Point groups and morphological symmetry. Introduction to the stereographic projection

Didactic material for the MaThCryst schools

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Lattice planes and Miller indices
Planes passing through lattice nodes are called “rational planes”

Equation of the plane: \( x'/pa + y'/qb + z'/rc = 1 \)
Define: \( x = x'/a; y = y'/b; z = z'/c \)
Equation of the plane: \( x/p + y/q + z/r = 1 \)

\((qr)x + (pr)y + (pq)z = pqr\)
\(hx + ky + lz = m\)

Making \( m \) variable, we obtain a family of lattice planes, \((hkl)\), where \( h, k \) and \( l \) are called the Miller indices.

First plane of the family \((hkl)\) for \( m = 1 \)
\(hx + ky + lz = 1\)

Intercepts of the first \( (m = 1) \) plane of the family \((hkl)\) on the axes
\( p = pqr/qr = m/h = 1/h \)
\( q = pqr/pr = m/k = 1/k \)
\( r = pqr/pq = m/l = 1/l \)

The values \( h, k \) and \( l \) are called the Miller indices of the lattice plane and give its orientation.

All lattice planes in the same family have the same orientation \( \rightarrow (hkl) \) represents the whole family of lattice planes.
Why the *reciprocal* of the intersection \((1/p)\) rather than the intersection \((p)\) itself?

Consider a plane parallel to an axis – for example \(c\)

What is the intersection of this plane with the axis \(c\)? \(\infty\)

What is the \(l\) Miller intersection of this plane? \(1/\infty = 0\)
Example: family (112) in a primitive lattice

Intercepts of the first plane of the family:
on $a$: 1/1
on $b$: 1/1
on $c$: 1/2

Intercepts of the second plane of the family:
on $a$: 2/1
on $b$: 2/1
on $c$: 2/2
Example: family (326) in a primitive lattice

Intercepts of the first plane of the family:
- on \(a\): 1/3
- on \(b\): 1/2
- on \(c\): 1/6

Intercepts of the sixth plane of the family:
- on \(a\): 6/3
- on \(b\): 6/2
- on \(c\): 6/6
Miller indices for a primitive lattice are relatively prime integers

Intercepts of the first plane of a hypothetic family (222):
on $a$: 1/2
on $b$: 1/2
on $c$: 1/2

This plane does not pass through any lattice node – it is an *irrational* plane

The first rational plane of this family has intercepts:
on $a$: 1/1
on $b$: 1/1
on $c$: 1/1

**In a primitive lattice, the Miller indices of a family of lattice planes are relatively prime integers: (111)**
Miller indices for different types of lattice: \((h00)\) in \(oP\) and \(oC\) (projection on \(ab\))

In morphology, we do not see the lattice and thus the Miller indices of a face are usually relatively prime integers.

http://dx.doi.org/10.1107/S1600576715011206
The concept of form: set of faces equivalent by symmetry

Example in the cubic crystal system

Form \{100\}: the cube

Form \{111\}: the octahedron
Zone: set of faces whose intersection is parallel to a same direction, called the zone axis

Example in the cubic crystal system

![Diagram of zones in the cubic crystal system](image)
The stereographic projection: how to get rid of accidental morphological features of a crystal
Spherical projection and spherical poles
Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')
Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')
Stereographic projection: poles and symmetry planes
Example of decomposition of the morphology of a crystal
Stereographic vs. gnomonic projection

Stereographic projection

Gnomonic projection

Be careful - some textbooks exchange the two terms!
The most detailed book about stereographic and gnomonic projections of crystal
Site-symmetry groups (stabilizers) and Wyckoff positions of point groups

Let $P$ be a crystallographic (thus finite) point group and $X$ a point in space.

The finite set of points $\{PX\} = \{X, X', X''\ldots\}$ is the orbit of $X$ under the action of $P$.

A subgroup $S$ of $P$ ($S \subset P$, possibly trivial, i.e. $S = 1$) leave $X$ invariant, i.e. $SX = X$

$S$ is called the site-symmetry group (or stabilizer) of $X$.

