Point groups and morphological symmetry. Introduction to the stereographic projection

UNIVERSITÉ DE LORRAINE

CRM²

Cristallographie, Résonance Magnétique et Modélisations

cnrs

iJB Institut Jean Barriol

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Lattice planes and Miller indices

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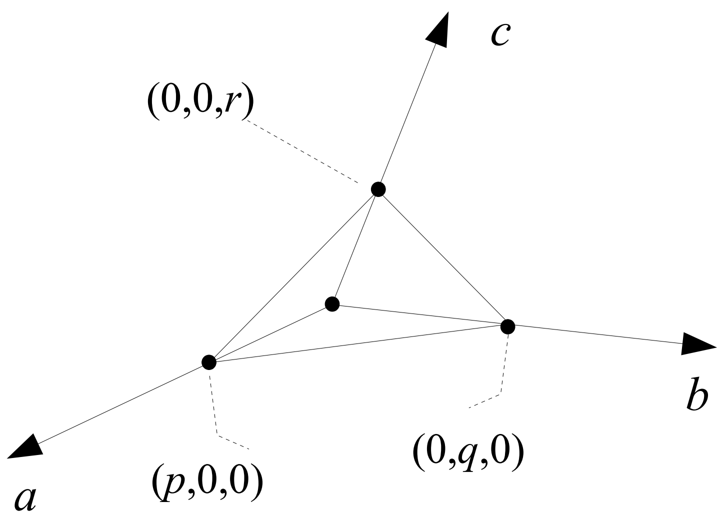
Planes passing through lattice nodes are called "rational planes"



Largest common integer factor for $p,q,r = 1 \rightarrow$ the plane shown is the first one for the chosen inclination passing through lattice node on ***all*** the three axes

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**.

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

$p = pqr/qr = m/h = 1/h$

$q = pqr/pr = m/k = 1/k$

$r = pqr/pq = m/l = 1/l$

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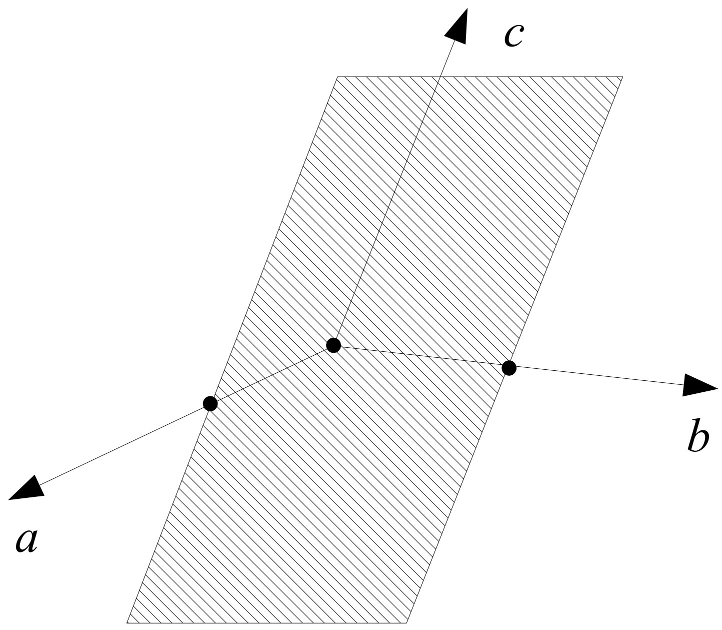
Why the *reciprocal* of the intersection (1/p) rather than the intersection (p) itself?

Consider a plane parallel to an axis – for example *c*



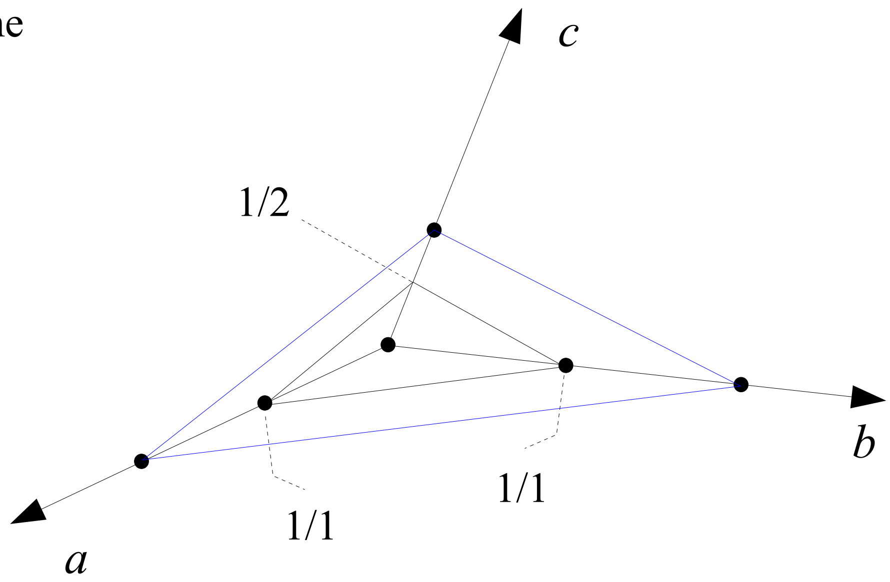
What is the intersection of this plane with the axis *c*? ∞

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

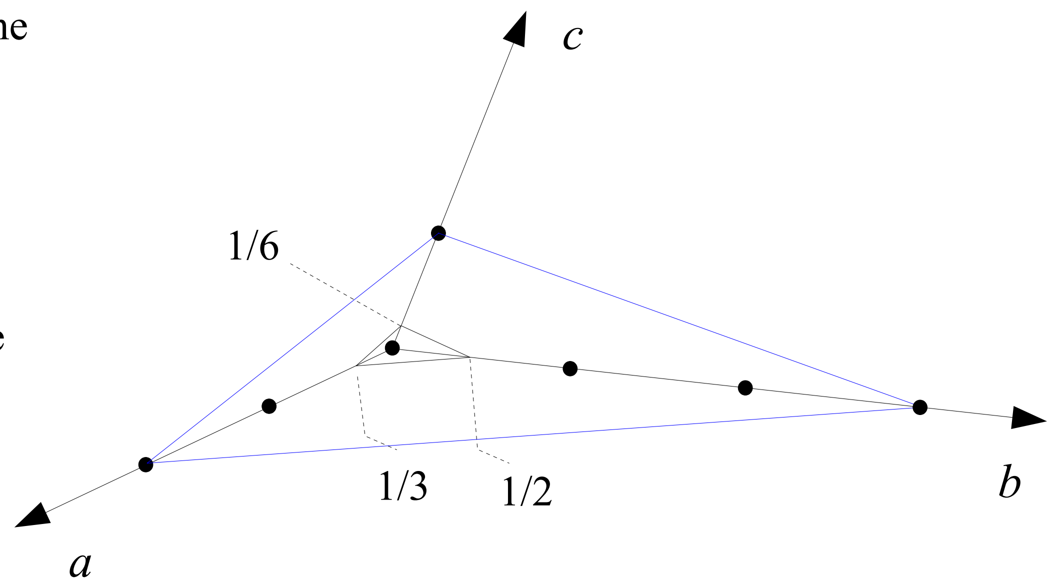
Intercepts of the second plane of the family:
on ***a***: 2/1
on ***b***: 2/1
on ***c***: 2/2



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



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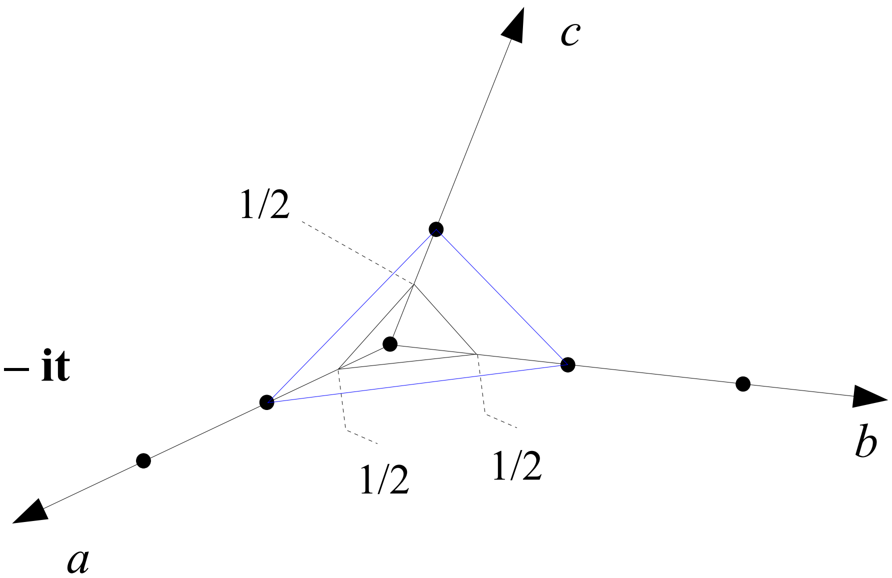
Miller indices for a primitive lattice are relatively prime integers

