Study of layer and multilayer materials using the Bilbao Crystallographic Server

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- Bilbao Crystallographic Server
- Subperiodic Groups: Layer, Rod and Frieze Groups
  - Crystallographic database available at the BCS
- Relationship between layer and space groups
  - Layer groups Brillouin-zone database
- Identification of layer symmetry of periodic sections
- The site-symmetry induced representations of layer groups
- Conclusions
Bilbao Crystallographic Server

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Point-group symmetry
Plane-group symmetry
Double point and space groups

Quick access to some tables
Space Groups
Plane Groups
Layer Groups
Rod Groups
Frieze Groups
2D Point Groups
3D Point Groups
Magnetic Space Groups

Bilbao Crystallographic Server in forthcoming schools and workshops

News:
- New program: MSAIO61, CORREPRESENTATIONS, CORREPRESENTATIONS PO, MOPMORPH, MLYM, Check Topological Magnetic Mat
- 16/2023 now both in the sections "Magnetic Symmetry and Applications" and "Representations and Applications". More info
- New section: TOPOLOGICAL QUANTUM CHEMISTRY 16/2023 tools for the identification of the topological character of non-magnetic and magnetic materials.
- MAGNADAT reaches 1,000 entries
Crystallographic Databases

Point groups
Plane groups
Space groups

Space groups

Subperiodic groups
- Frieze groups
- Rod groups
- Layer groups
Crystallographic Databases

- Magnetic groups
- Brillouin zones and $k$-vector
- Magnetic structures database
- Double groups

Bilbao Incommensurate Structures Database

B-IncStrDB
Subperiodic Groups: Layer, Rod and Frieze Groups

- Crystallographic information
- Brillouin-zone database for layer groups
- Identification of layer symmetry of periodic sections
- Site-symmetry induced representations of layer groups
Subperiodic Groups: Layer, Rod and Frieze Groups

There are three types of subperiodic groups:

Frieze groups
2D groups with 1D translations

Rod groups
3D groups with 1D translations

Layer groups
3D groups with 2D translations
Subperiodic Groups: Layer, Rod and Frieze Groups

Polymers

Nanotubes

Layered materials
Volume E – International Tables

**p222**

**No. 19**

**Orthorhombic/Rectangular**

Patterson symmetry $p_{mmm}$

**Generators selected**

(3): $r(1,0,0)$; $r(0,1,0)$; (2): (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>General: no conditions Special: no extra conditions</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**GENPOS**

- **4** $m$ 1
- (1): $x,y,z$
- (2): $x,5,z$
- (3): $x,y,2$
- (4): $x,5,z$

**Symmetry of special projections**

- Along [001] $p_{222}$
- Along [010] $p_{222}$
- Along [001] $p_{222}$

**WYCKPOS**

- Origin at (0,0,0)
- Origin at (0,0,0)
- Origin at (0,0,0)

**Maximal non-isotypic subgroups**

- I: $[1] \ p_{222} (p_{211} 1.8) ; 1 ; 3$
- II: $[2] \ p_{222} (p_{211} 1.8) ; 1 ; 4$
- III: $[3] \ p_{222} (1.8) ; 1 ; 2$

- Maximal isotopic subgroups of lowest index
  - I: $[1] \ p_{222} (1.8)$
  - II: $[2] \ p_{222} (1.8)$

**Minimal non-isotypic supergroups**

- I: $[2] \ p_{222}$
- II: $[2] \ p_{222}$
# Programs: GENPOS, WYCKPOS & MAXSUB

## GENPOS

<table>
<thead>
<tr>
<th>No.</th>
<th>Coordinate triplets</th>
<th>Matrix form</th>
<th>Symmetry operation</th>
<th>ITE</th>
<th>Seitz</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x,y,z$</td>
<td>$\begin{pmatrix} 1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>1</td>
<td>{}{1</td>
<td>0}</td>
</tr>
<tr>
<td>2</td>
<td>$-x,y,z$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>200,2</td>
<td>{}{2</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>$-x,y,-z$</td>
<td>$\begin{pmatrix} -1 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; -1 \end{pmatrix}$</td>
<td>200,0</td>
<td>{}{2</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>$x,-y,-z$</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 \ -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 \end{pmatrix}$</td>
<td>2x0,0</td>
<td>{}{2</td>
<td>0</td>
</tr>
</tbody>
</table>

