic $k$-subgroups:

$P1(pa,b,c)$: $p > 1$, prime

$P1(a,qb,c)$: $q > 1$, prime

... etc.

Subgroups of space groups

$\{ T_H < T_G \}$

$P_H = P_G$

$H = T_e$

$t_a(1,0,0)$

$T_e$

$T_e t_a$

$(l,0)$  $(l,t_a)$

$(l,t_1)$  $(l,t_1 + t_a)$

$(l,t_2)$  $(l,t_2 + t_a)$

...  ...

$(l,t_j)$  $(l,t_j + t_a)$

...  ...

INFINITE number of maximal isomorphic subgroups
Series of maximal isomorphic subgroups

\[ P \bar{1} \]

No. 2

\[ P \bar{1} \]

- Series of maximal isomorphic subgroups

\([p] a' = pa, \; b' = qa + b, \; c' = ra + c \]

\( P \bar{1} \) (2)

\[ \langle 2 + (2u, 0, 0) \rangle \]

\( p > 2; \; 0 \leq q < p; \; 0 \leq r < p; \; 0 \leq u < p \)

\( p \) conjugate subgroups for each triplet of \( q, r, \) and

prime \( p \)

\( pa, qa + b, ra + c \)

\( u, 0, 0 \)

\([p] b' = pb, \; c' = qb + c \]

\( P \bar{1} \) (2)

\[ \langle 2 + (0, 2u, 0) \rangle \]

\( p > 2; \; 0 \leq q < p; \; 0 \leq u < p \)

\( p \) conjugate subgroups for each pair of \( q \) and prime \( p \)

\( a, pb, qb + c \)

\( 0, u, 0 \)

\([p] c' = pc \]

\( P \bar{1} \) (2)

\[ \langle 2 + (0, 0, 2u) \rangle \]

\( p > 2; \; 0 \leq u < p \)

\( p \) conjugate subgroups for the prime \( p \)

\( a, b, pc \)

\( 0, 0, u \)
Klassengleiche subgroups $H \triangleleft G$: **non-isomorphic**

$\{T_H < T_G, P_H = P_G\}$

**Example:** $C_2$

**Coset decomposition**

$C_2 = T_c + T^-_c 2$

$T^-_i + T^-_i t_c$

$t_i = \text{integer} \quad t_c = 1/2, 1/2, 0$

**non-isomorphic $k$-subgroups:**

$H_1 = T^-_i \cup T^-_i 2$

$P_2$

$H_2 = T^-_i \cup T^-_i t_c 2$

$P_{2_1}$

<table>
<thead>
<tr>
<th>$T_i$</th>
<th>$T^-_i t_c$</th>
<th>$T^-_i 2$</th>
<th>$T^-_i t_c 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1,0)$</td>
<td>$(1,t_c)$</td>
<td>$(2,0)$</td>
<td>$(2,t_c)$</td>
</tr>
<tr>
<td>$(1,t_1)$</td>
<td>$(1,t_1 + t_c)$</td>
<td>$(2, t_1)$</td>
<td>$(2, t_1 + t_c)$</td>
</tr>
<tr>
<td>$(1,t_2)$</td>
<td>$(1,t_2 + t_c)$</td>
<td>$(2, t_2)$</td>
<td>$(2, t_2 + t_c)$</td>
</tr>
<tr>
<td>$(1,t_j)$</td>
<td>$(1,t_j + t_c)$</td>
<td>$(2, t_j)$</td>
<td>$(2, t_j + t_c)$</td>
</tr>
</tbody>
</table>

...
Maximal subgroups of space groups

### Example: P4mm

<table>
<thead>
<tr>
<th>Group</th>
<th>No.</th>
<th>Translationengleich</th>
<th>Enlarged unit cell</th>
<th>Series of maximal isomorphic subgroups</th>
</tr>
</thead>
<tbody>
<tr>
<td>P4mm</td>
<td>99</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**I Maximal translationengleich subgroups**

- [2] $\text{P411 (75, P4)}$; $1; 2; 3; 4$
- [2] $\text{P21m (35, Cmm2)}$; $1; 2; 7; 8$
- [2] $\text{P2m1 (25, Pmm2)}$; $1; 2; 5; 6$

**II Maximal klassengleich subgroups**

- **Enlarged unit cell**
  - [2] $c' = 2c$
    - $\text{P4}_{\text{m}} \text{c} \ (105)$
    - $\langle 2; 5; 3 + (0, 0, 1) \rangle$
    - $a, b, 2c$
  - $\text{P4}_{\text{c}} \text{c} \ (103)$
    - $\langle 2; 3; 5 + (0, 0, 1) \rangle$
    - $a, b, 2c$
  - $\text{P4}_{\text{2}} \text{cm} \ (101)$
    - $\langle 2; (3; 5) + (0, 0, 1) \rangle$
    - $a, b, 2c$
  - $\text{P4} \text{mm} \ (99)$
    - $\langle 2; 3; 5 \rangle$
    - $a, b, 2c$