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

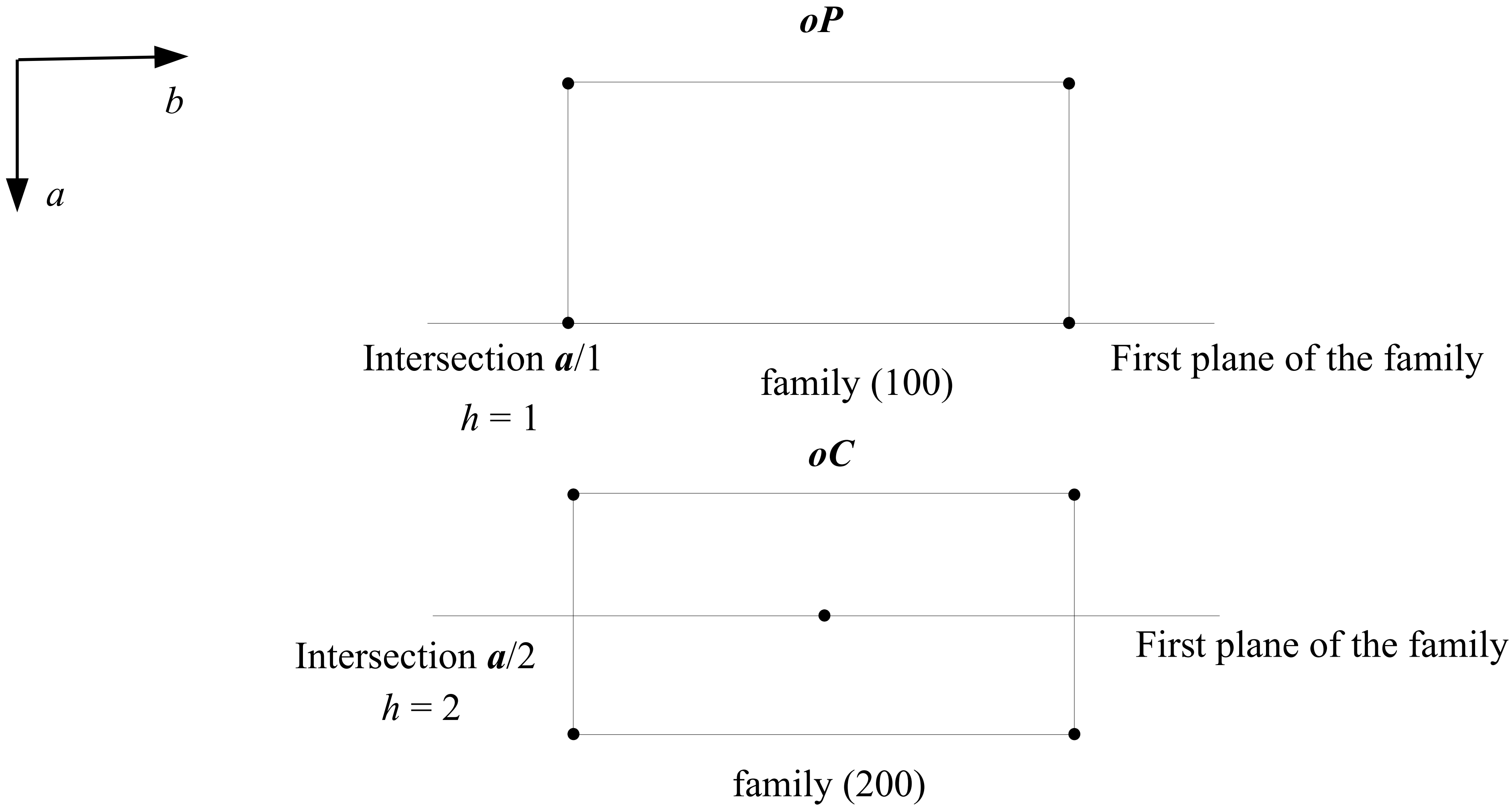
This plane does not pass through any lattice node – it is an *irrational* plane



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 : (*h*00) in *oP* and *oC* (projection on *ab*)



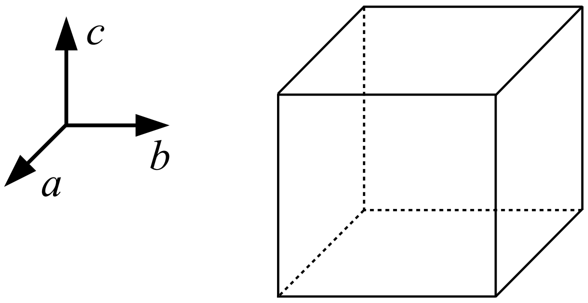
In morphology, we do not see the lattice and thus the Miller indices of a face are usually relatively prime integers

http://dx.doi.org/10.1107/S1600576715011206

The concept of form: set of faces equivalent by symmetry

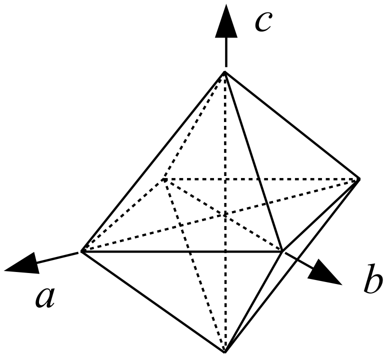
Example in the cubic crystal system

Form {100}: the cube



Multiplicity 6

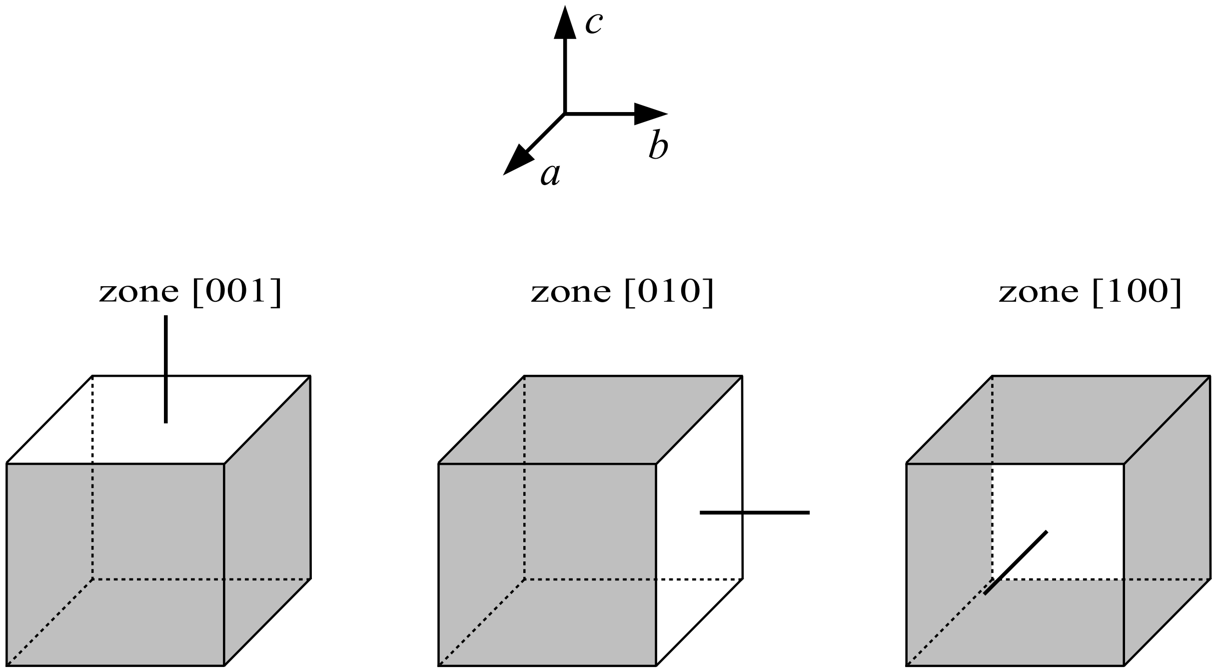
Form {111}: the octahedron



Multiplicity 8

Zone: set of faces whose intersection is parallel to a same direction, called the zone axis

Example in the cubic crystal system



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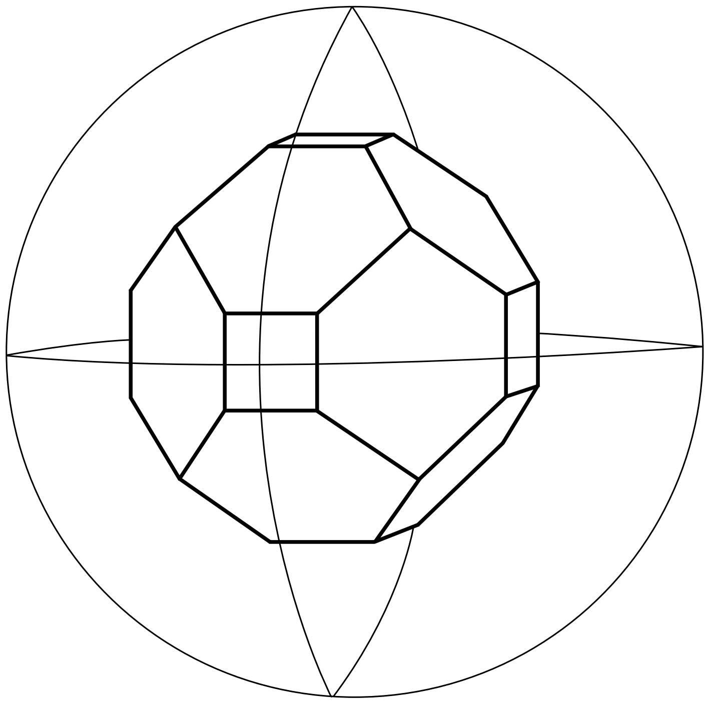
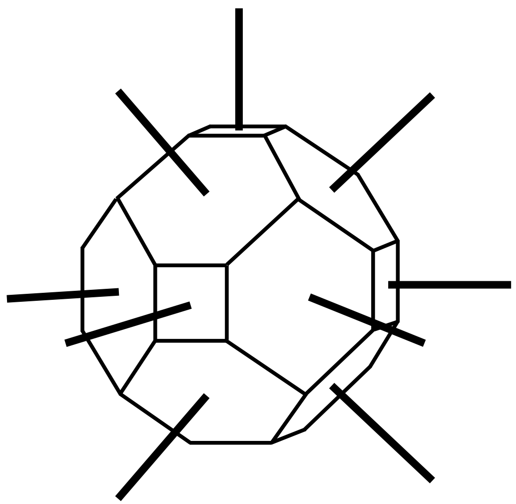
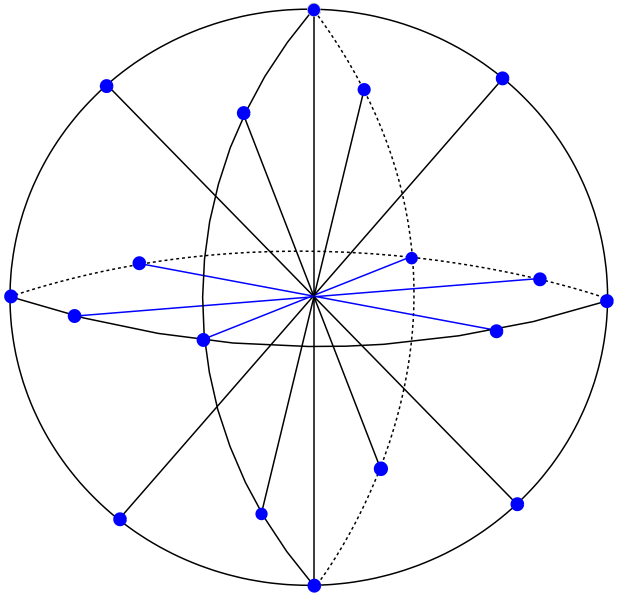
The stereographic projection: how to get rid of accidental morphological features of a crystal