## WYCKPOS

### Wyckoff Positions of Layer Group $p\overline{2}2\overline{2}$ (No. 19)

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>m</td>
<td>1</td>
<td>$(x,y,z)$, $(-x,y,z)$, $(-x,-y,z)$, $(x,-y,z)$</td>
</tr>
<tr>
<td>2</td>
<td>i</td>
<td>2</td>
<td>$(1/2,1/2,1/2)$, $(1/2,1/2,-1/2)$</td>
</tr>
<tr>
<td>2</td>
<td>k</td>
<td>2</td>
<td>$(0,1/2,1/2)$, $(0,1/2,-1/2)$</td>
</tr>
<tr>
<td>2</td>
<td>j</td>
<td>2</td>
<td>$(1/2,0,1/2)$, $(1/2,0,-1/2)$</td>
</tr>
<tr>
<td>2</td>
<td>l</td>
<td>2</td>
<td>$(0,0,0)$, $(0,0,-1)$</td>
</tr>
<tr>
<td>2</td>
<td>g</td>
<td>2</td>
<td>$(1/2,1/2,0)$, $(1/2,1/2,0)$</td>
</tr>
<tr>
<td>2</td>
<td>f</td>
<td>2</td>
<td>$(x,1/2,0)$, $(-x,1/2,0)$</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>2</td>
<td>$(0,0,0)$, $(0,0,-1)$</td>
</tr>
</tbody>
</table>

### Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)

<table>
<thead>
<tr>
<th>Variable parameters</th>
<th>Parameter $x$, $y$, $z$ are also accepted</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$</td>
<td>$y$</td>
</tr>
<tr>
<td>$z$</td>
<td></td>
</tr>
</tbody>
</table>

## MAXSUB

### Maximal Subgroups of Layer Group $p\overline{2}2\overline{2}$ (No. 19)

Note: The program uses the default settings

In the following table the list of maximal subgroups is given. Click over "show." to see the possible setting(s) for the given subgroup.

<table>
<thead>
<tr>
<th>Subgroup</th>
<th>HM Symbol</th>
<th>Index</th>
<th>Type</th>
<th>Transformations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>p 1 1 2</td>
<td>2</td>
<td>t</td>
<td>show.</td>
</tr>
<tr>
<td>2</td>
<td>p 2 1 1</td>
<td>2</td>
<td>t</td>
<td>show.</td>
</tr>
<tr>
<td>3</td>
<td>p 2 2 2</td>
<td>2</td>
<td>k</td>
<td>show.</td>
</tr>
<tr>
<td>4</td>
<td>p 2 2 2</td>
<td>3</td>
<td>k</td>
<td>show.</td>
</tr>
<tr>
<td>5</td>
<td>p 2 2 2</td>
<td>2</td>
<td>k</td>
<td>show.</td>
</tr>
<tr>
<td>6</td>
<td>p 2 2 2</td>
<td>2</td>
<td>k</td>
<td>show.</td>
</tr>
</tbody>
</table>

1 represents the translationengleichen subgroups
k represents the kiassengleichen subgroups

GENPOS & WPOS provide the data in standard and non-standard settings.
Relationship between layer and space groups

- Layer groups ($\mathcal{L}$) form a subgroup of space groups ($\mathcal{G}$): $\mathcal{L} < \mathcal{G}$
- $\mathcal{L} < \mathcal{G}$ is essential to derive the layer groups $k$ vectors and Brillouin zones
- The space group $\mathcal{G}$ can be expressed as $\mathcal{G} = \mathcal{L} \triangleleft T_3 \quad \Rightarrow \quad \mathcal{L} \cong G / T_3$
- The $k$ vectors of $\mathcal{L}$ can be deduced from $\mathcal{G}$ based on the isomorphism $\mathcal{L} \cong G / T_3$
- The reciprocal-group approach is applied to classify the $k$ vectors of $\mathcal{L}$
- The reciprocal space of layer groups is described by reciprocal-plane groups
Procedure: $k$-vector and BZ figures derivation

Brillouin Zone of the space group P4mm (No. 99)

Brillouin Zone of the layer group $p4mm$ (No. 55)
Procedure: k-vector and BZ figures derivation

1. Identify the space group $G$ to which the layer group $L$ is related to
2. Identify the reciprocal-space-group $(G)^*$ of $G$
3. Calculate the section of $(G)^*$ along $(001) \rightarrow (L_{\text{section}})$
4. Determine the reciprocal plane group of $L$: the $[001]$ projection of $L_{\text{section}}$ is calculated

The classification scheme of the $k$ vectors derived in this work is compared with the classification of Litvin & Wike in *Character Tables and Compatibility Relations of the Eighty Layer Groups*
The program LKVEC

