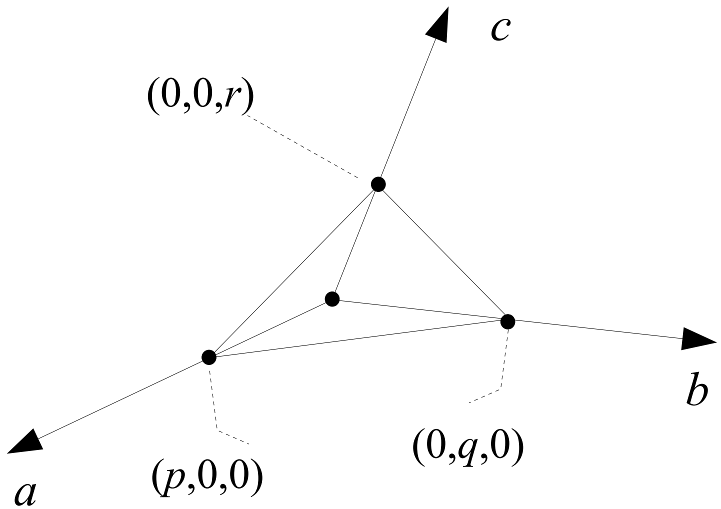
# Point groups and morphological symmetry. Introduction to the stereographic projection

Didactic material for the MaThCryst schools

**Massimo Nespolo, Université de Lorraine, France**
massimo.nespolo@univ-lorraine.fr

# Lattice planes and Miller indices

# 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**.

* https://mathemerize.com/intercept-form-of-a-plane/

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 $m = 1$

$$hx + ky + lz = 1$$

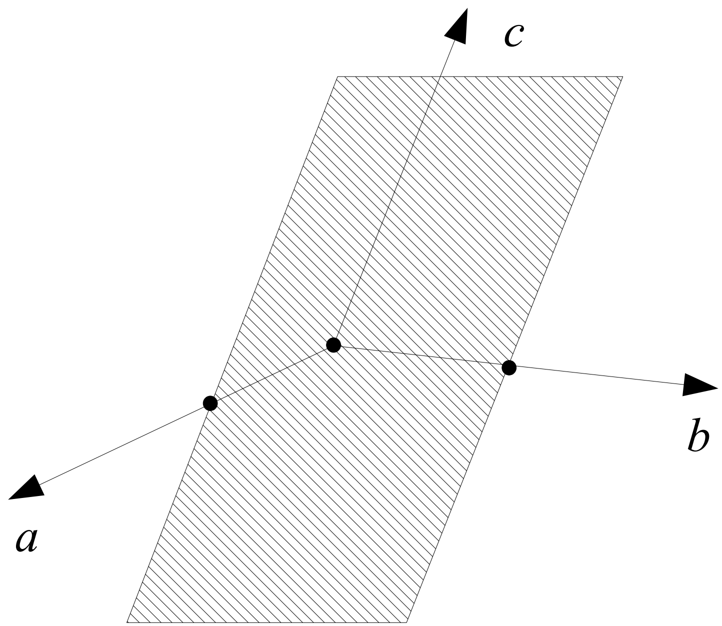
Intercepts of the first ($m = 1$) plane of the family ($hkl$) on the axes

$$p = pqr/qr = m/h = 1/h$$
$$q = pqr/pr = m/k = 1/k$$
$$r = pqr/pq = m/l = 1/l$$


Massimo Nespolo, Université de Lorraine

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

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



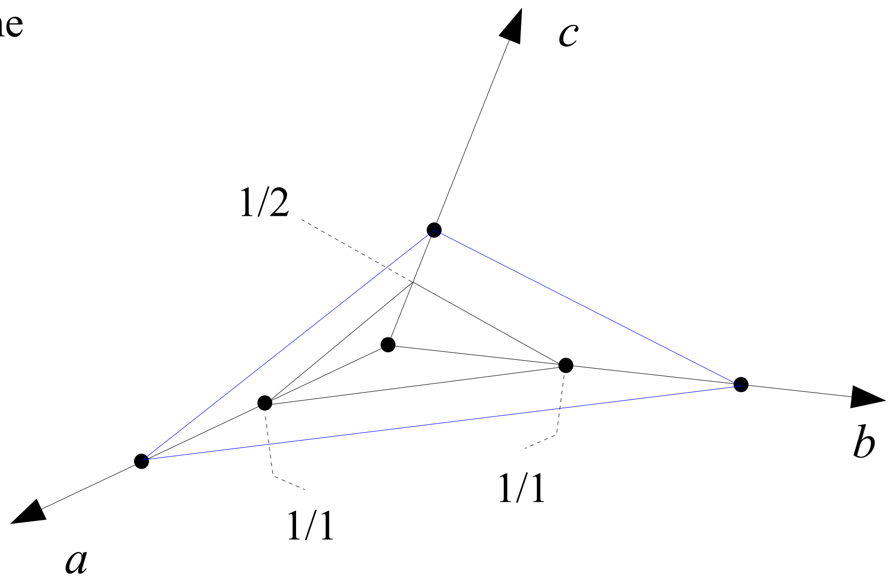

What is the intersection of this plane with the axis $c$? $\infty$

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

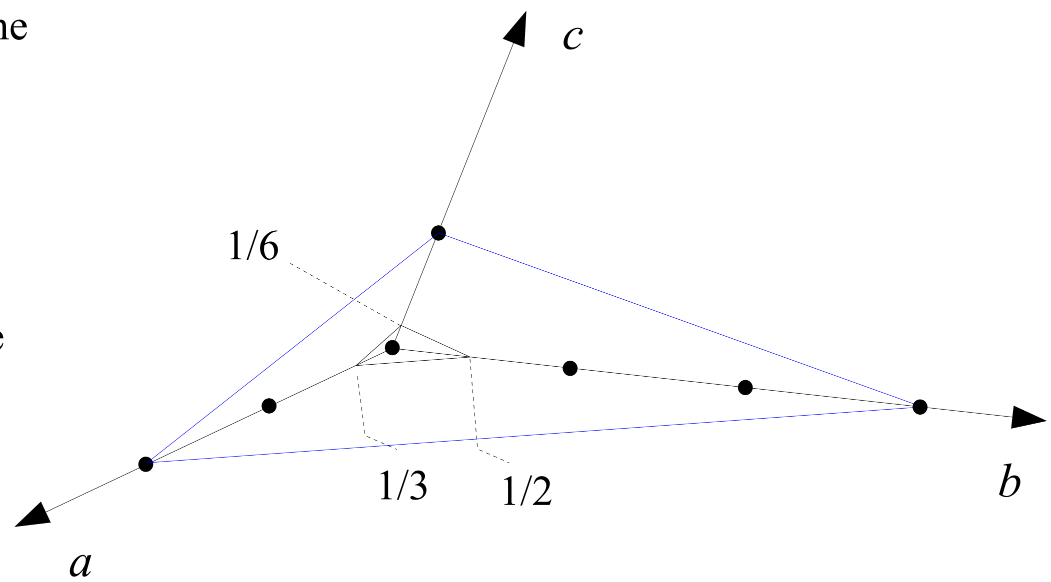
Intercepts of the second
plane of the family:
on ***a***: 2/1
on ***b***: 2/1
on ***c***: 2/2



# 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

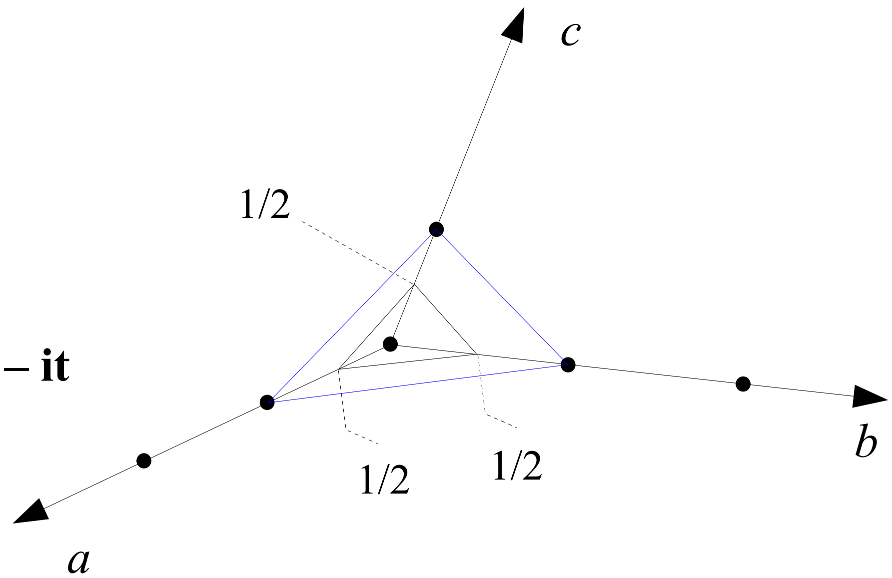
Intercepts of the sixth plane of the family:
on ***a***: 6/3
on ***b***: 6/2
on ***c***: 6/6