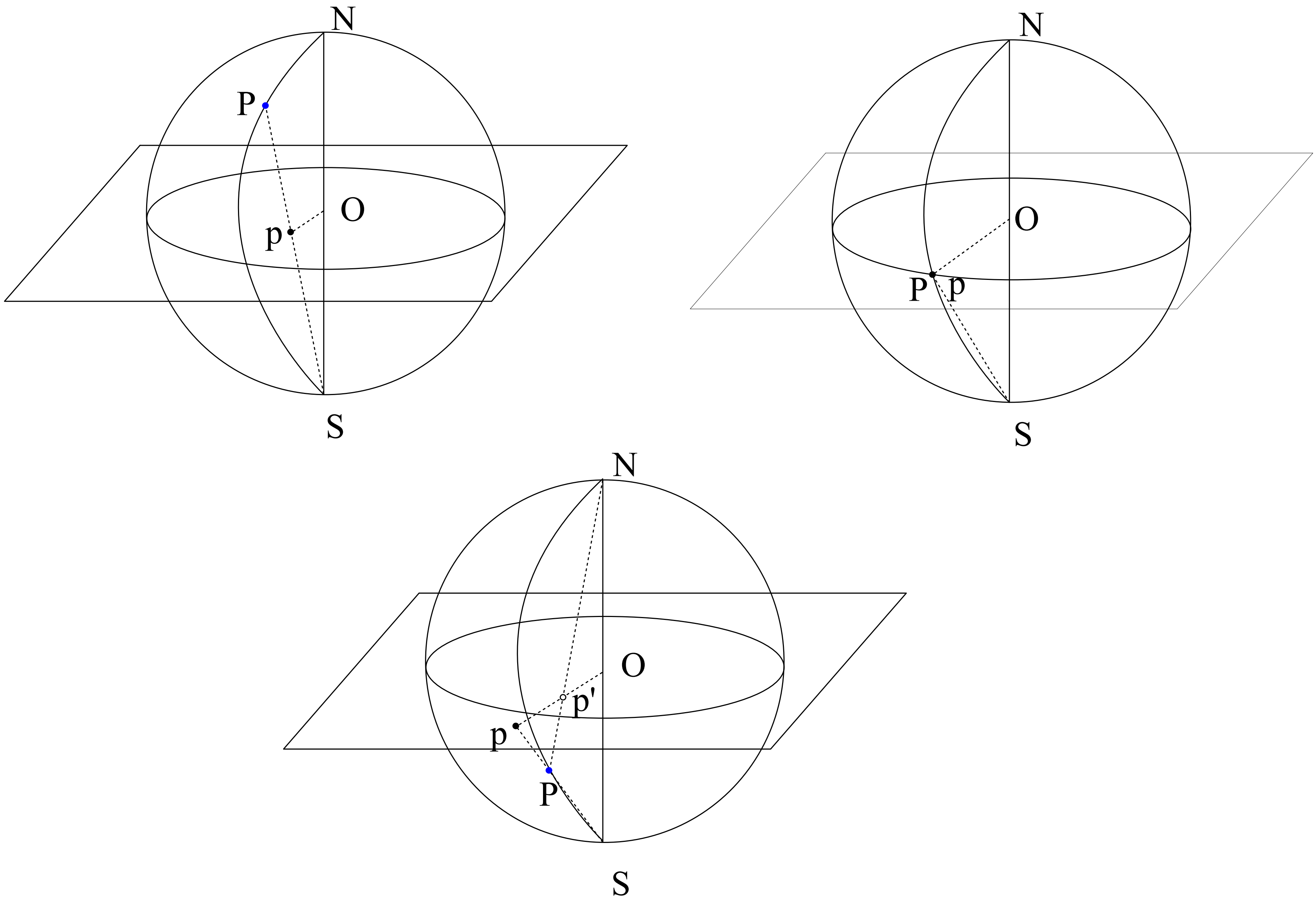
Spherical projection and spherical poles



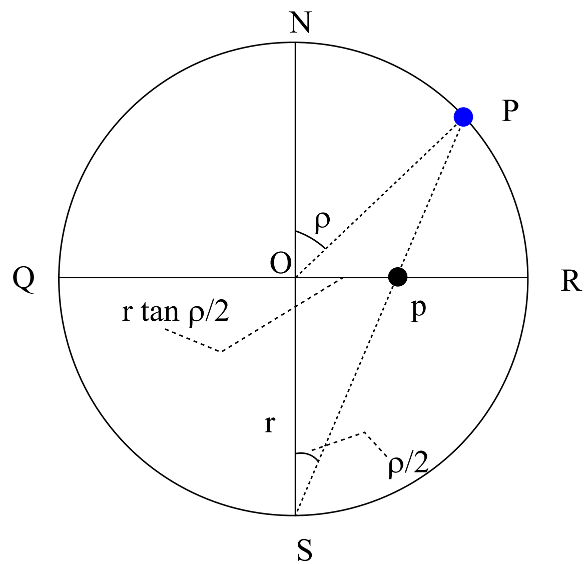


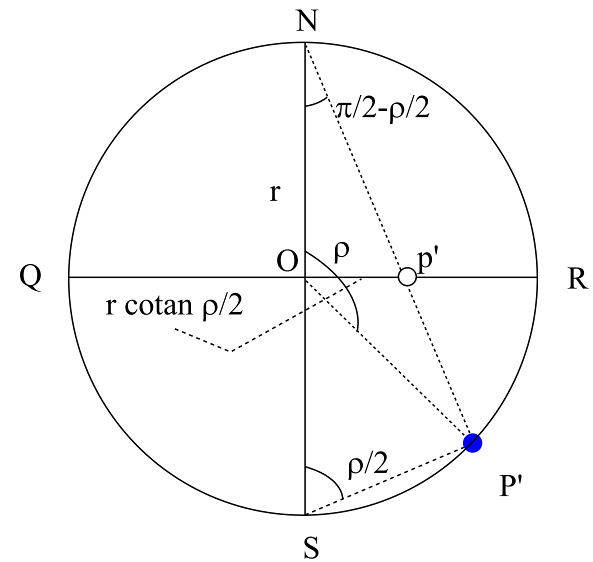


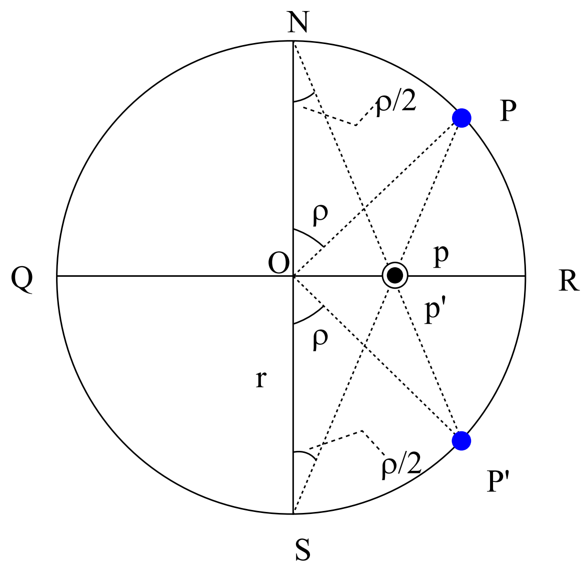
Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')

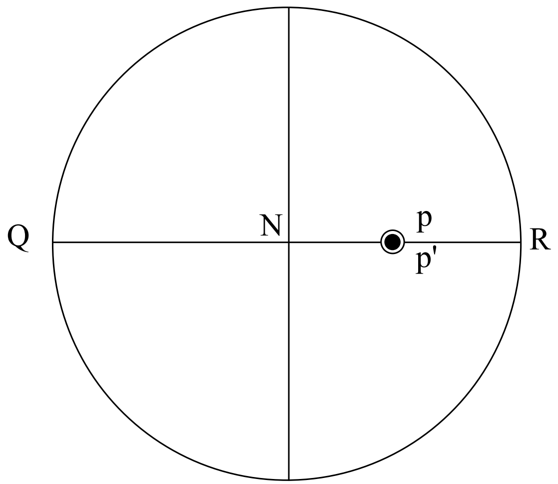


Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')