**Input** of the program: layer group number

### The k-vector types of layers group $p\, 4\, m\, m$ (No. 55)

*(Table for arithmetic crystal class 4mmp)*

$p4mm$ (No. 55), $p4bm$ (No. 56)

Reciprocal plane group ($p4mm$)* (No. 11)

Brillouin zone

<table>
<thead>
<tr>
<th>k-vector description</th>
<th>Plane-group description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Label(1)</td>
<td>Coefficients</td>
</tr>
<tr>
<td>GM</td>
<td>0,0</td>
</tr>
<tr>
<td>M</td>
<td>1/2,1/2</td>
</tr>
<tr>
<td>X</td>
<td>0,1/2</td>
</tr>
<tr>
<td>DT</td>
<td>0,u</td>
</tr>
<tr>
<td>Y</td>
<td>u,1/2</td>
</tr>
<tr>
<td>SM</td>
<td>u,u</td>
</tr>
<tr>
<td>D=[GM, X, M]</td>
<td>u,v</td>
</tr>
</tbody>
</table>
The program LKVEC

**Input** of the program: layer group number

The **k-vector types of layers group p 4 m m (No. 55)**

*(Table for arithmetic crystal class 4mmp)*

*p4mm (No. 55), p4bm (No. 56)*

Reciprocal plane group (p4mm)* (No. 11)

Brillouin zone

<table>
<thead>
<tr>
<th>k-vector description</th>
<th>Plane-group description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Label</strong></td>
<td><strong>Coefficients</strong></td>
</tr>
<tr>
<td>GM</td>
<td>0,0</td>
</tr>
<tr>
<td>M</td>
<td>1/2,1/2</td>
</tr>
<tr>
<td>X</td>
<td>0,1/2</td>
</tr>
<tr>
<td>DT</td>
<td>0,u</td>
</tr>
<tr>
<td>Y</td>
<td>u,1/2</td>
</tr>
<tr>
<td>SM</td>
<td>u,u</td>
</tr>
<tr>
<td>D-[GM,X,M]</td>
<td>u,v</td>
</tr>
</tbody>
</table>

---

**The k-vector types of layers group p 4 m m (No. 55)**

- Layer Group: p 4 m m (No. 55)
- The reciprocal bases: primitive
- The k-vector coordinates: 0, 1
- k-vector label: GM
- The star of the k-vector has 1 arm:
  - 0,000 1,000
- GM is a k-vector point
- Layer little co-group: 4mm
- ITA classification: 1a
- Site-symmetry group: 4mm
Identification of layer symmetry of periodic sections

- The symmetries of planes intersecting the crystal are called the \textit{sectional layer groups}.

Scanning tables

\[ G = P4mm \]

<table>
<thead>
<tr>
<th>Orientation orbit (hkl)</th>
<th>Conventional basis of the scanning group ( a', b', c )</th>
<th>Scanning group ( H )</th>
<th>Linear orbit ( sd )</th>
<th>Sectional layer group ( L_{sd} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(001) ( (hkl) )</td>
<td>( a \ b \ c )</td>
<td>( P4mm )</td>
<td>( sd )</td>
<td>( p4mm )</td>
</tr>
<tr>
<td>(100) ( (hkl) )</td>
<td>( b \ c \ a )</td>
<td>( Pm2n )</td>
<td>( 0d, \frac{1}{2}d )</td>
<td>( pm2n )</td>
</tr>
<tr>
<td>(010) ( (hkl) )</td>
<td>( -a \ c \ b )</td>
<td></td>
<td>( [sd, -sd] )</td>
<td>( pm11 )</td>
</tr>
<tr>
<td>(110) ( (hkl) )</td>
<td>( (a + b) \ c \ (a + b) )</td>
<td>( Bm2n )</td>
<td>( [0d, \frac{1}{2}d] )</td>
<td>( pm2n )</td>
</tr>
<tr>
<td>(1T0) ( (hkl) )</td>
<td>( (a + b) \ c \ (a - b) )</td>
<td></td>
<td>( \frac{1}{2}d, \frac{1}{2}d )</td>
<td>( pm2a (a'/4) )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( \pm sd, (\pm s + \frac{1}{2})d )</td>
<td>( pm11 )</td>
</tr>
</tbody>
</table>

[Image of book cover]
The program SECTIONS

For a given space group the program identifies the full set of possible layer symmetries of periodic sections defined by their common normal vector