Points whose site-symmetry groups $S$ are conjugate under $P$ belong the same Wyckoff position

The number of points obtained as $\{PX\}$ is the multiplicity $M$ of the orbit, which is equal to the index of $S$ in $P$: $M = |P|/|S|$
Site-symmetry groups (stabilizers) and Wyckoff positions of point groups

Coordinates

\[ xyz, \ yxz, \ x\bar{yz}, \ y\bar{xz}, \ \bar{xyz}, \ \bar{yxz}, \ x\bar{yz}, \ y\bar{xz} \]

S = \{1\}, M = 8

General position
S = \{1\}, M = |P|

Coordinates

\[ xx0, \ \bar{xx}0: \ S = \{1,2_{[110]}\} \]
\[ xx0, \ \bar{xx}0: \ S = \{1,2_{[11\bar{1}0]}\} \]

S = \{..2\}, M = 4

Special position
S \supset \{1\}, M = |P|/|S|

\[ \forall p_j \in P \]
\[ p_j 1 p_j^{-1} = 1 \]
\[ p_j 2_{[110]} p_j^{-1} = \{2_{[110]}, 2_{[1\bar{1}0]}\} \]
Subgroups vs. supergroups: to remove symmetry operations is easier than to add them

\[ G \supseteq H \quad \text{ and } \quad i = \frac{|G|}{|H|} \]
To remove symmetry operations is easier than to add them.

Orthorhombic subgroups of index 2

Tetragonal supergroups of 222. index 2
Indexing crystals of the hexagonal family: Bravais-Miller indices
Hexagonal axes: Bravais-Miller indices

abc \rightarrow A_1A_2A_3C

hkl \rightarrow hkil
Miller indices \quad Bravais-Miller indices

A_3 = -A_1 - A_2

i = -h - k
Bravais-Miller indices: example

If you use Miller indices the symmetry is less evident!

(100)  
(010)  
(110)  
(100)  
(010)  
(110)

Bravais-Miller indices: example

parallel to $C \rightarrow l = 0$
parallel to $A_2 \rightarrow k = 0$

$(hki l) \rightarrow (h0i0) \rightarrow (h0h0) \rightarrow (10\bar{1}0)$
$i = -h - 0$
divide by the common factor
If you use Miller indices the symmetry is less evident!

\[(h0l)\]
\[(0hl)\]
\[(\bar{h}hl)\]
\[(\bar{h}0l)\]
\[(0\bar{h}l)\]
\[(h\bar{h}l)\]

Bravais-Miller indices: example

\[(hkl) \rightarrow (h0il) \quad \rightarrow (h0\bar{hl})\]

\[i = -h-0\]

parallel to \(A_2 \rightarrow k = 0\)

\[A_1\]

\[A_2\]

\[A_3\]
**Bravais-Miller indices: example**

- Parallel to $C \rightarrow l = 0$
- Same intersection on $A_1$ and $A_2 \rightarrow k = h$

$$ (hkl) \rightarrow (hhi0) \rightarrow (hh\bar{2}h0) \rightarrow (1\bar{1}20) $$

If you use Miller indices, the symmetry is less evident!

- $(110)$
- $(120)$
- $(\bar{2}10)$
- $(110)$
- $(1\bar{2}0)$
- $(2\bar{1}0)$
same intersection on $A_1$ and $A_2 \rightarrow k = h$

$\begin{align*}
(hkil) &\rightarrow (hhil) & \rightarrow & (hh2hl) \\
i = -h &-h
\end{align*}$

If you use Miller indices the symmetry is less evident!

$\begin{align*}
(hhl) &\rightarrow (h2hl) \\
(hhl) &\rightarrow (2hhl) \\
(hhl) &\rightarrow (h2hl) \\
(2hhl) &\rightarrow (2hhl)
\end{align*}$
We you don’t see $3/m$ in crystallography?

Trigonal bipyramid

$3/m \equiv \bar{6}$

Mirror visible in the morphology (absent in the structure)

Contradiction!
For trigonal and hexagonal crystal, an extension to a four-axes axial setting exists also for lattice directions, known as the **Weber indices**. The Weber indices of the direction perpendicular to a lattice plane are the same as the Bravais-Miller indices of that plane.