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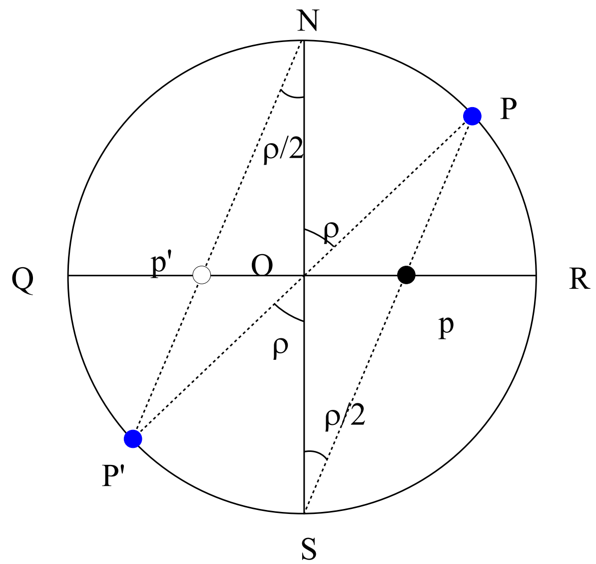
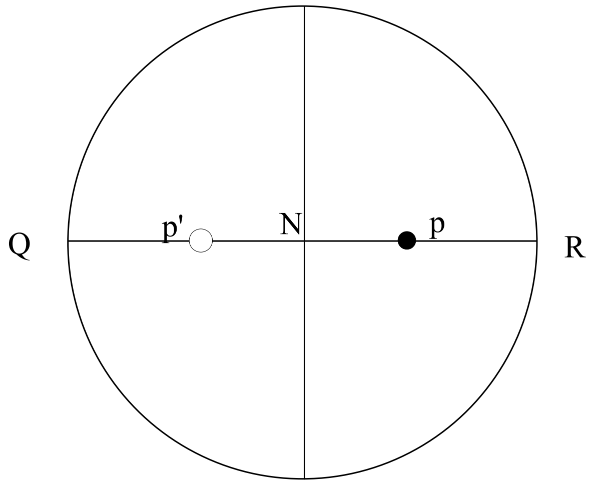
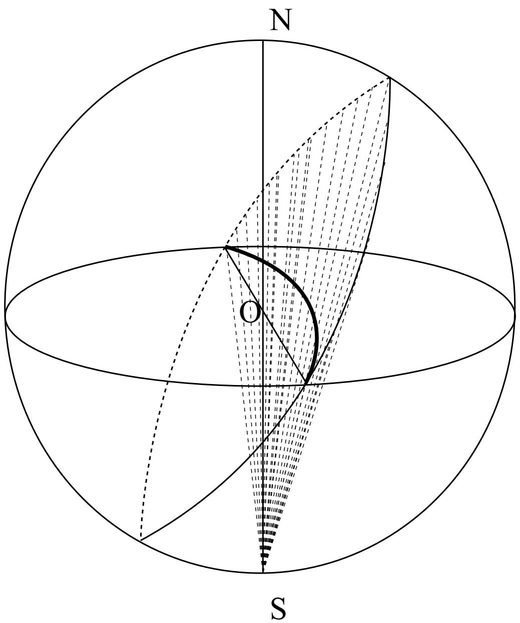
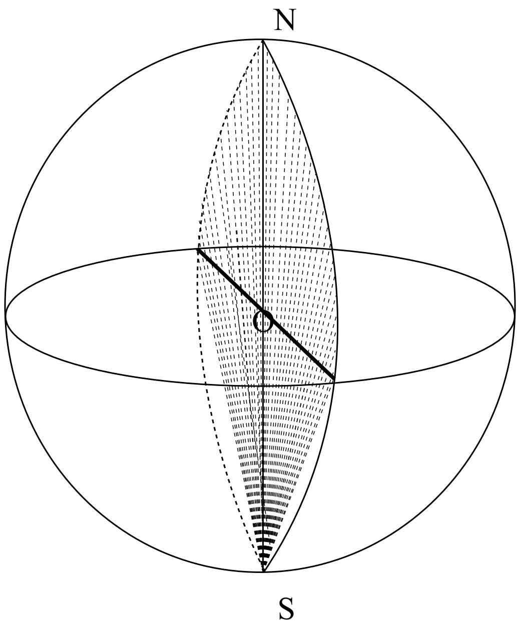
Stereographic projection: poles and symmetry planes









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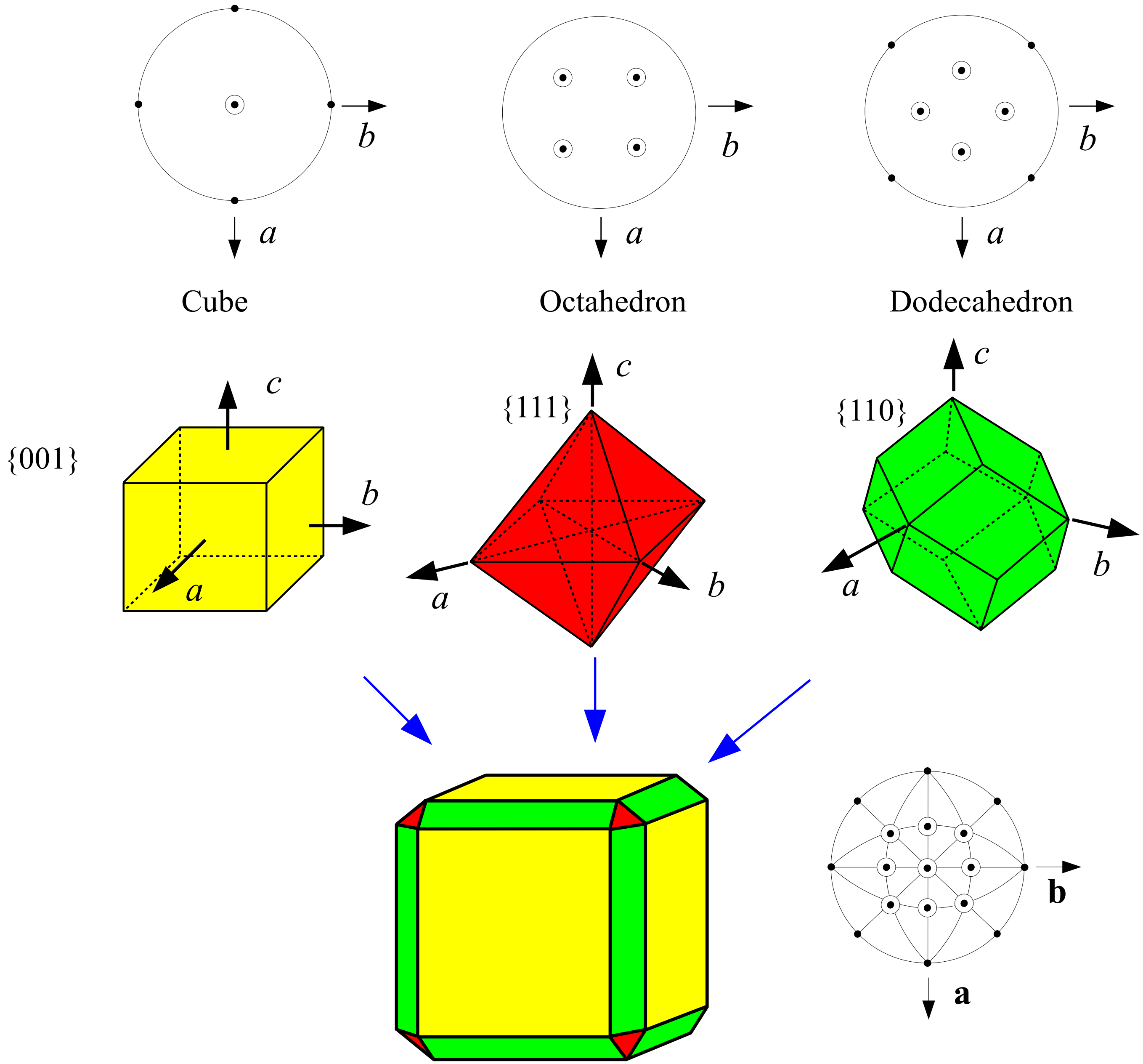
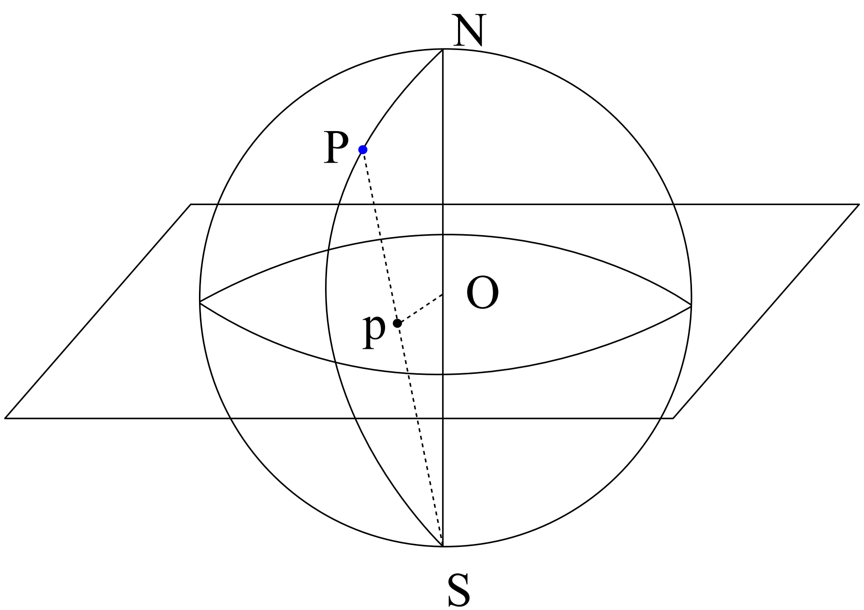
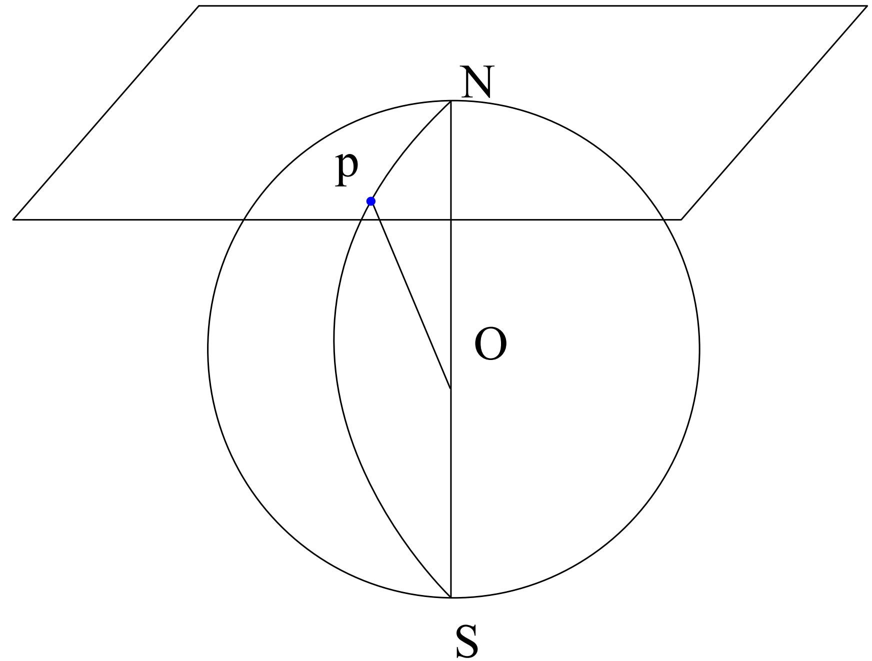
Example of analysis of the morphology of a crystal



Stereographic vs. gnomonic projection



Stereographic projection



Gnomonic projection

Be careful - some textbooks exchange the two terms!