# 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

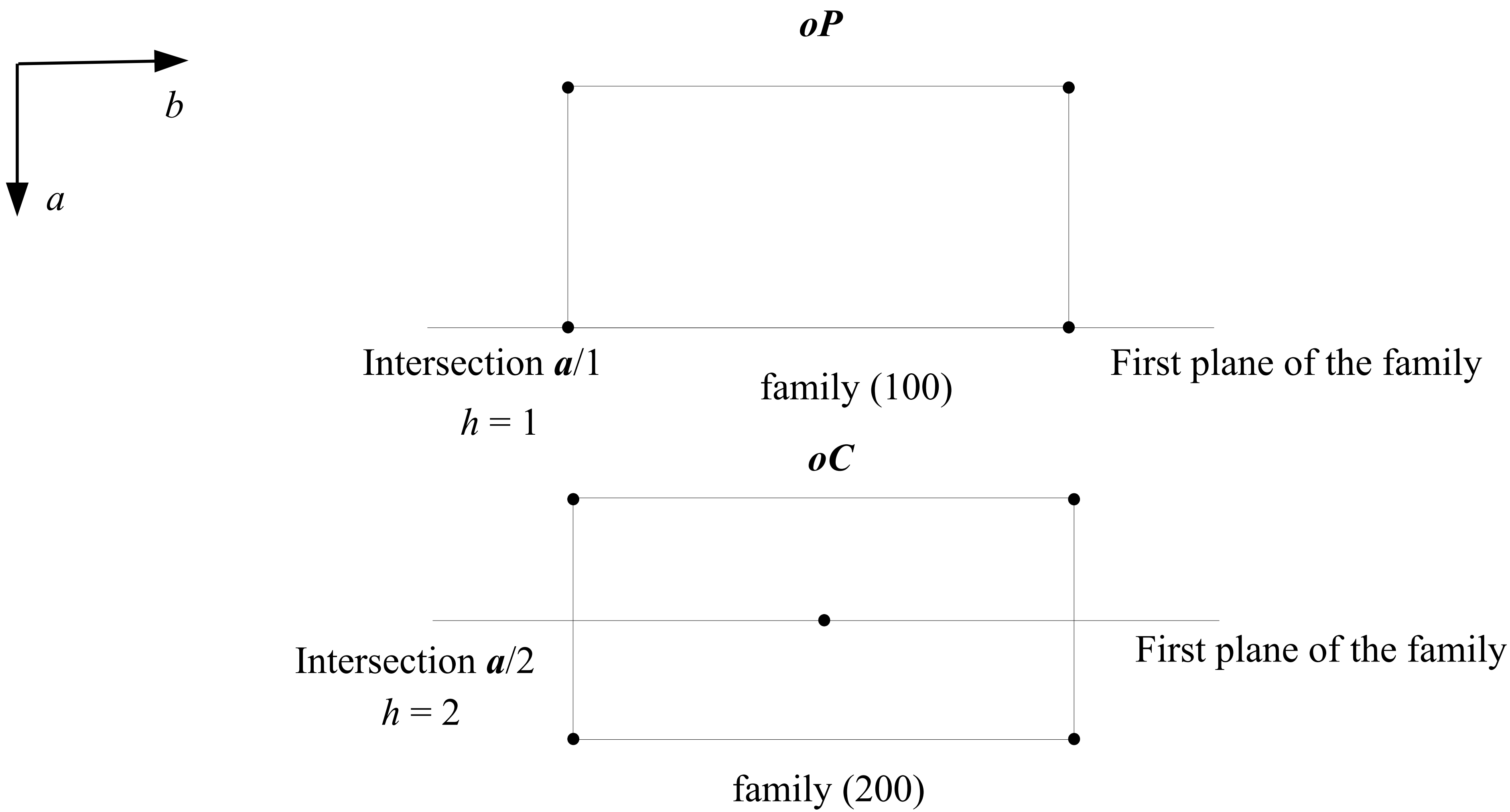
**This plane does not pass through any lattice node – it is an *irrational* plane**




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



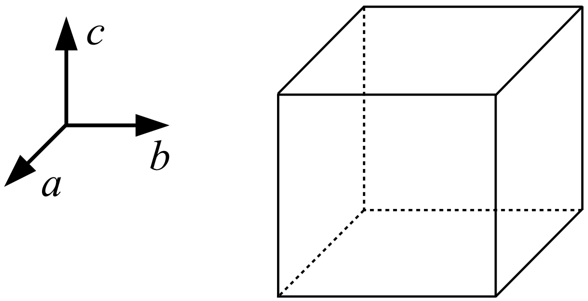

**In morphology, we do not see the lattice and thus the Miller indices of a face are usually relatively prime integers**

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

# The concept of form: set of faces equivalent by symmetry

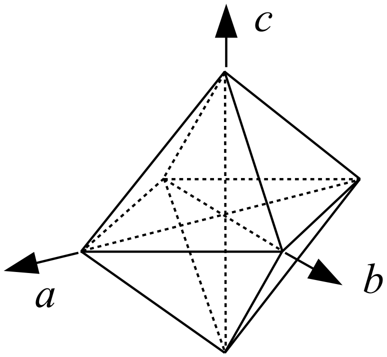
## Example in the cubic crystal system

Form {100}: the cube




Multiplicity 6

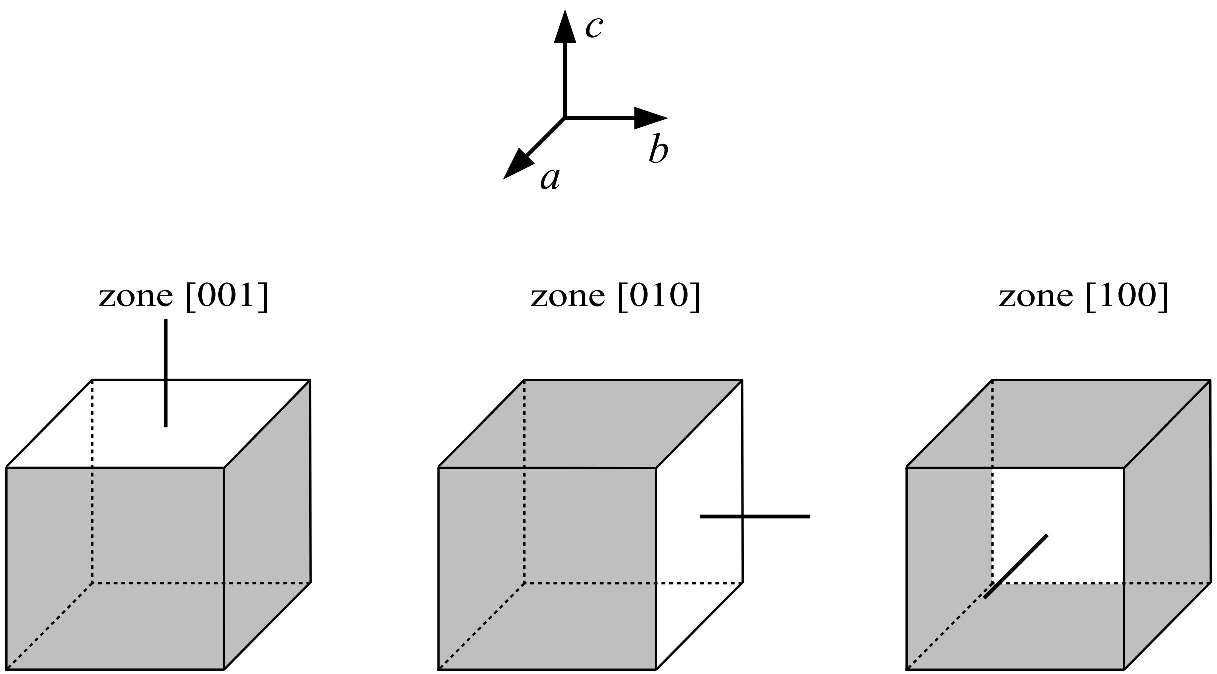
Form {111}: the octahedron




Multiplicity 8

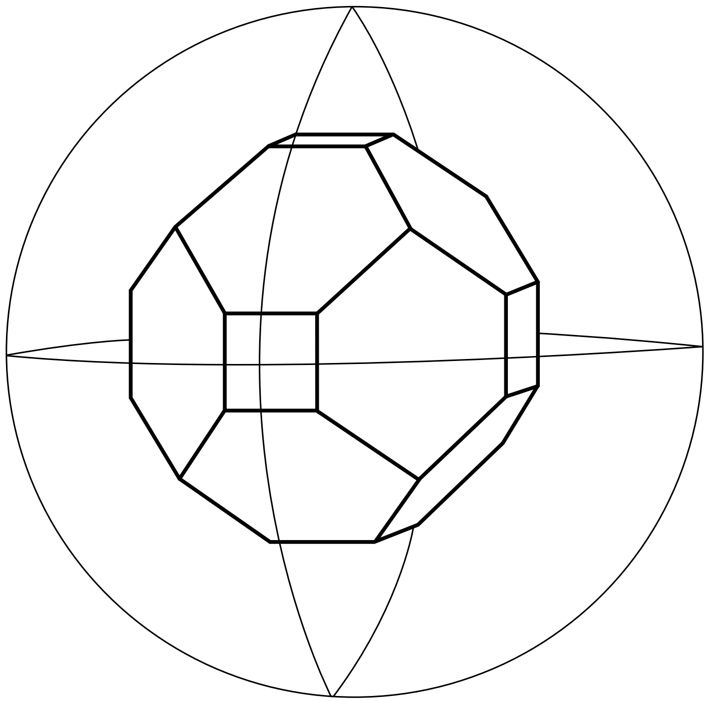
# Zone: set of faces whose intersection is parallel to a same direction, called the zone axis