Scanning tables for the space group $P4mm$ (No. 99) along $(1\ 0\ 0)$

<table>
<thead>
<tr>
<th>Scanning group</th>
<th>Conventional basis of the scanning group $a', b', c', d, p_1, p_2, p_3$</th>
<th>Linear orbit $sd$</th>
<th>Sectional layer group</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Pmm2$ (No. 25)</td>
<td>$b, c, a$; 0, 0, 0</td>
<td>$\pm sd$</td>
<td>$pm11$ (No. 11) $-a, -b, c$; 0, 0, 0</td>
</tr>
<tr>
<td></td>
<td>$[0d, 1/2d]$</td>
<td>$pm2m$ (No. 27) $a, b, c$; 0, 0, 0</td>
<td></td>
</tr>
</tbody>
</table>
Example: Program SECTIONS – CdI₂

Scanning tables for the space group P-3m1 (No. 164)

<table>
<thead>
<tr>
<th>Scanning group</th>
<th>Conventional basis of the scanning group</th>
<th>Linear orbit sd</th>
<th>Sectional layer group</th>
</tr>
</thead>
<tbody>
<tr>
<td>P.3m1 (No. 164)</td>
<td>a,b,c, 0,0,0</td>
<td>±sd</td>
<td>p3m1 (No. 69) a,b,c, 0,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[0d, 1/2d]</td>
<td>p-3m1 (No. 72) a,b,c, 0,0,0</td>
</tr>
</tbody>
</table>

For planes of this orientation at any other height p3m1

P₃m1 (No. 164)
The program LSITESYM

**Site-symmetry approach**: It establishes the local properties of atoms in crystals with the symmetry of states of the whole crystalline system.

**Bulk crystal**: \( P6_3/mmc \) (No. 194)

- Mo: 2c \((1/3, 2/3, 1/4)\)
- S: 4f \((1/3, 2/3, z)\)

**Single layer**: \( p\text{-}6m2 \) (No. 78)

- Mo: 1c \((2/3, 1/3, 0)\)
- S: 2e \((1/3, 2/3, z)\)
The program LSITESYM

**Site-symmetry approach**: It establishes the local properties of atoms in crystals with the symmetry of states of the whole crystalline system.

**Bulk crystal**: \( P6_3/mmc \) (No. 194)

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyckoff position</th>
<th>( \mathbf{D}_\sigma )</th>
<th>( \Gamma (0, 0) , 62m )</th>
<th>( K (\frac{1}{2}, \frac{1}{2}) , 00m )</th>
<th>( M (\frac{1}{2}, 0) , m2m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo</td>
<td>1c ( (\frac{1}{2}, \frac{1}{2}, 0) )</td>
<td>( A_2^0 ) (z)</td>
<td>3</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>( 6m2 )</td>
<td>( E' ) (x, y)</td>
<td>5</td>
<td>1, 3</td>
<td>1, 2</td>
</tr>
<tr>
<td>S</td>
<td>2e ( (\frac{1}{2}, \frac{1}{2}, z) )</td>
<td>( A_1 ) (z)</td>
<td>1, 3</td>
<td>3, 4</td>
<td>1, 3</td>
</tr>
<tr>
<td></td>
<td>( 3m )</td>
<td>( E ) (x, y)</td>
<td>5, 6</td>
<td>1, 2, 5, 6</td>
<td>1, 2, 3, 4</td>
</tr>
</tbody>
</table>

**Single layer**: \( p-6m2 \) (No. 78)

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyckoff position</th>
<th>( \mathbf{D}_\sigma )</th>
<th>( \Gamma (0, 0) , 62m )</th>
<th>( K (\frac{1}{2}, \frac{1}{2}) , 00m )</th>
<th>( M (\frac{1}{2}, 0) , m2m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo</td>
<td>1c ( 2/3, 1/3, 0 )</td>
<td>( E' ) (x, y)</td>
<td>5, 6</td>
<td>1, 2, 5, 6</td>
<td>1, 2, 3, 4</td>
</tr>
<tr>
<td>S</td>
<td>2e ( 1/3, 2/3, z )</td>
<td>( E' ) (x, y)</td>
<td>5, 6</td>
<td>1, 2, 5, 6</td>
<td>1, 2, 3, 4</td>
</tr>
</tbody>
</table>
Conclusions

- The *Bilbao Crystallographic Server* is in constant development

- New features and programs have been recently included in the section dedicated to Subperiodic Groups: layer, rod and frieze groups

- Set of tools dedicated to the study of layered and multilayered materials

- New tools are under development and will be soon available in the server
THANK YOU FOR YOUR ATTENTION

Questions

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