- **Series of maximal isomorphic subgroups**
  - $[p] c' = pc$
    - $\text{P4} \text{mm} \ (99)$
    - $\langle 2; 3; 5 \rangle$
    - $a, b, pc$
    - $p > 1$
    - No conjugate subgroups
  - $[p^2] a' = pa, b' = pb$
    - $\text{P4} \text{mm} \ (99)$
    - $\langle 2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (0, 2v, 0) \rangle$
    - $pa, pb, c$
    - $u, v, 0$
    - $p > 2$; $0 \leq u < p$; $0 \leq v < p$
    - $p^2$ conjugate subgroups for the prime $p$
GENERAL SUBGROUPS OF SPACE GROUPS
General subgroups $H \lhd G$:

Graph of maximal subgroups

Group-subgroup pair

$\mathcal{G} > \mathcal{H} : \mathcal{G}, \mathcal{H}, [i], (P, p)$

Pairs: group - maximal subgroup

$\mathcal{Z}_k > \mathcal{Z}_{k+1}, (P, p)_k$

$(P, p) = \prod_{k=1}^{n} (P, p)_k$
Subgroups of space groups

General subgroups $H < G$:

For each pair $G > H$, there exists a uniquely defined intermediate subgroup $M$, $G \geq M \geq H$, such that:

- $M$ is a $t$-subgroup of $G$
- $H$ is a $k$-subgroup of $M$

$[i] = [i_P] \cdot [i_L]$

Corollary

A maximal subgroup is either a $t$- or $k$-subgroup
PROBLEM: Domain-structure analysis

number of domain states

twins and antiphase domains states

twinning operation

symmetry groups of the domain states; multiplicity and degeneracy
A connected homogeneous part of a domain structure or of a twinned crystal is called a domain. Each domain is a single crystal. The number of such crystals is not limited; they differ in their locations in space, in their orientations, in their shapes and in their space groups but all belong to the same space-group type of H.

The domains belong to a finite (small) number of domain states. Two domains belong to the same domain state if their crystal patterns are identical, i.e. if they occupy different regions of space that are part of the same crystal pattern.

The number of domain states which are observed after a phase transition is limited and determined by the group-subgroup relations of the space groups G and H.
Hermann, 1929:

For each pair $G \succ H$, index $[i]$, there exists a uniquely defined intermediate subgroup $M$, $G \supseteq M \supseteq H$, such that:

- $M$ is a $t$-subgroup of $G$
- $H$ is a $k$-subgroup of $M$

with $[i] = [i_P] \cdot [i_L]$

- $i_P = P_G / P_H$
- $i_L = Z_{H,p} / Z_{G,p} = V_{H,p} / V_{G,p}$

Domains-structure analysis

**SUBGROUPS CALCULATIONS: HERMANN**
Index $[i]$ for a group-subgroup pair $G \supset H$

Lead vanadate $\text{Pb}_3(\text{VO}_4)_2$

**INDEX:** $[i] = [i_P] \cdot [i_L]$
Pb$_3$(VO$_4$)$_2$: Ferroelastic Domains in P2$_1$/c phase

**Group-Subgroup Lattice**

Maximal-subgroup graph

Number of domain states = index $[i] = [i_P][i_L] = 6$

Number of ferroelastic domain states: $i_P = 12:4 = 3$

Number of different subgroups P2$_1$/c: 3
Problem: CLASSIFICATION OF DOMAINS

Quartz

$G = P_{6222}$

$t$-subgroup

$H = P_{32121}$

$i = i_t = 2$

twin domains

Cu$_3$Au

$G = Fm\bar{3}m$

$k$-subgroup

$H = Pm\bar{3}m$

$i = i_k = 4$

antiphase domains

Gd$_2$(MoO$_4$)$_3$

$G = P\bar{4}2_1m$

$H = Cmm2$

$i_t = 2$

$t$-subgroup

twin and antiphase domains

$i_k = 2$

$k$-subgroup
EXERCISES

Problem 2.3.3

(A) High symmetry phase: P2/m
Low symmetry phase: P1, small unit-cell deformation
How many and what kind of domain states?

Hint: Determine the index \([i]=[i_P],[i_L]\)

(B) High symmetry phase: P2/m
Low symmetry phase: P1, duplication of the unit cell
How many and what kind of domain states?

(C) High symmetry phase: P4mm
Low symmetry phase: P2, index 8
How many and what kind of domain states?

(D) High symmetry phase: P4_2bc
Low symmetry phase: P2_1, index 8
How many and what kind of domain states?