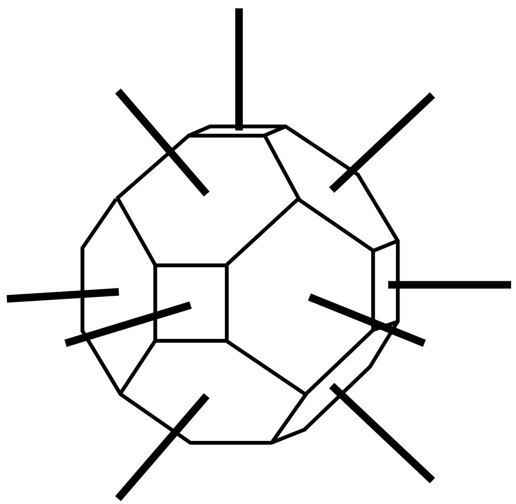
## Example in the cubic crystal system

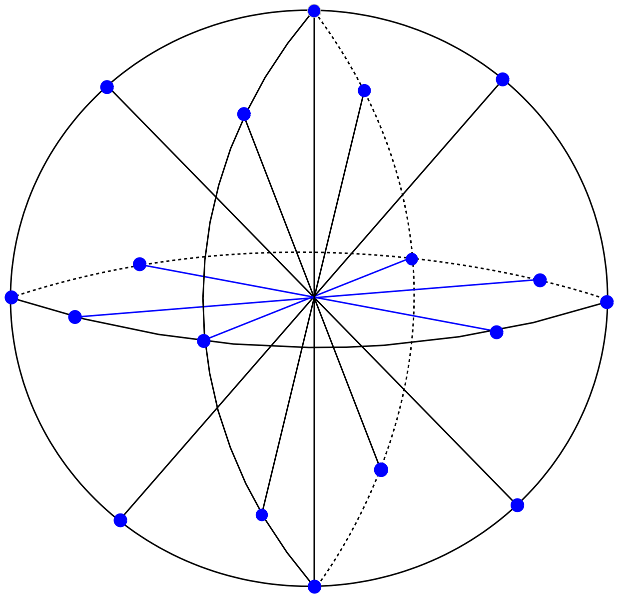


# The stereographic projection: how to get rid of accidental morphological features of a crystal

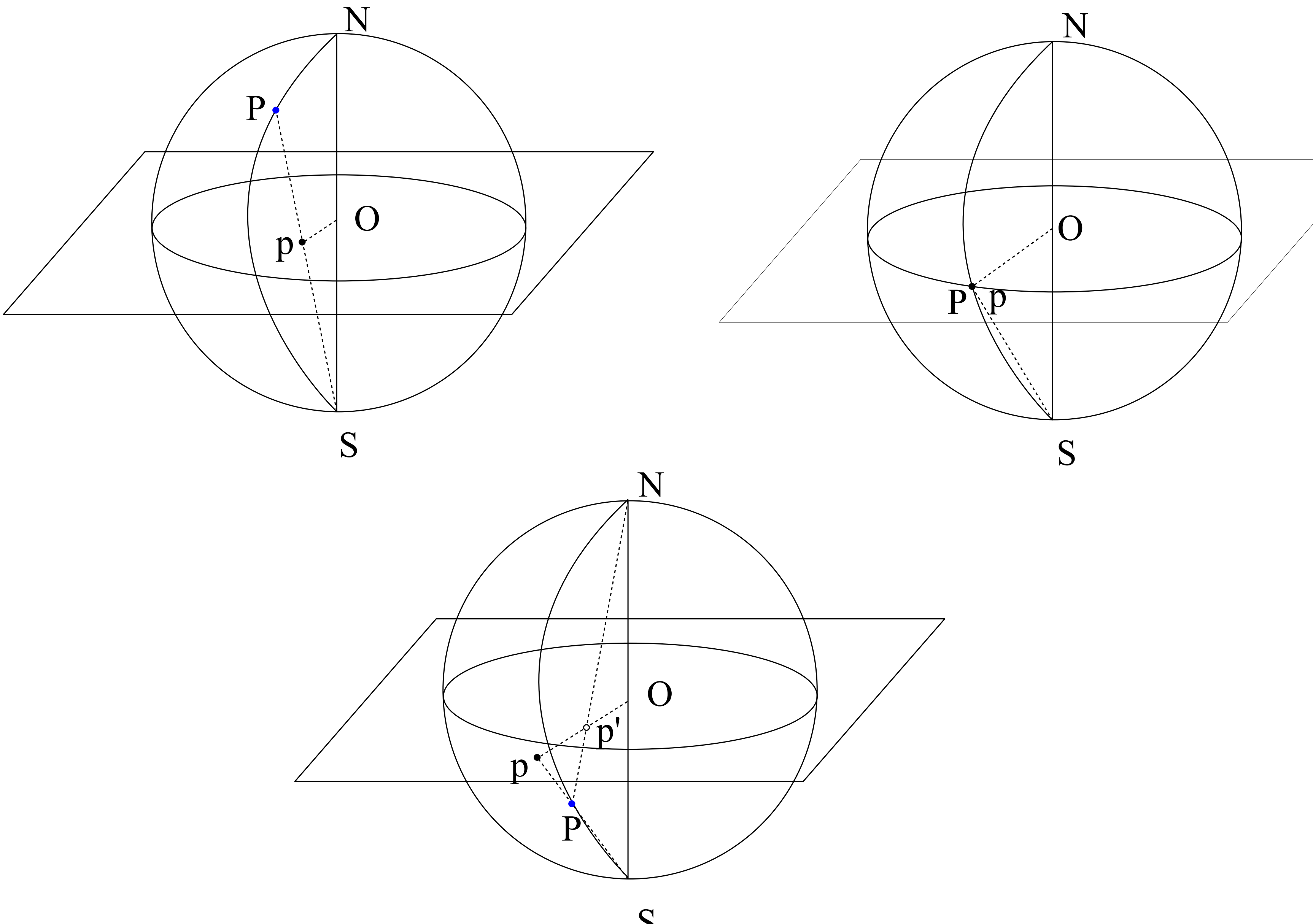
# Spherical projection and spherical poles



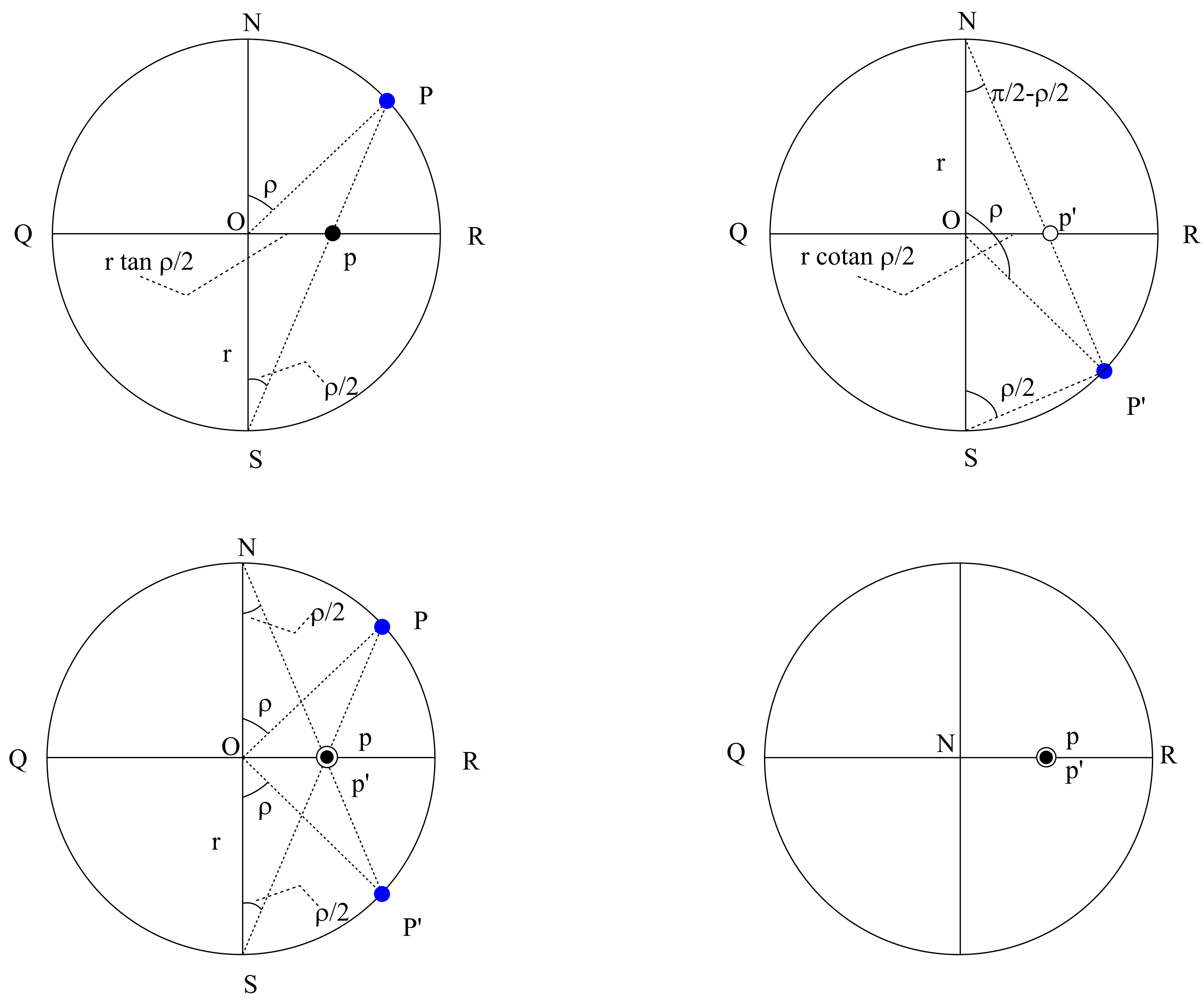




# Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')



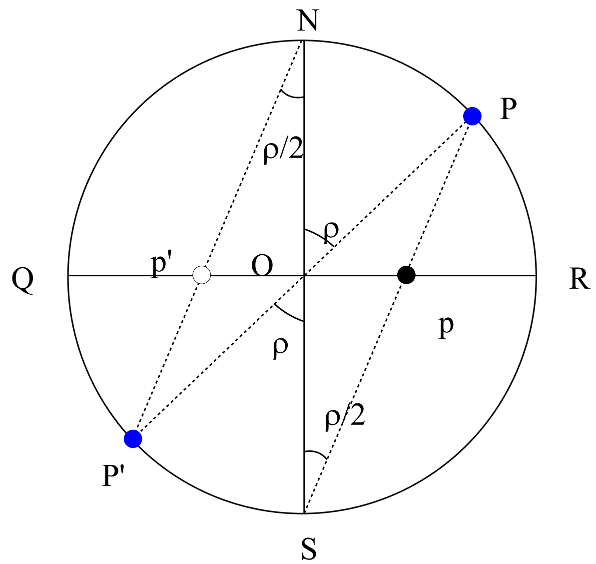
# Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')