Let $A_1, A_2, A_3, C$ be the four hexagonal axes, and let be $uvw$ and $UVTW$ the indices of a direction with respect to $A_1, A_2, C$ or $A_1, A_2, A_3, C$ respectively. The relations between $uvw$ and $UVTW$ are:

\[
\begin{align*}
uw &= 2U + V; \quad v = U + 2V; \quad w = W \\
U &= (2u - v)/3; \quad V = (2v - u)/3; \quad T = -(u + v)/3.
\end{align*}
\]

The relation $T = -U - V$ holds for $U$ and $V$ but not for $u$ and $v$, whereas for the Bravais-Miller indices the addition of the third axis does not modify $h$ and $k$ so that the relation $i = -h - k$ is applied directly. For this reason, the Bravais-Miller indices are widely used in crystallography, whereas the Weber indices are more used in fields like electron microscopy and metallurgy but seldom in crystallography.

<table>
<thead>
<tr>
<th>Miller indices</th>
<th>Bravais-Miller indices</th>
<th>Perpendicular direction</th>
<th>Perpendicular direction (Weber indices)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(hkl0)$</td>
<td>$(hki0)$</td>
<td>$[2h+k, h+2k, 0]$</td>
<td>$[hki0]$</td>
</tr>
<tr>
<td>Ex. (100)</td>
<td>(1010)</td>
<td>[210]</td>
<td>[1010]</td>
</tr>
<tr>
<td>Ex. (210)</td>
<td>(2110)</td>
<td>[100]</td>
<td>[2110]</td>
</tr>
</tbody>
</table>

With the exception of $[0001]$ and $[UVT0]$, the Weber indices correspond to a mixture of direct and reciprocal space, which should be avoided.

https://doi.org/10.1107/S1600576718007033

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Diffraction and Laue indices
Every point of the grid is the source of a spherical wave. Waves which differ by an integer number of wavelengths interfere positively, resulting in diffracted waves. Waves from neighbour points which differ by \( n \) wavelengths result in the \( n \)-th order diffraction.

From M.J. Burger, *X-ray crystallography*
One-dimensional diffraction

From M.J. Burger, *X-ray crystallography*
Two-dimensional diffraction

From M.J. Burger, *X-ray crystallography*
Interpreting diffraction as “reflection”
Bragg’s law

Path difference of BD and AC: FGH

Condition for positive interference

\[ \text{FGH} = n\lambda \]
\[ \text{FG} = \frac{n\lambda}{2} \]

\[ n\lambda/2 = dsin\vartheta \]

\[ n\lambda = 2dsin\vartheta \text{ Bragg’s law} \]

From M.J. Burger, *X-ray crystallography*
Miller indices vs. Laue indices

Miller indices (within parentheses)

(hkl) planes

First-order diffraction: hkl
Second-order diffraction: 2h2k2l
Third-order diffraction: 3h3k3l
n-th-order diffraction: nhnknl

Laue indices (without parentheses!)

Direct beam
000
1st-order
hkl
2nd-order
2h2k2l
3rd-order
3h3k3l
Curie’s law applied to crystals
Curie groups

Cylindrical system

Spherical system

∞
∞/m (∞)
∞2
∞m
∞/mm

2∞ (∞∞)

m∞
(2/m∞, ∞∞, ∞∞m)
Apply a field to a crystal, observe an effect

K: point group of the crystal

F: point group of the field applied to the crystal

G: point group of the resulting phenomenon

Necessary (but not sufficient) condition for the phenomenon to occur

\[ G \supseteq K \cap F \]
Pyroelectric effect

Change of polarization in a dielectric undergoing a change of temperature

\[ F = m \infty \rightarrow K \cap F = K \]

G (point group of an electric field) : \( \infty m \)

Necessary condition for the phenomenon to occur

\[ K \subset \infty m \]

The point group of the crystal must be compatible with the existence of a polar direction.

The 10 types of point groups satisfying this conditions are called pyroelectric groups

1, 2, 3, 4, 6

m, 2mm, 3m, 4m, 6mm
Piezoelectric effect

Change of polarization in a dielectric undergoing a compression

\[ F = \infty/mm = \infty/m2/m \quad G (\text{point group of the electric field}) : \infty m \]

Necessary condition for the phenomenon to occur

\[ K \cap \infty/m2/m \subset \infty m \]

The intersection group of the point group of the crystal and of the point group of the compression must belong to one of the 10 pyroelectric types of point group.