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"…} 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: $M = |P|/|S|$

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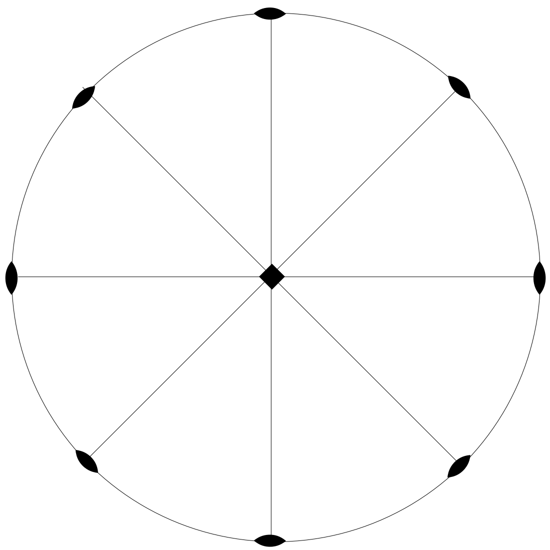
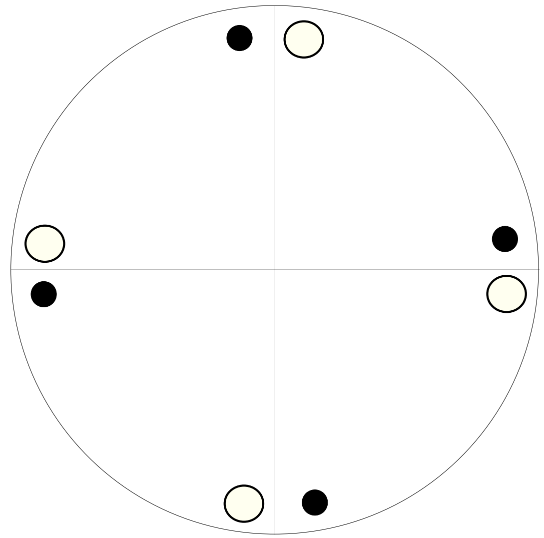
Site-symmetry groups (stabilizers) and Wyckoff positions of point groups





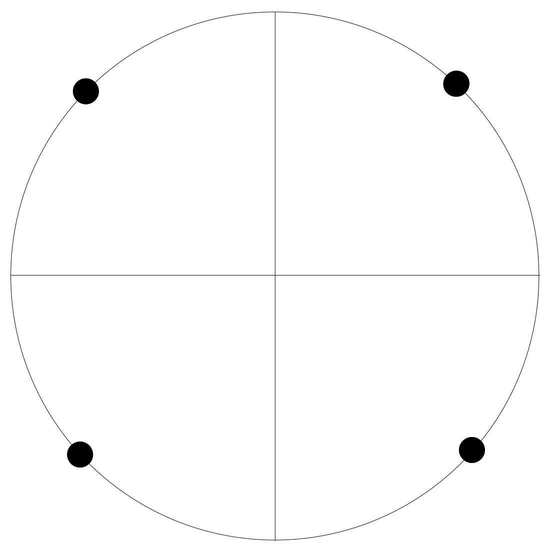
Coordinates

xyz, $\bar{y}xz$, $\bar{x}\bar{y}z$, $y\bar{x}z$,
$x\bar{y}\bar{z}$, $\bar{y}\bar{x}\bar{z}$, $\bar{x}y\bar{z}$, $yx\bar{z}$

S = {1}, M = 8

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

$\forall p_j \in P$
$p_j 1 p_j^{-1} = 1$
$p_j 2_{[110]} p_j^{-1} = \{2_{[110]}, 2_{[1\bar{1}0]}\}$



Coordinates

$xx0$, $\bar{x}\bar{x}0$: $S = \{1, 2_{[110]}\}$
$\bar{x}x0$, $\bar{x}x0$: $S = \{1, 2_{[1\bar{1}0]}\}$

S = {..2}, M = 4

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

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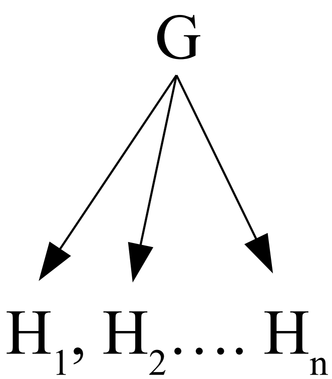
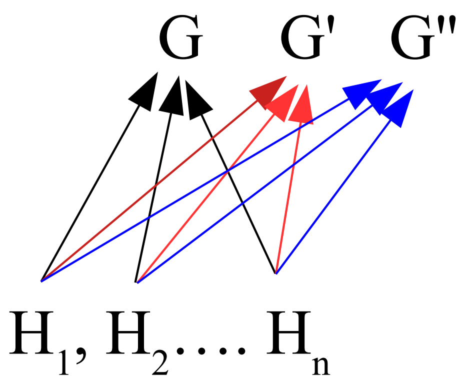
Subgroups vs. supergroups: to remove symmetry operations is easier than to add them

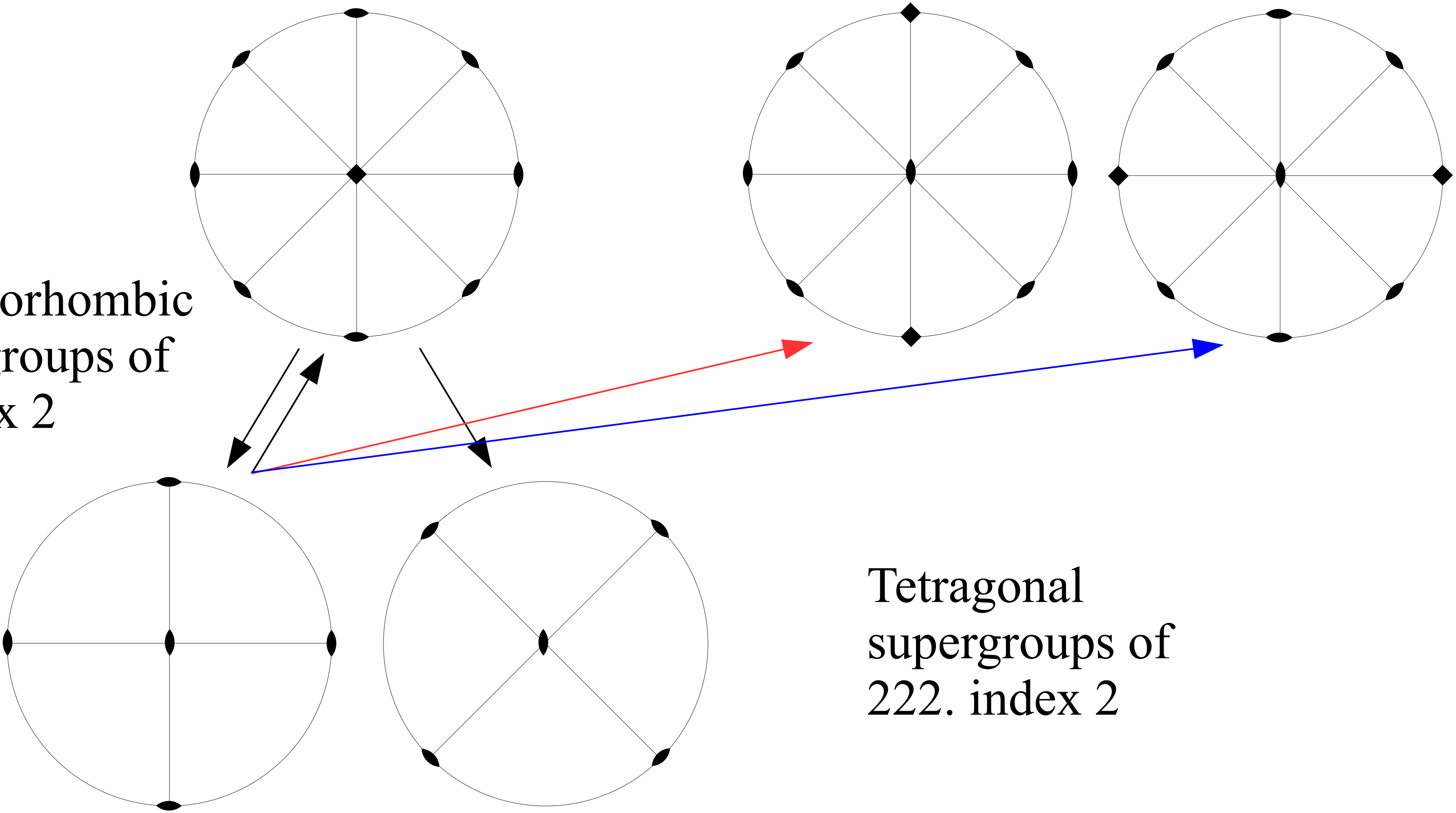
$G \supset H$ $\qquad$ $i = |G|/|H|$





To remove symmetry operations is easier than to add them

422



222.