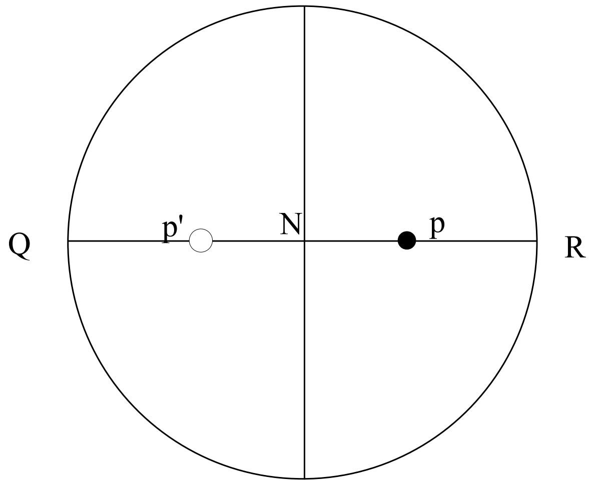


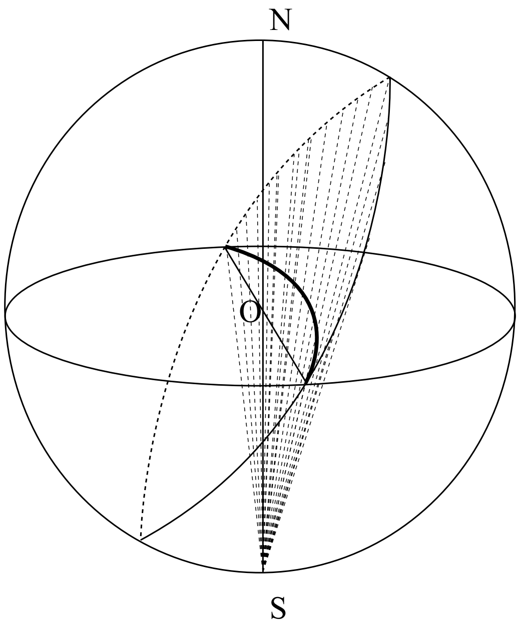


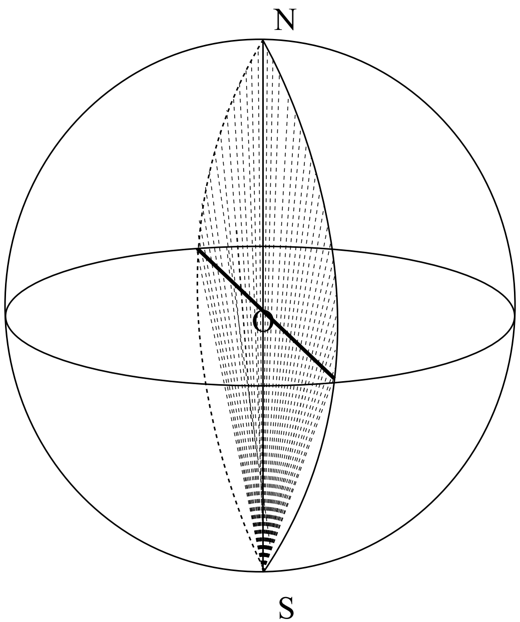
Massimo Nespolo, Université de Lorraine

# Stereographic projection: poles and symmetry planes



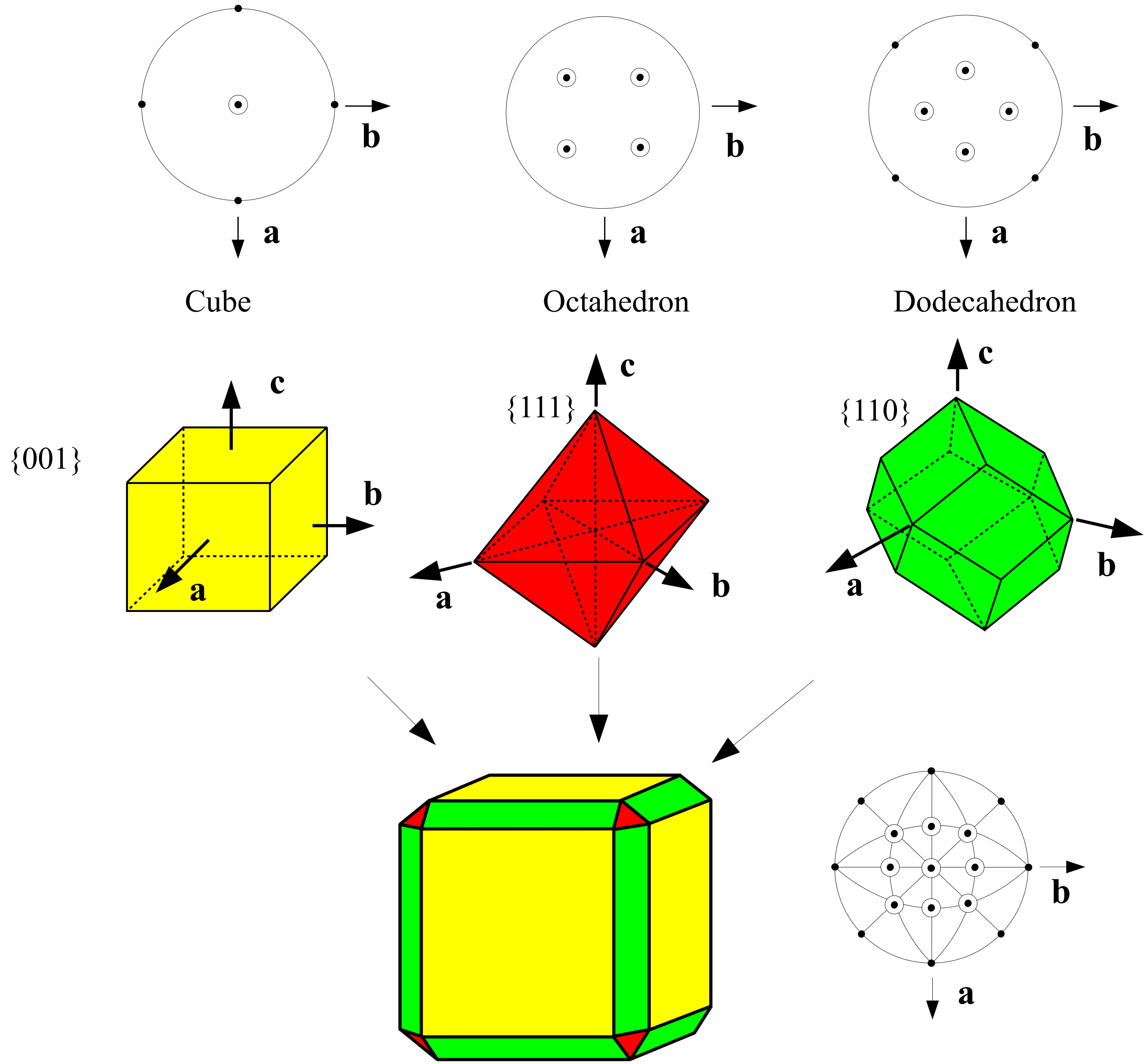



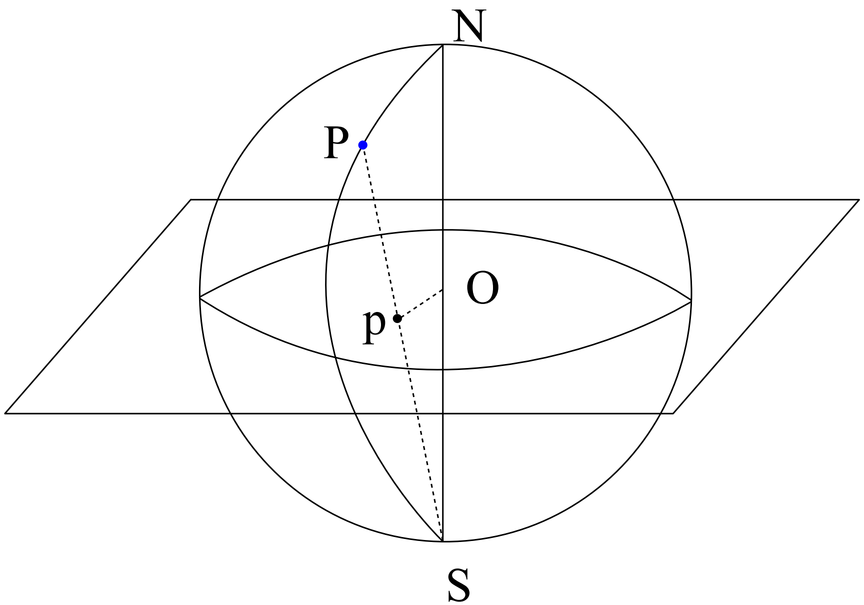


Massimo Nespolo, Université de Lorraine

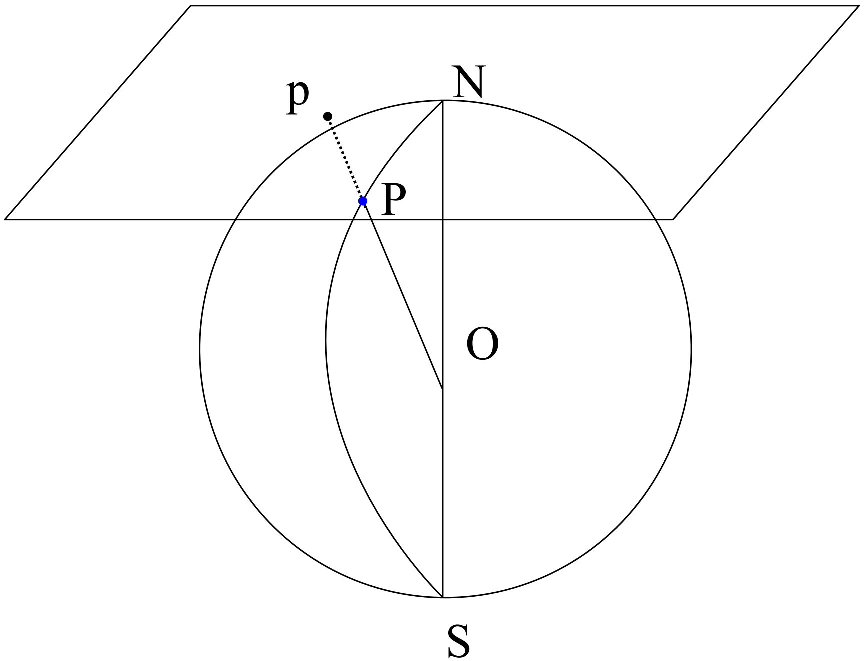
# Example of decomposition of the morphology of a crystal



# Stereographic vs. gnomonic projection



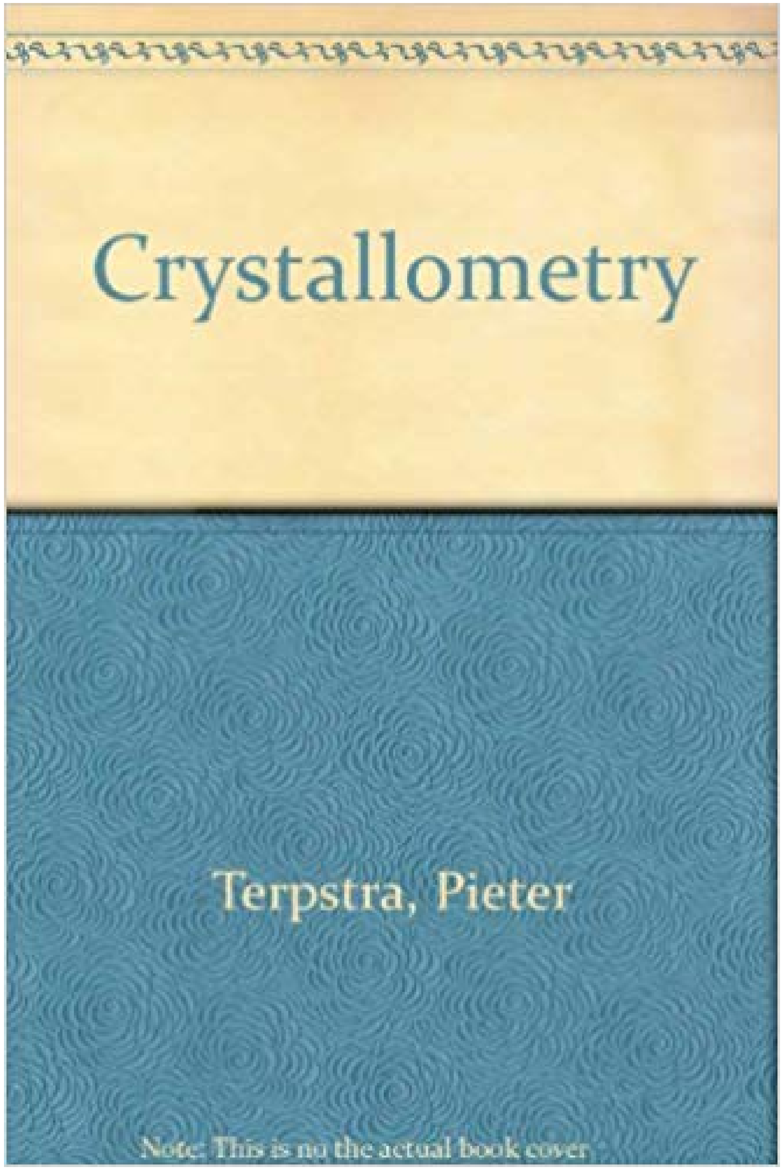

Stereographic projection




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"…} 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

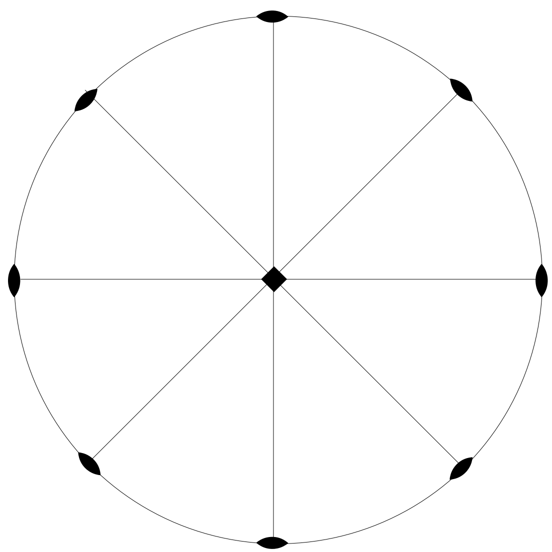
S is called the site-symmetry group (or stabilizer) of X.

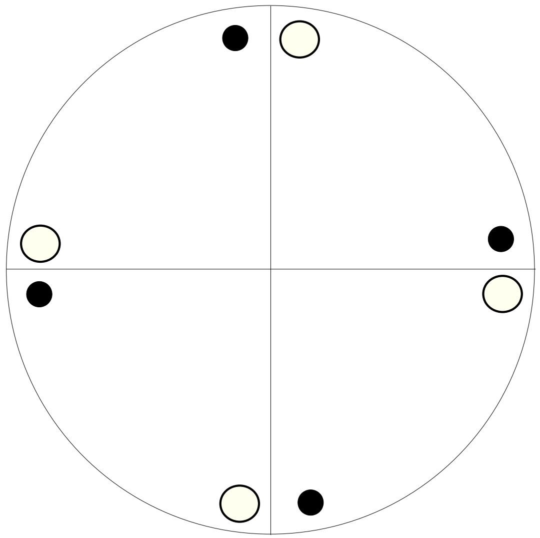
Points whose site-symmetry groups S are conjugate under P belong the same Wyckoff position

The number of points obtained as {PX} is the multiplicity M of the orbit, which is equal to the index of S in P: $M = |P|/|S|$


Massimo Nespolo, Université de Lorraine

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





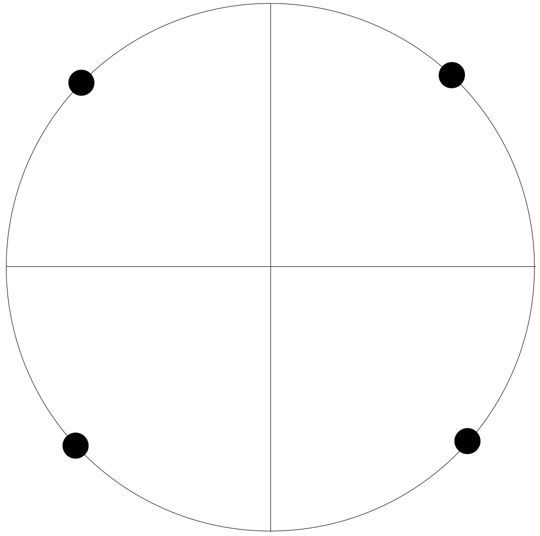
Coordinates

$x\underline{yz}$, $\underline{\bar{y}xz}$, $\underline{\bar{x}}\bar{y}\underline{z}$, $y\bar{x}\underline{z}$,
$xyz$, $yxz$, $xyz$, $yxz$

S = {1}, M = 8

**General position**

S = {1}, M = |P|



Coordinates

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

S = {..2}, M = 4

**Special position**

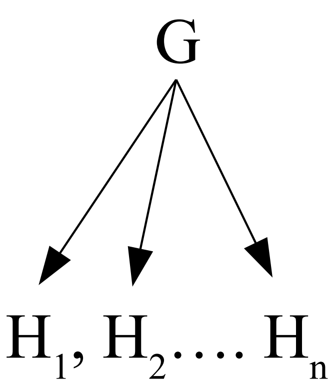
S $\supset$ {1}, M = |P|/|S|

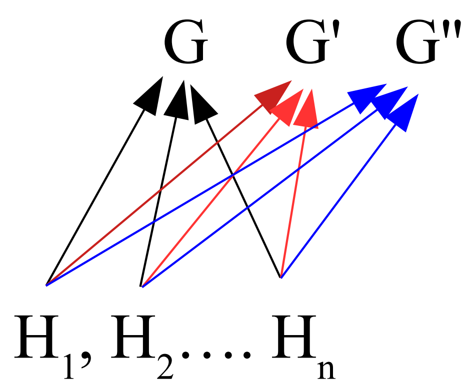
$\forall p_j \in P$
$p_j 1 p_j^{-1} = 1$
$p_j 2_{[110]} p_j^{-1} = \{2_{[110]}, 2_{[1\bar{1}0]}\}$