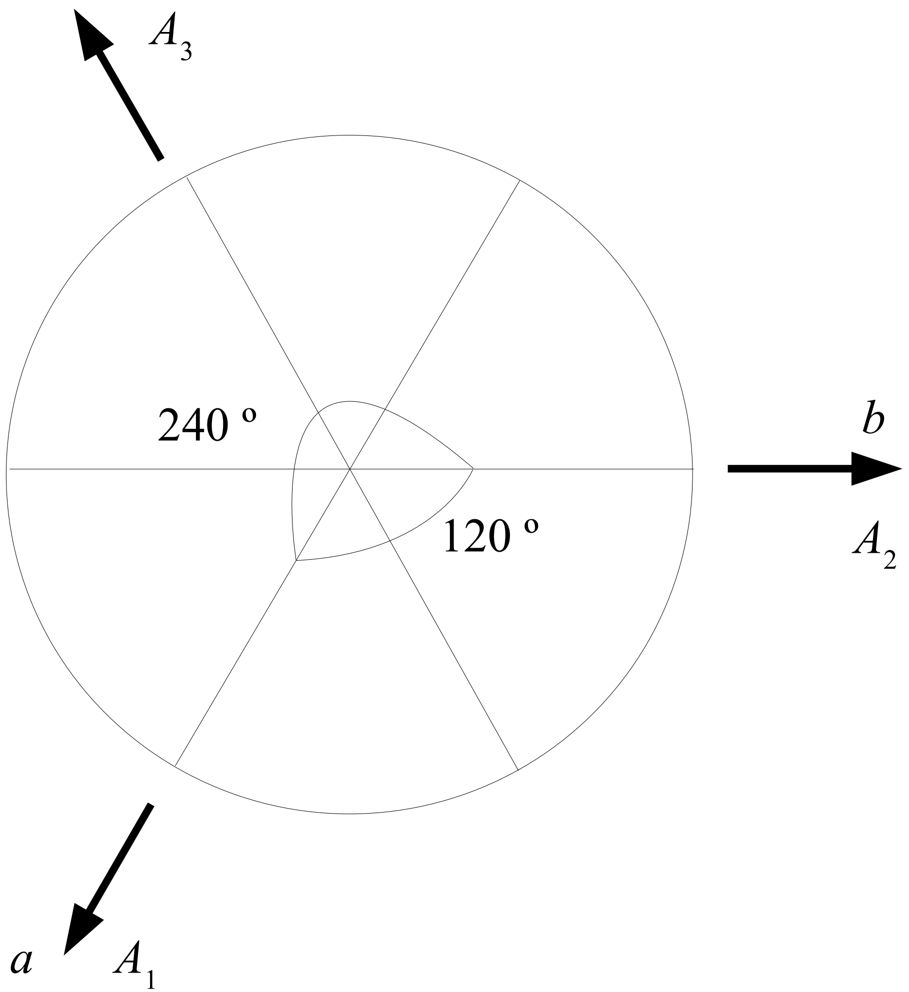
2.22

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



$$\mathbf{abc} \rightarrow \mathbf{A_1A_2A_3C}$$

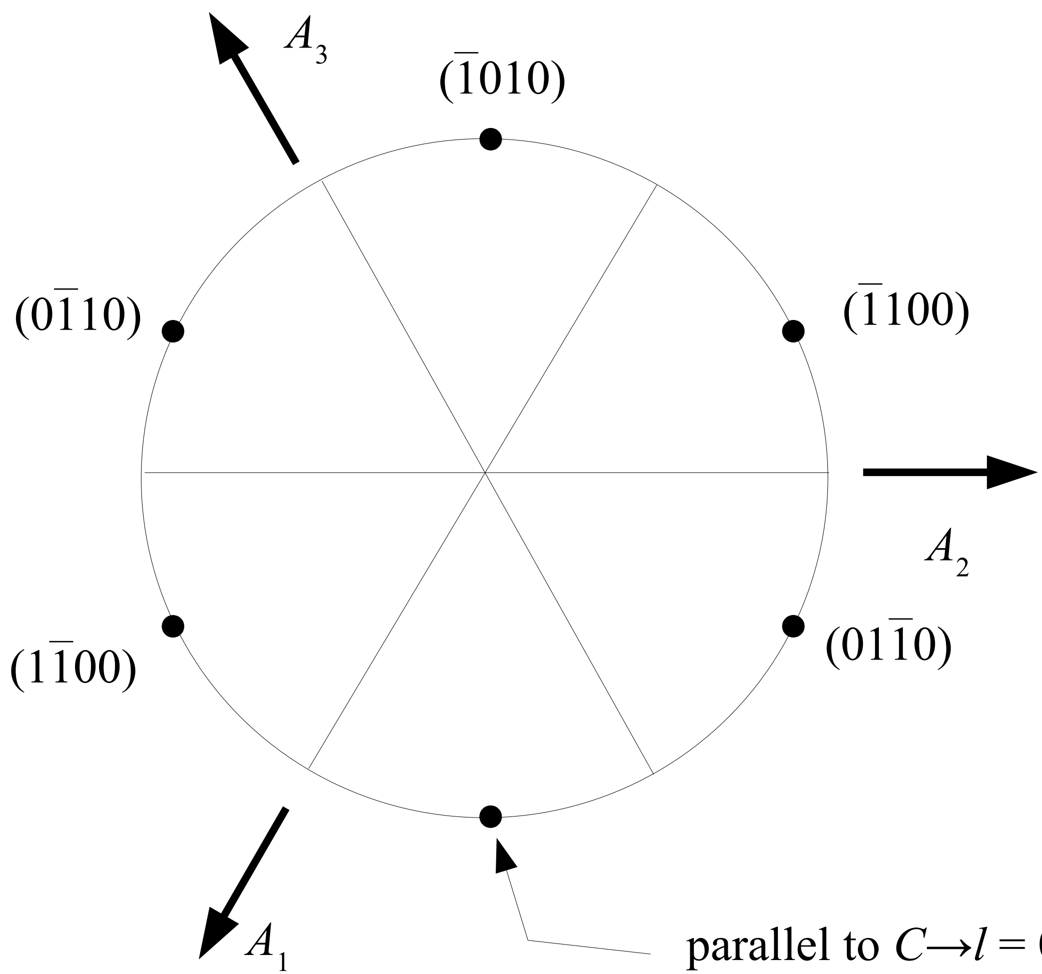
$$hkl \rightarrow hkil$$

Miller indices — Bravais-Miller indices

$$\mathbf{A_3} = -\mathbf{A_1} - \mathbf{A_2}$$

$$i = -h-k$$

Bravais-Miller indices: example



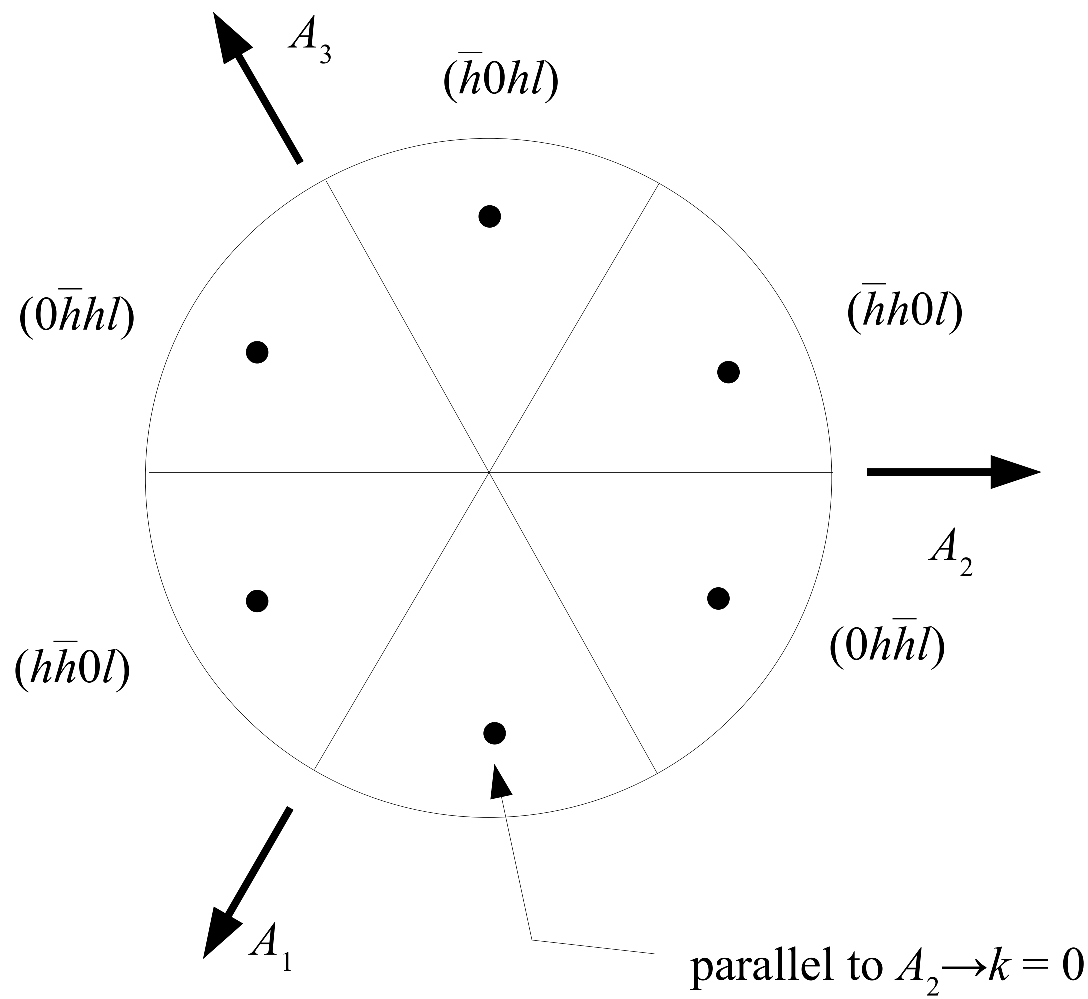
If you use Miller indices the symmetry is less evident!

(100)
(010)
$(\bar{1}10)$
$(\bar{1}00)$
$(0\bar{1}0)$
$(1\bar{1}0)$

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

$(hkil) \rightarrow (h0i0) \xrightarrow{i = -h-0} (h0\bar{h}0) \xrightarrow{\text{divide by the common factor}} (10\bar{1}0)$

Bravais-Miller indices: example



If you use Miller indices the symmetry is less evident!