Massimo Nespolo, Université de Lorraine

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

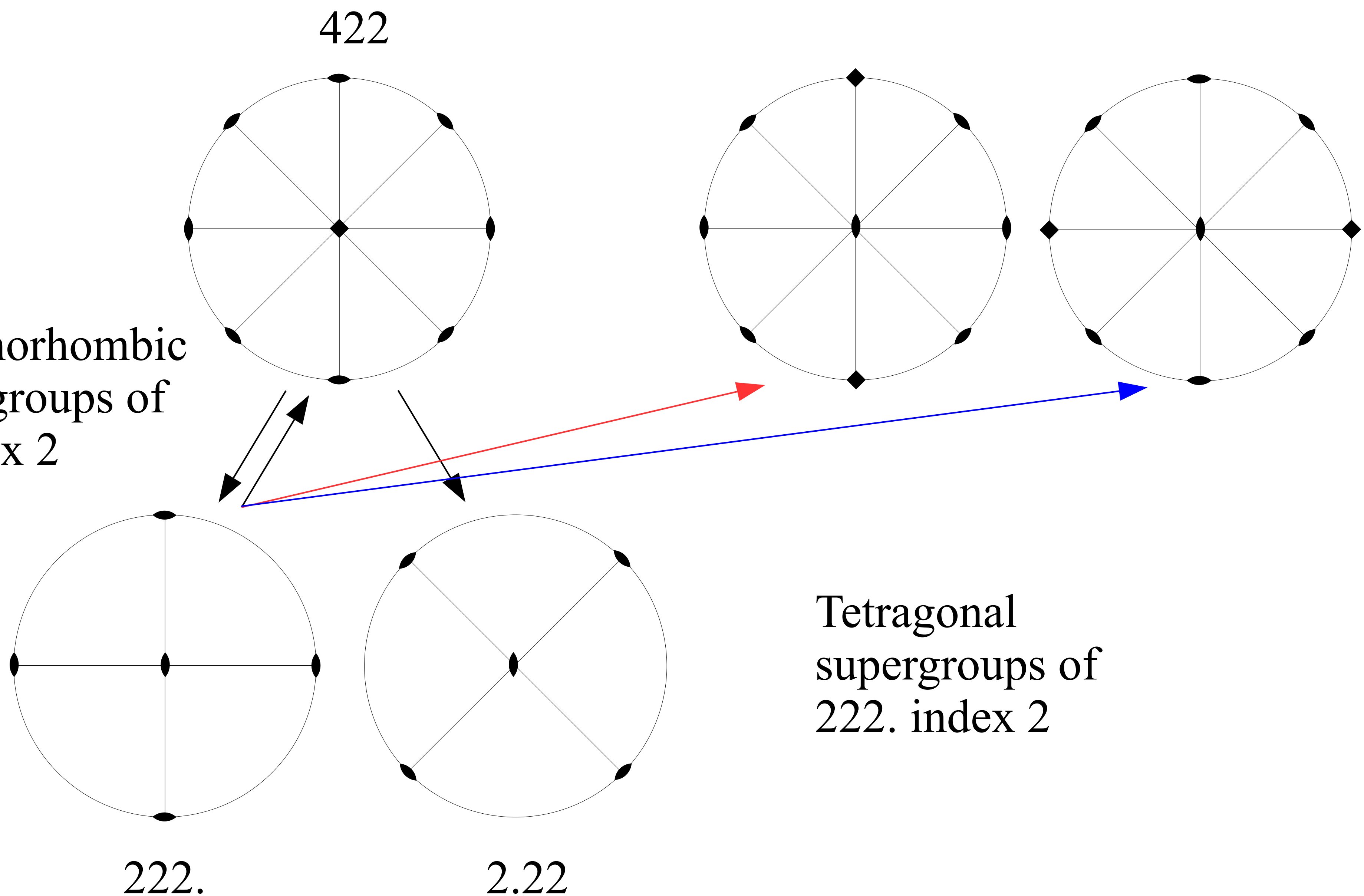
$G \supset H$ $\qquad$ $i = |G|/|H|$



# To remove symmetry operations is easier than to add them

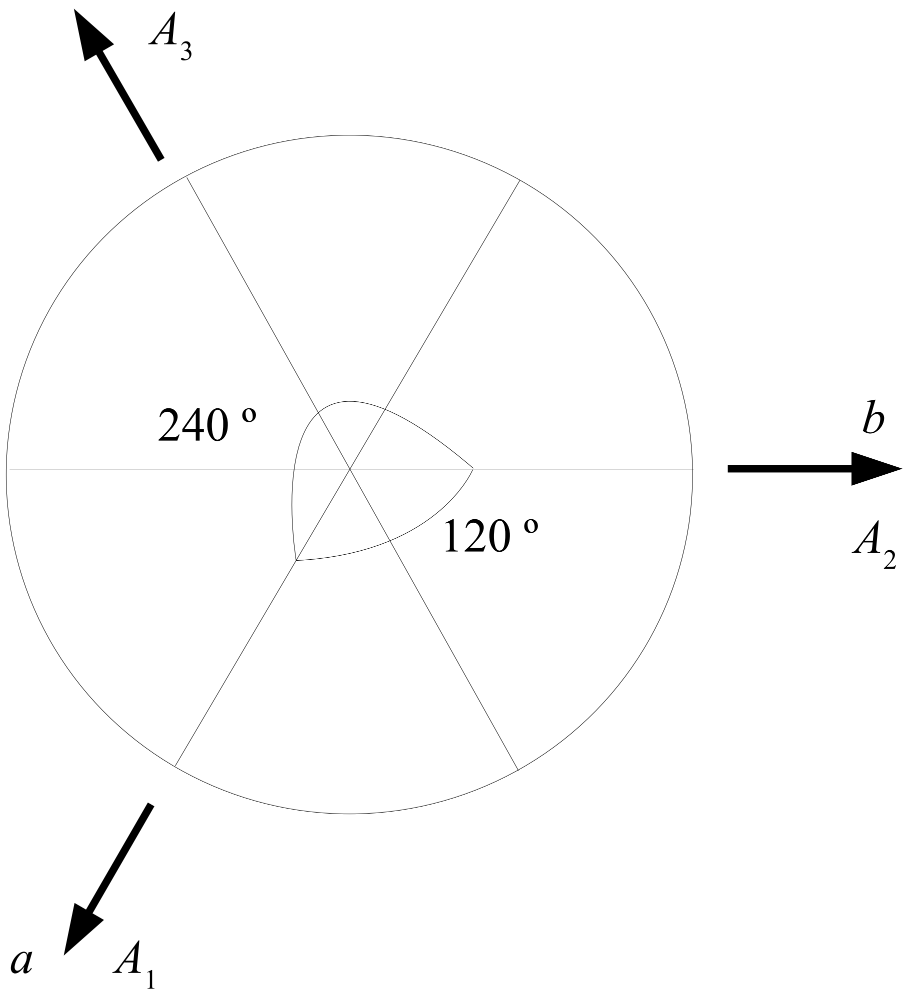
Orthorhombic subgroups of index 2



# Indexing crystals of the hexagonal family: Bravais-Miller indices


Massimo Nespolo, Université de Lorraine

# Hexagonal axes: Bravais-Miller indices




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

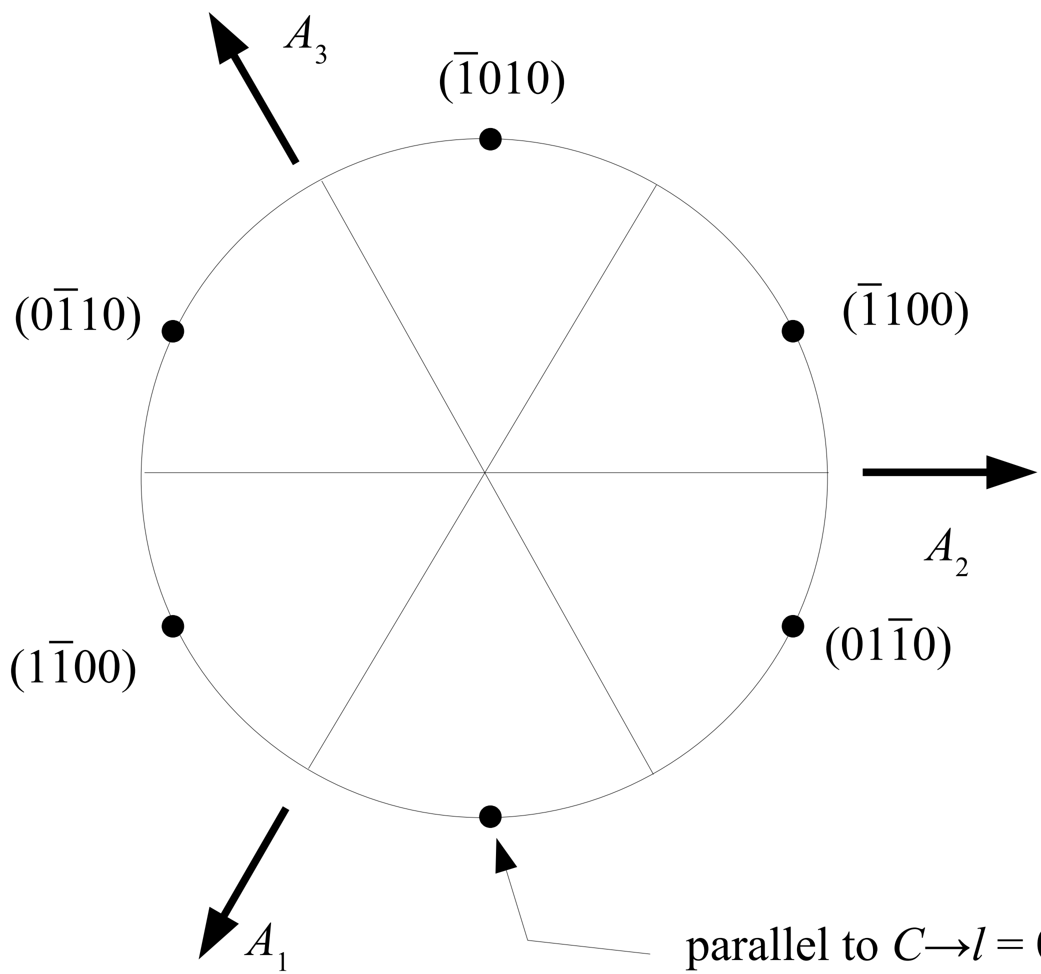
$$hkl \rightarrow hkil$$

Miller indices | Bravais-Miller indices

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

$$i = -h-k$$

# Bravais-Miller indices: example



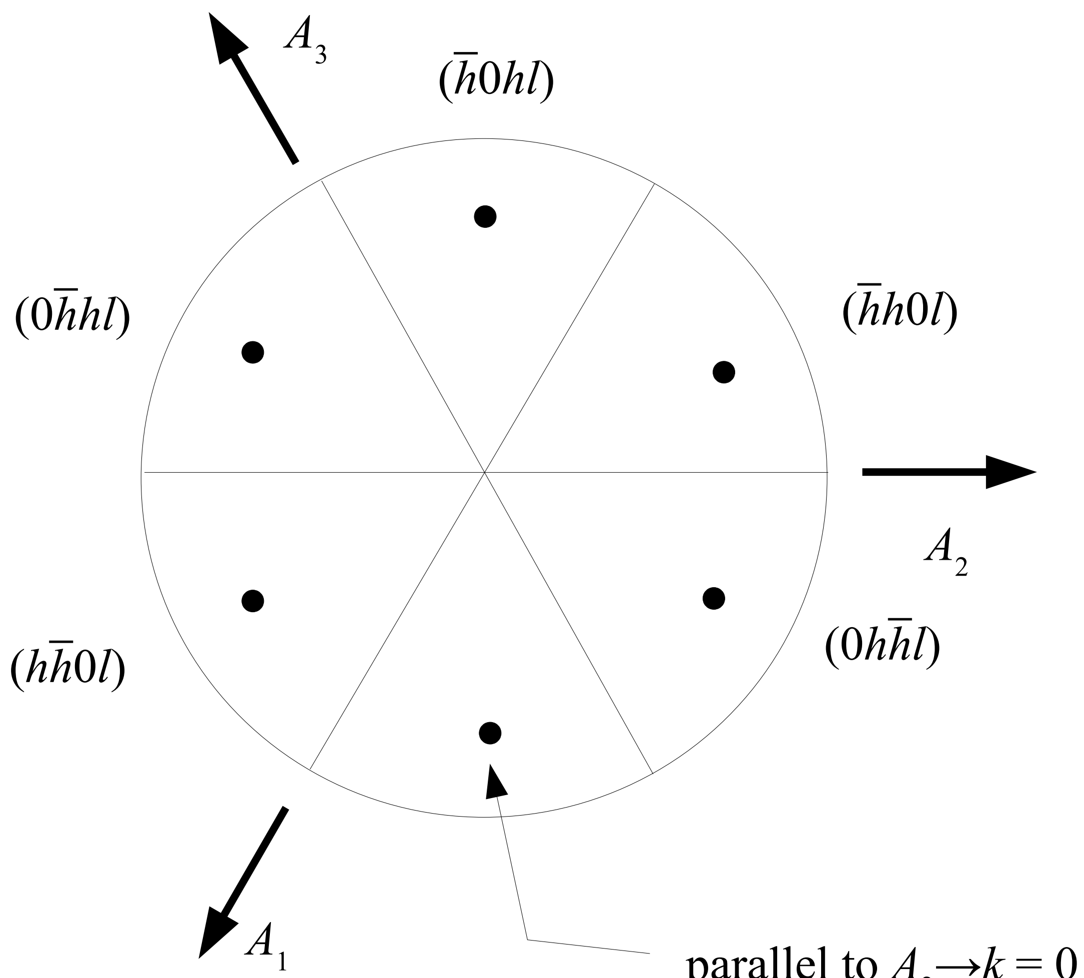

If you use Miller indices the symmetry is less evident!

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

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

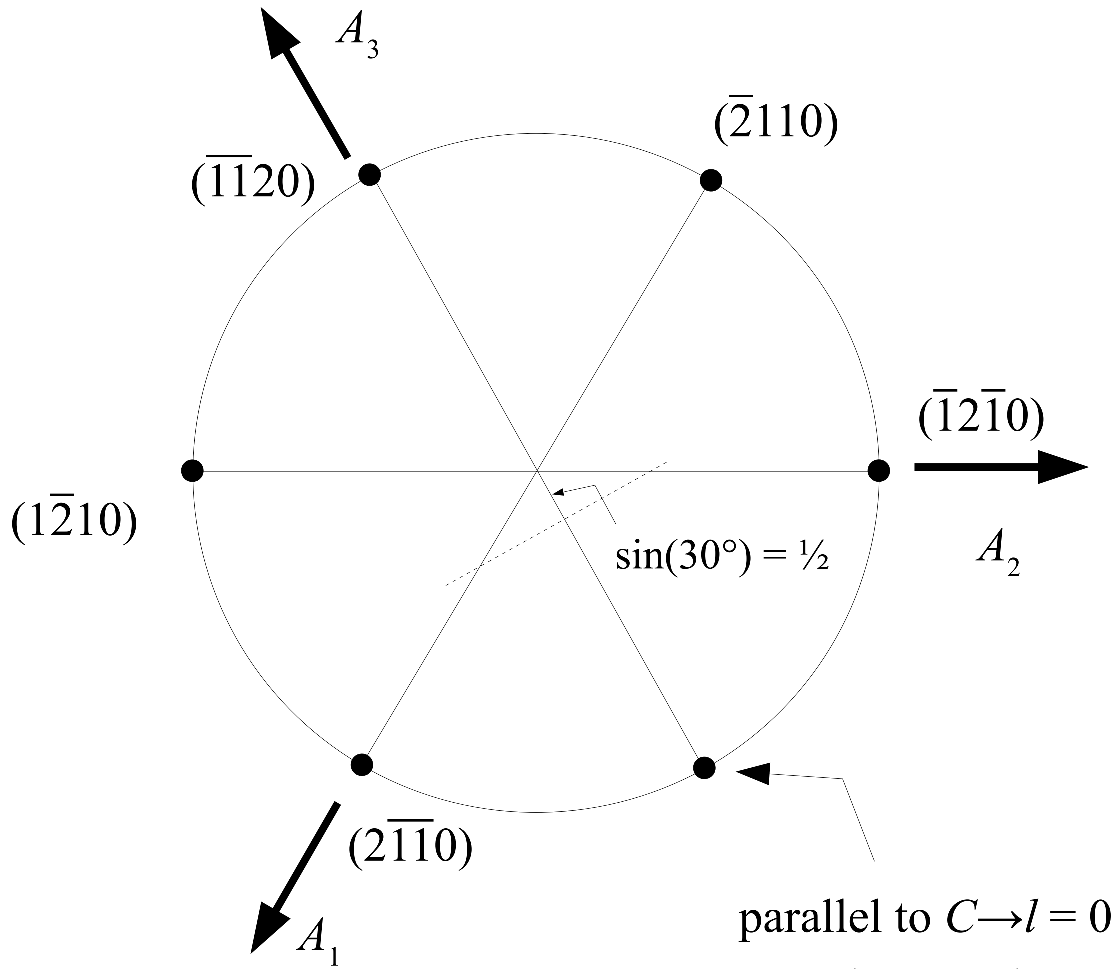



If you use Miller indices the symmetry is less evident!

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

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

# Bravais-Miller indices: example




If you use Miller indices the symmetry is less evident!

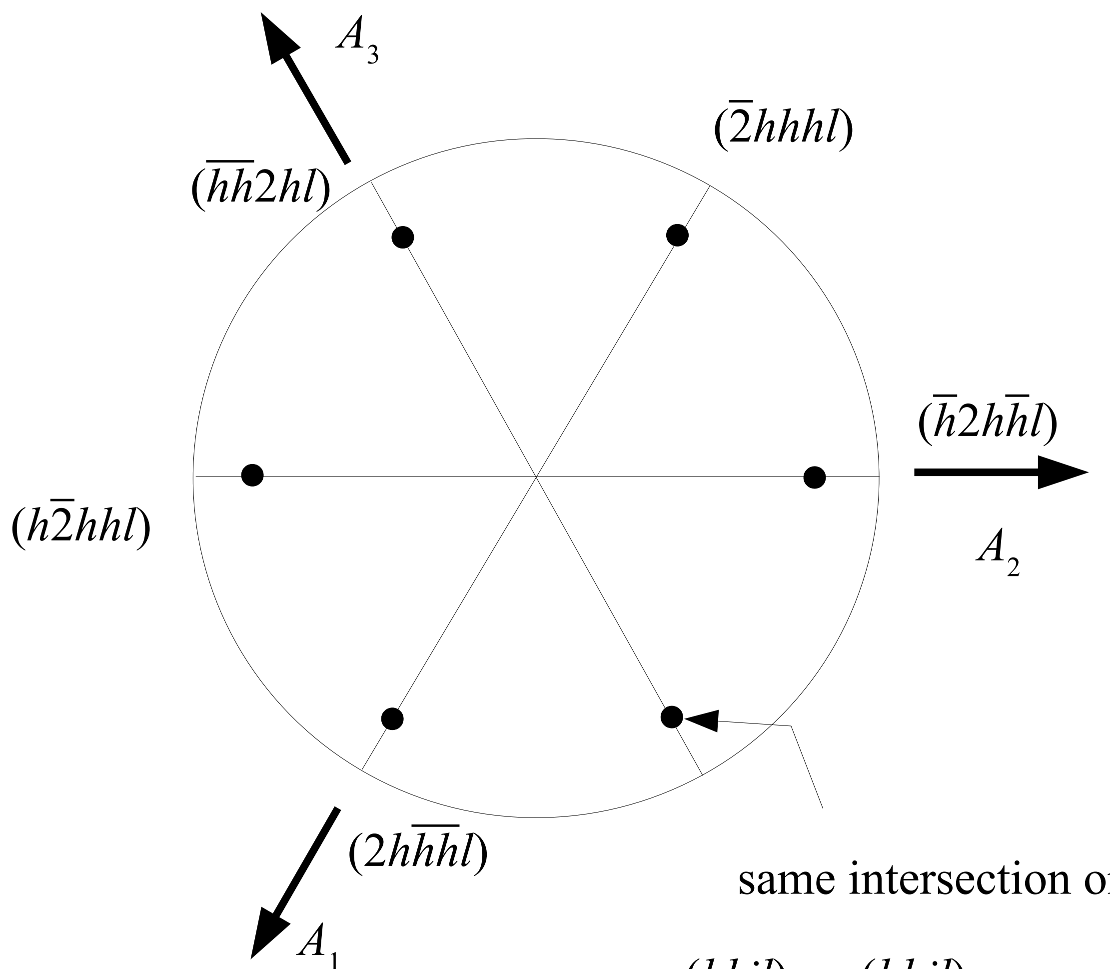
$(110)$
$(\bar{1}20)$
$(\bar{2}10)$
$(110)$
$(1\bar{2}0)$
$(2\bar{1}0)$

parallel to $C \rightarrow l = 0$

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

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

# Bravais-Miller indices: example




If you use Miller indices the symmetry is less evident!

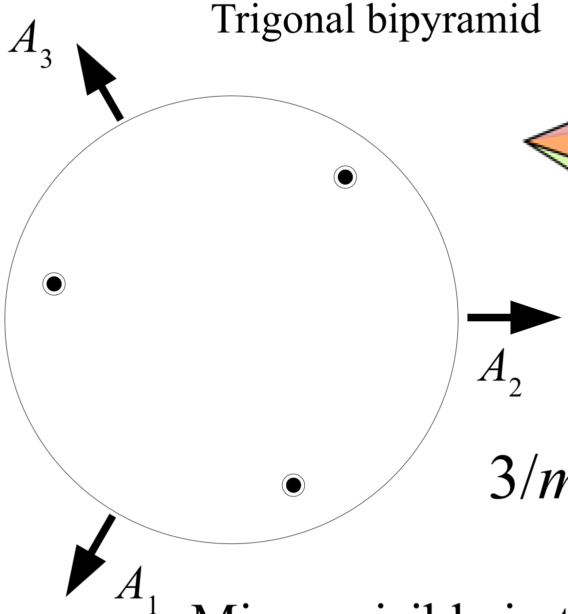
$(hhl)$
$(\bar{h}2hl)$
$(\bar{2}hhl)$
$(\bar{h}\bar{h}l)$
$(h\bar{2}hl)$
$(2h\bar{h}l)$

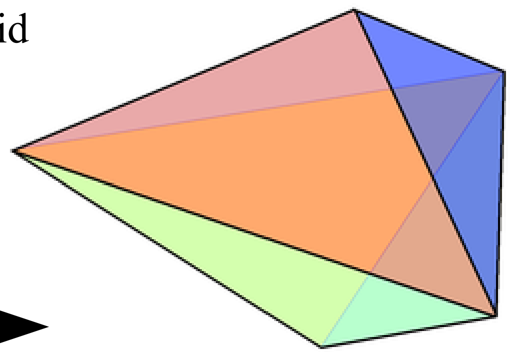
same intersection on $A_1$ and $A_2 \rightarrow k = h$

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

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

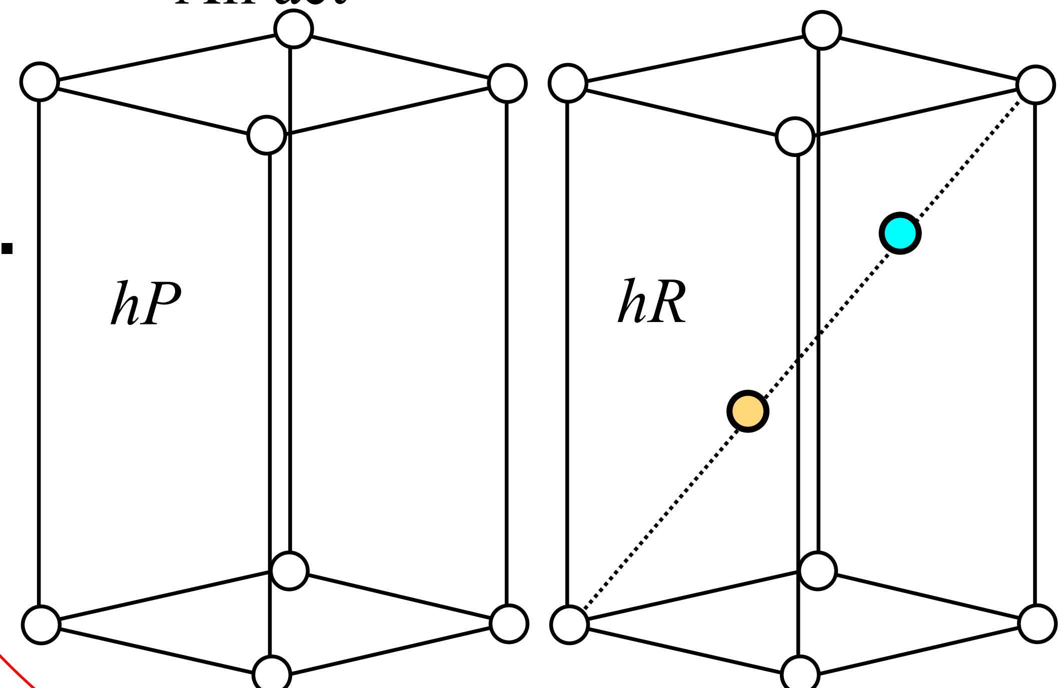
Trigonal bipyramid



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

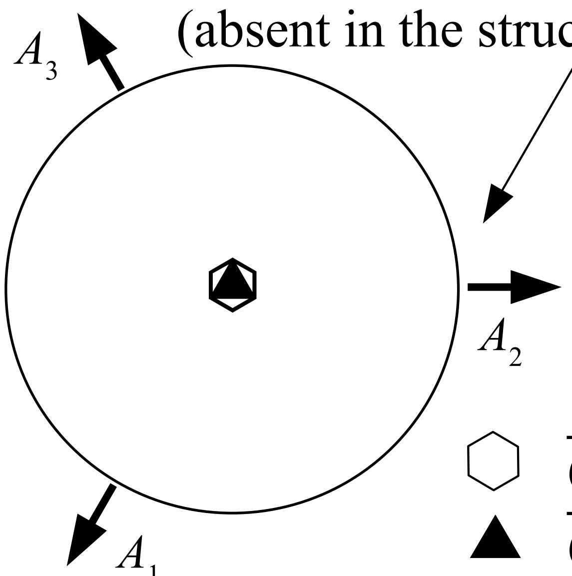
Only 3 and $\bar{3}$ act




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 $\boxed{hP}$ → trigonal system

~~$m$~~ ⟵ acts on $\boxed{hP}$ only → hexagonal system

**Contradiction !**



Massimo Nespolo, Université de Lorraine

# Weber indices

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 $\mathbf{A}_1,\mathbf{A}_2,\mathbf{A}_3,\mathbf{C}$ be the four hexagonal axes, and let be *uvw* and *UVTW* the indices of a direction with respect to $\mathbf{A}_1,\mathbf{A}_2,\mathbf{C}$ or $\mathbf{A}_1,\mathbf{A}_2,\mathbf{A}_3,\mathbf{C}$ respectively. The relations between *uvw* and *UVTW* are:

$$u = 2U+\mathrm{V};\ v = U+2V;\ w = W$$

$$U = (2u-v)/3;\ V = (2v-u)/3;\ T = -(u+v)/3.$$

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 $\boldsymbol{i = -h-k}$ 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.

| Miller indices | Bravais-Miller indices | Perpendicular direction | Perpendicular direction (Weber indices) |
|---|---|---|---|
| $(hkl0)$ | $(hki0)$ | $[2h+k,h+2k,0]$ | $[hki0]$ |
| Ex. $(100)$ | $(10\bar{1}0)$ | $[210]$ | $[10\bar{1}0]$ |
| Ex. $(2\bar{1}0)$ | $(2\bar{1}10)$ | $[100]$ | $[2\bar{1}10]$ |

With the exception of [0001] and [*UVT*0], the Weber indices correspond to a mixture of direct and reciprocal space, which should be avoided.