$(h0l)$
$(0hl)$
$(\bar{h}hl)$
$(\bar{h}0l)$
$(0\bar{h}l)$
$(h\bar{h}l)$

$$(hkil) \to (h0il) \xrightarrow[i = -h-0]{} (h0\bar{h}l)$$

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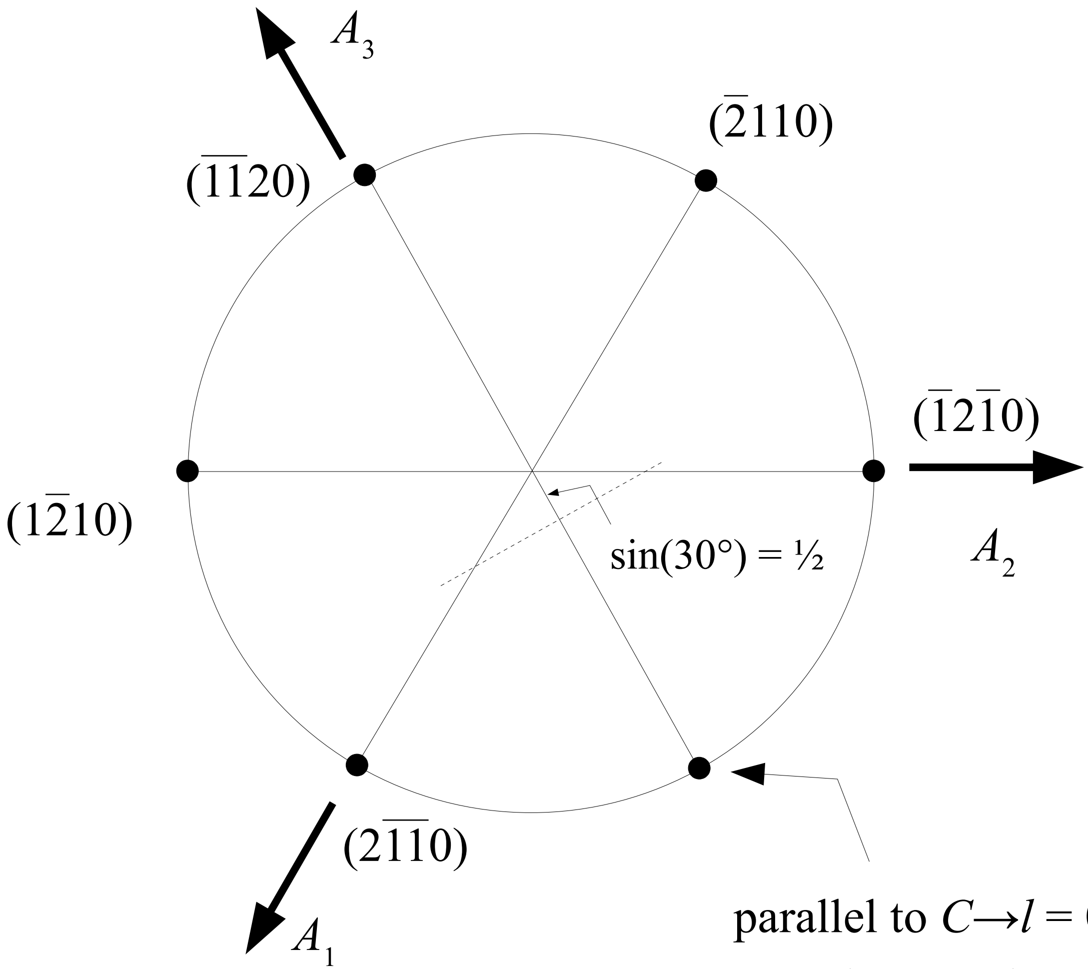
Bravais-Miller indices: example



If you use Miller indices the symmetry is less evident!

(110)
$(\bar{1}20)$
$(\bar{2}10)$
(110)
$(1\bar{2}0)$
$(2\bar{1}0)$

parallel to $C \rightarrow l = 0$

same intersection on A_1 and $A_2 \rightarrow k = h$

$(hkil) \rightarrow (hhi0) \xrightarrow[i = -h-h]{} (hh\bar{2}h0) \xrightarrow[\text{divide by the common factor}]{} (11\bar{2}0)$

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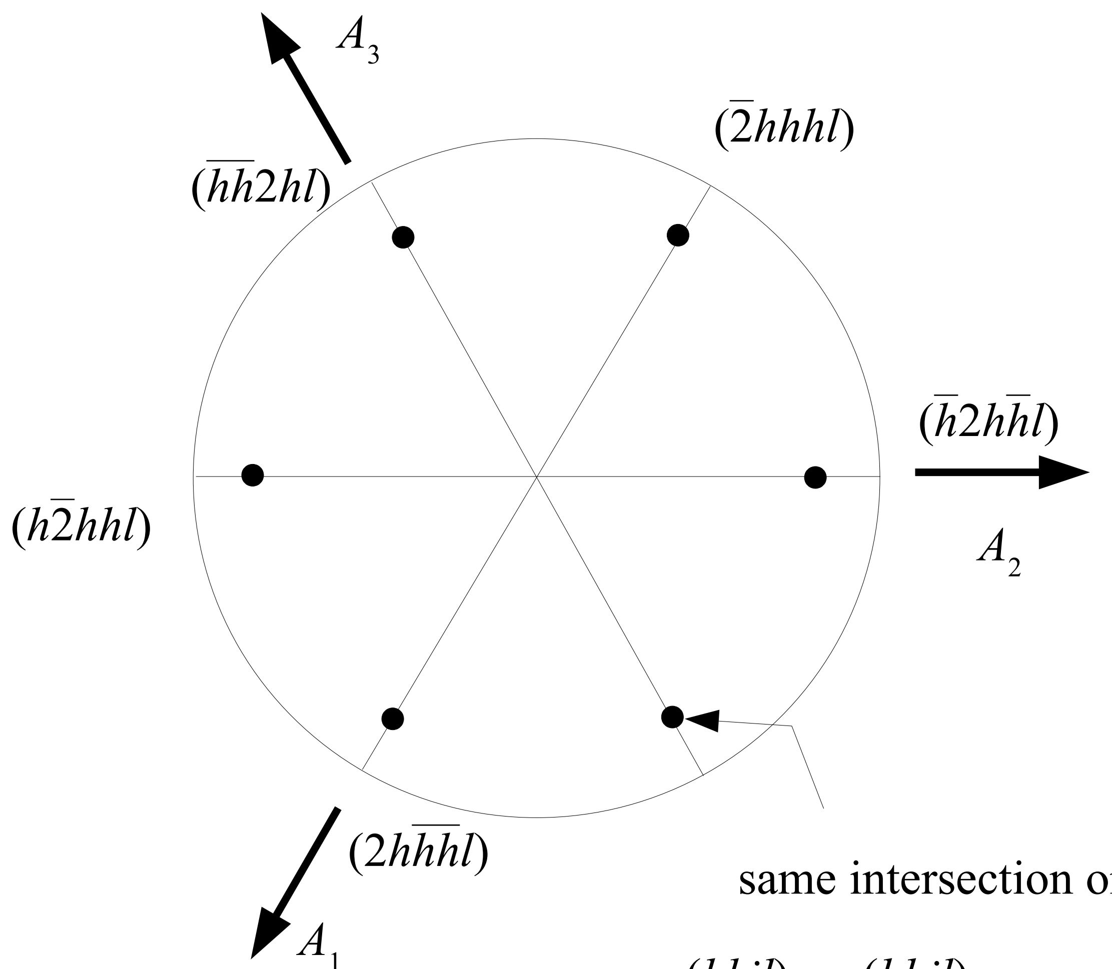


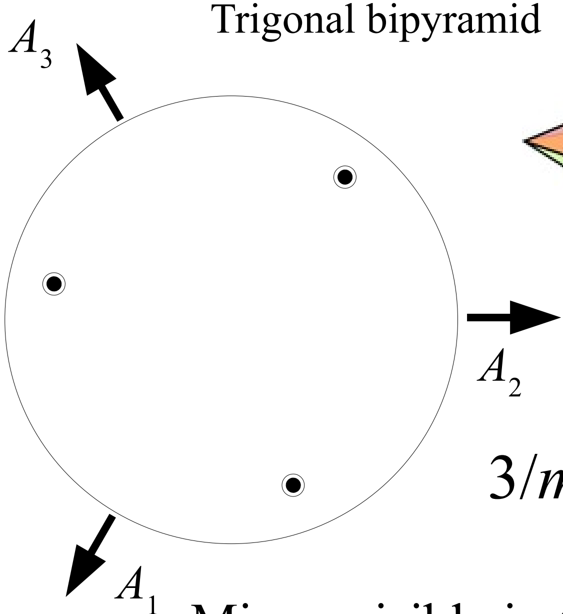
If you use Miller indices the symmetry is less evident!

(hhl)
$(\bar{h}2hl)$
$(\overline{2}hhl)$
$(\bar{h}\bar{h}l)$
$(h\overline{2}hl)$
$(2h\bar{h}l)$

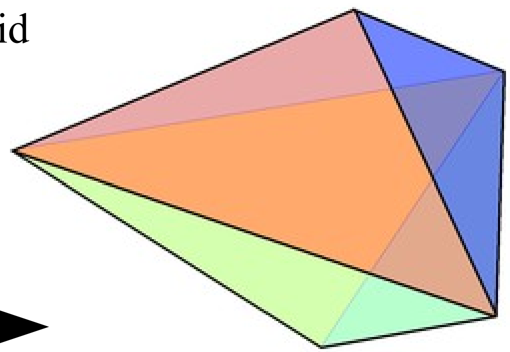
same intersection on A_1 and $A_2 \rightarrow k = h$

$$(hkil) \rightarrow (hhil) \xrightarrow[i\,=\,-h-h]{} (hh\overline{2}hl)$$

We you don’t see 3/*m* in crystallography ?

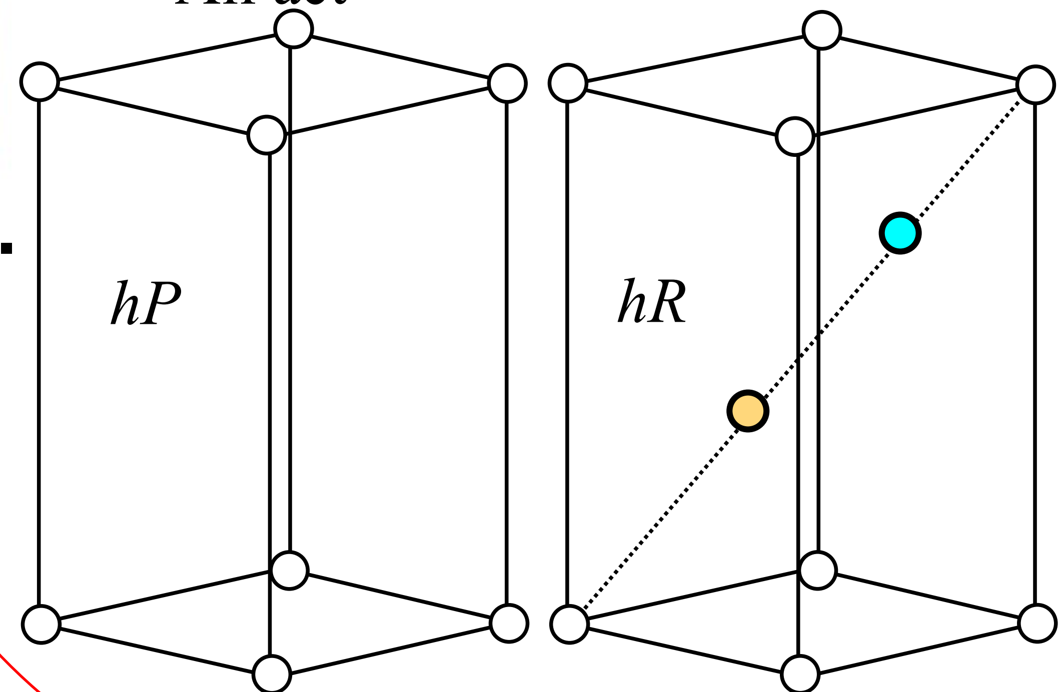


Trigonal bipyramid



$3, \bar{3}, 6, \bar{6}, m_{[001]}$
All act

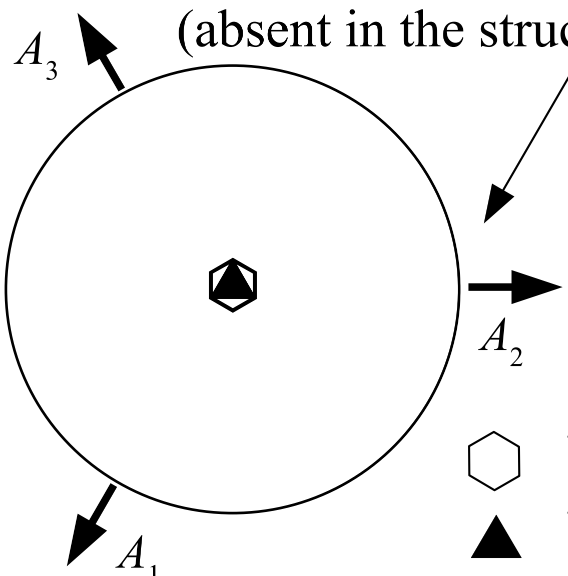
Only 3 and $\bar{3}$ act



However ....

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

Mirror visible in the morphology
(absent in the structure)



$\bar{6}$

$\bar{6}^2 = 3$

3 ⟵ acts on *hR* and *hP*→trigonal system

~~*m*~~ ⟵ acts on *hP* only→hexagonal system

Contradiction !

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Diffraction and Laue indices

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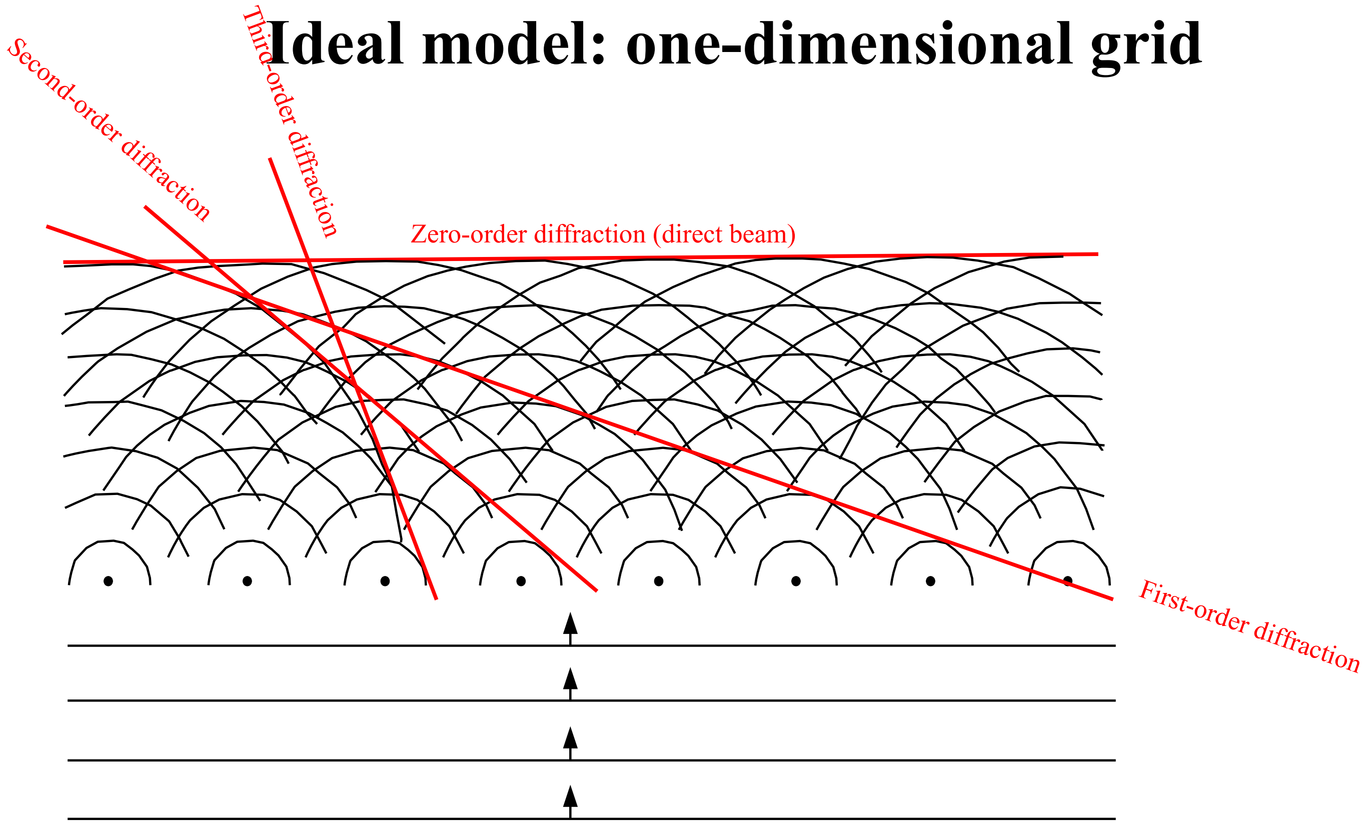
A hyper-simplified view at diffraction phenomenon

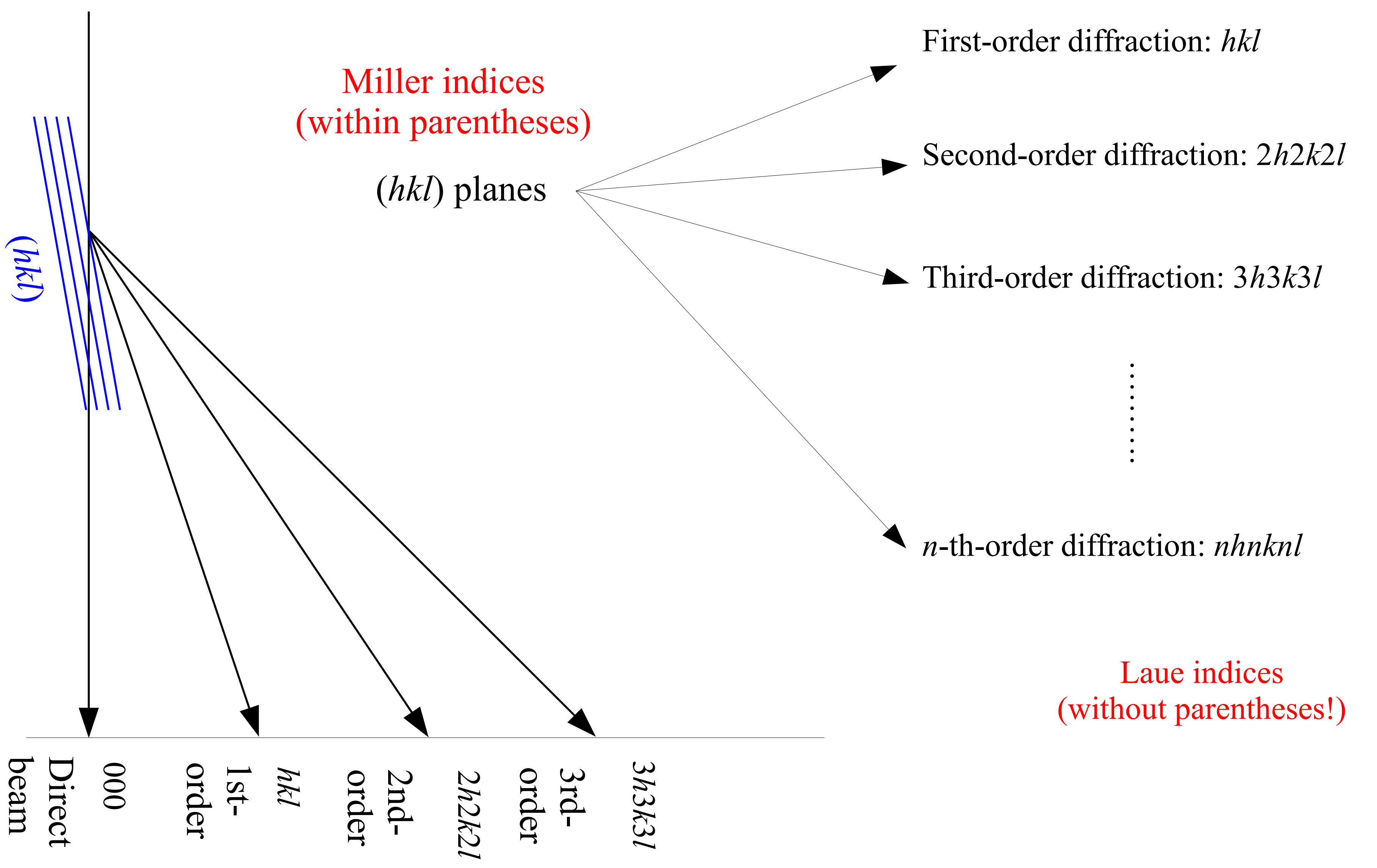
Ideal model: one-dimensional grid



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*

Miller indices vs. Laue indices



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