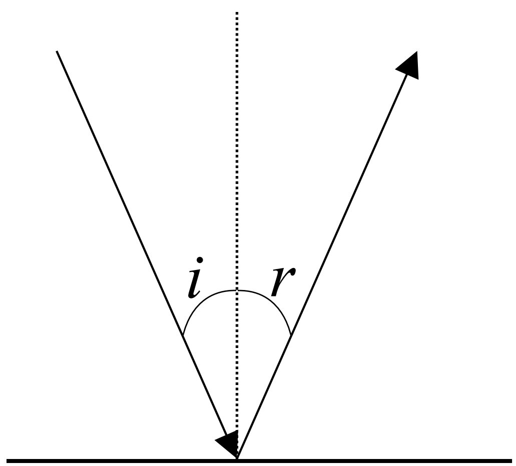
https://doi.org/10.1107/S1600576718007033

# Diffraction and Laue indices

# Reminder

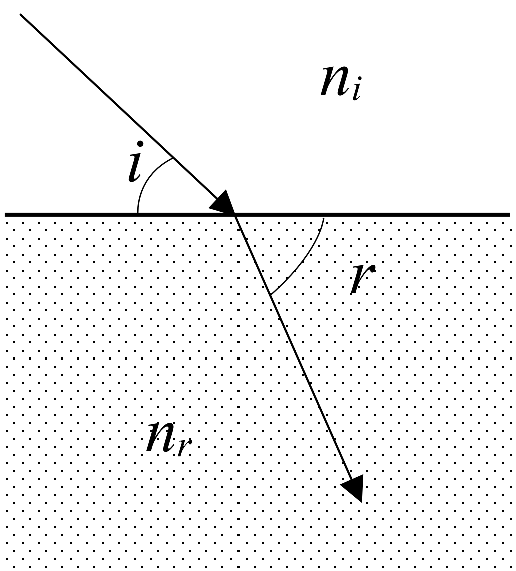
**Reflection** | **Refraction** | **Scattering**

Reflection

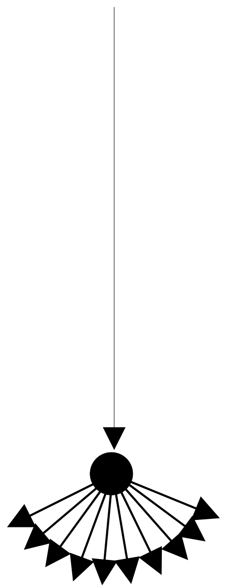



Refraction

$$\frac{\sin i}{\sin r} = \frac{n_r}{n_i}$$




Scattering

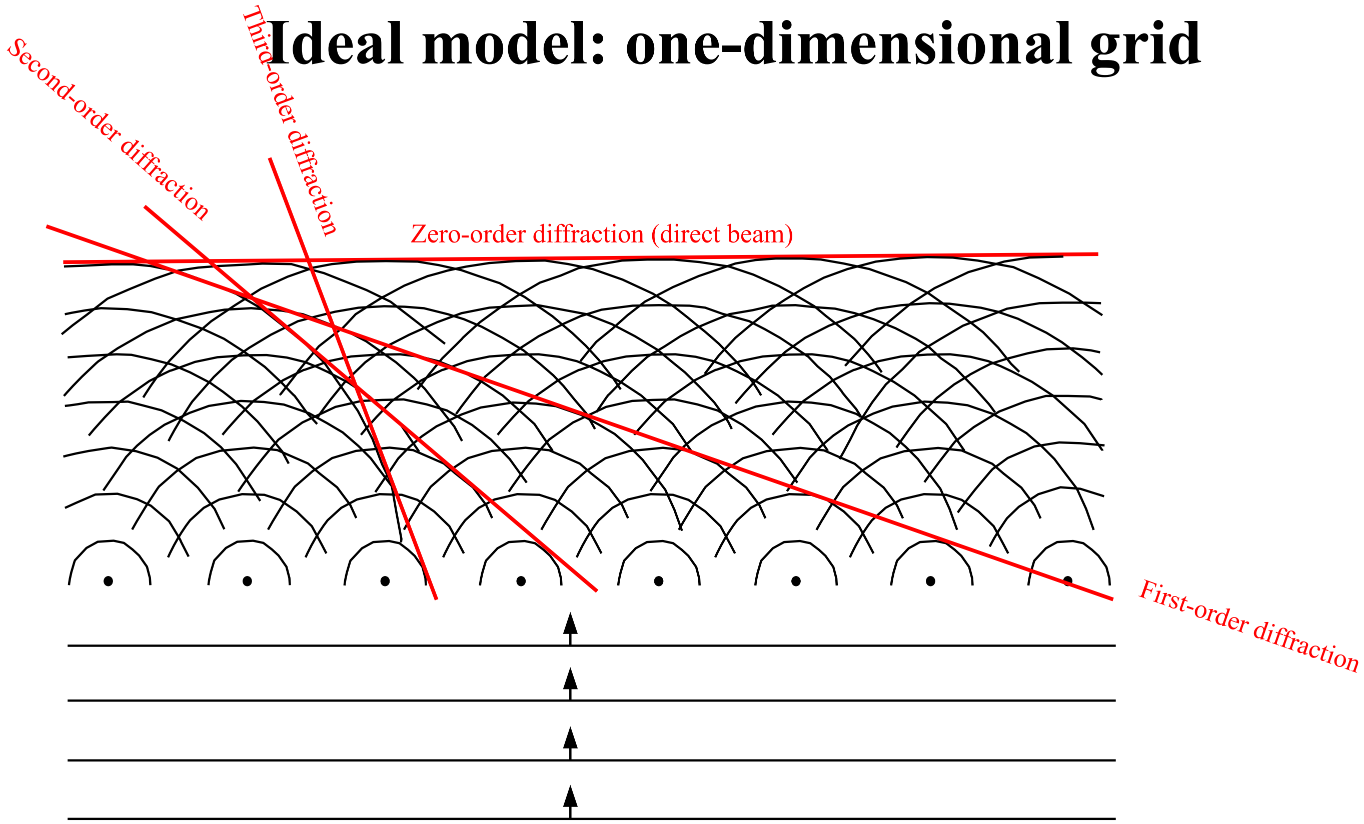


Diffraction: constructive interference of (elastically) scattered waves

approximation

# A hyper-simplified view at diffraction phenomenon

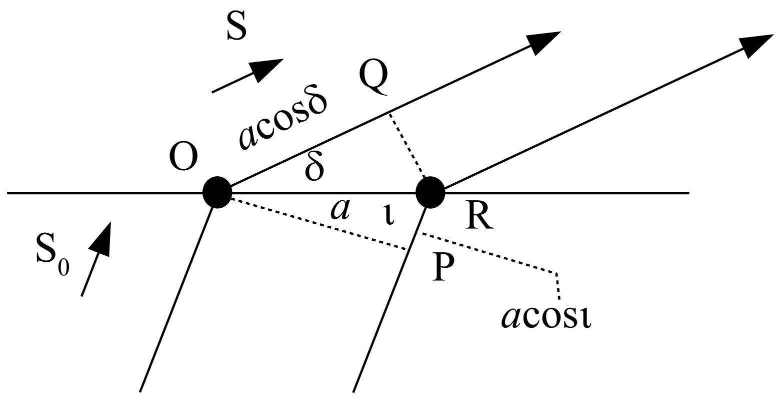
## Ideal model: one-dimensional grid

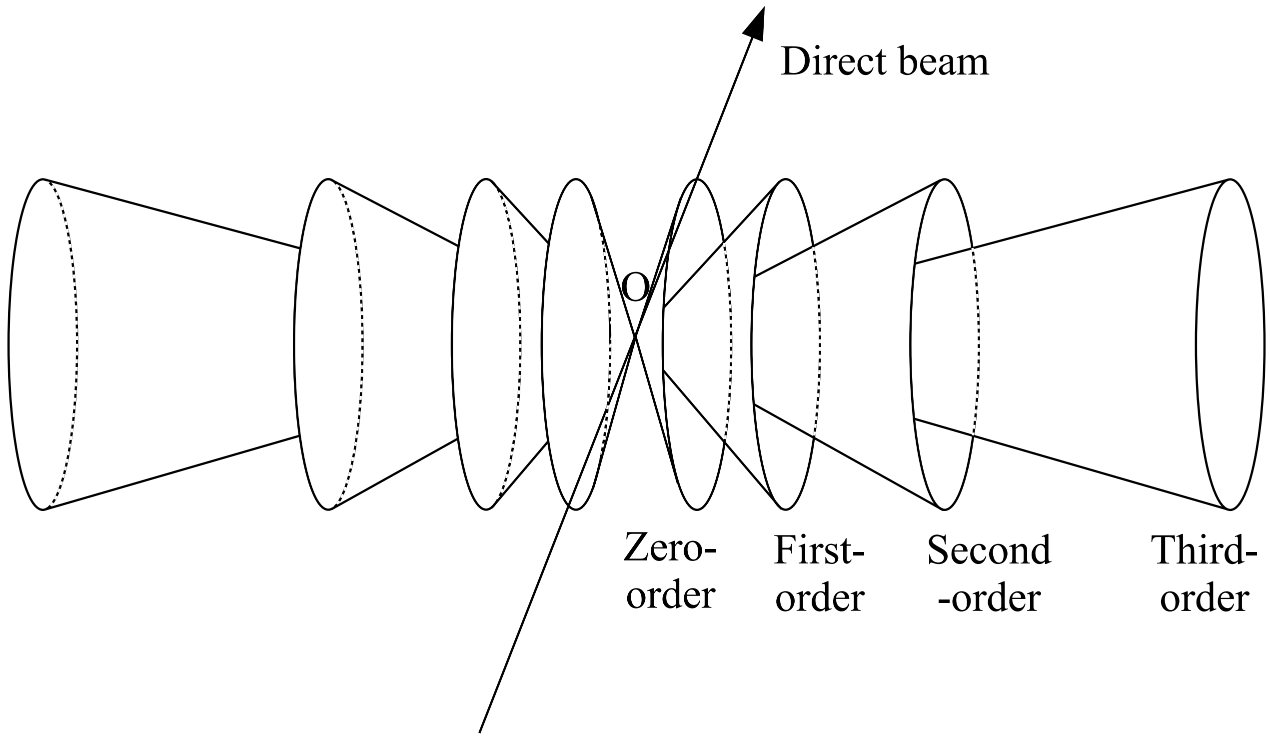



Every point of the grid is the source of a spherical wave. Waves which differ by an integer number of wavelengths interfere positively, resulting in diffracted waves. Waves from neighbour points which differ by $n$ wavelengths result in the $n$-th order diffraction.

From M..J. Burger, *X-ray crystallography*

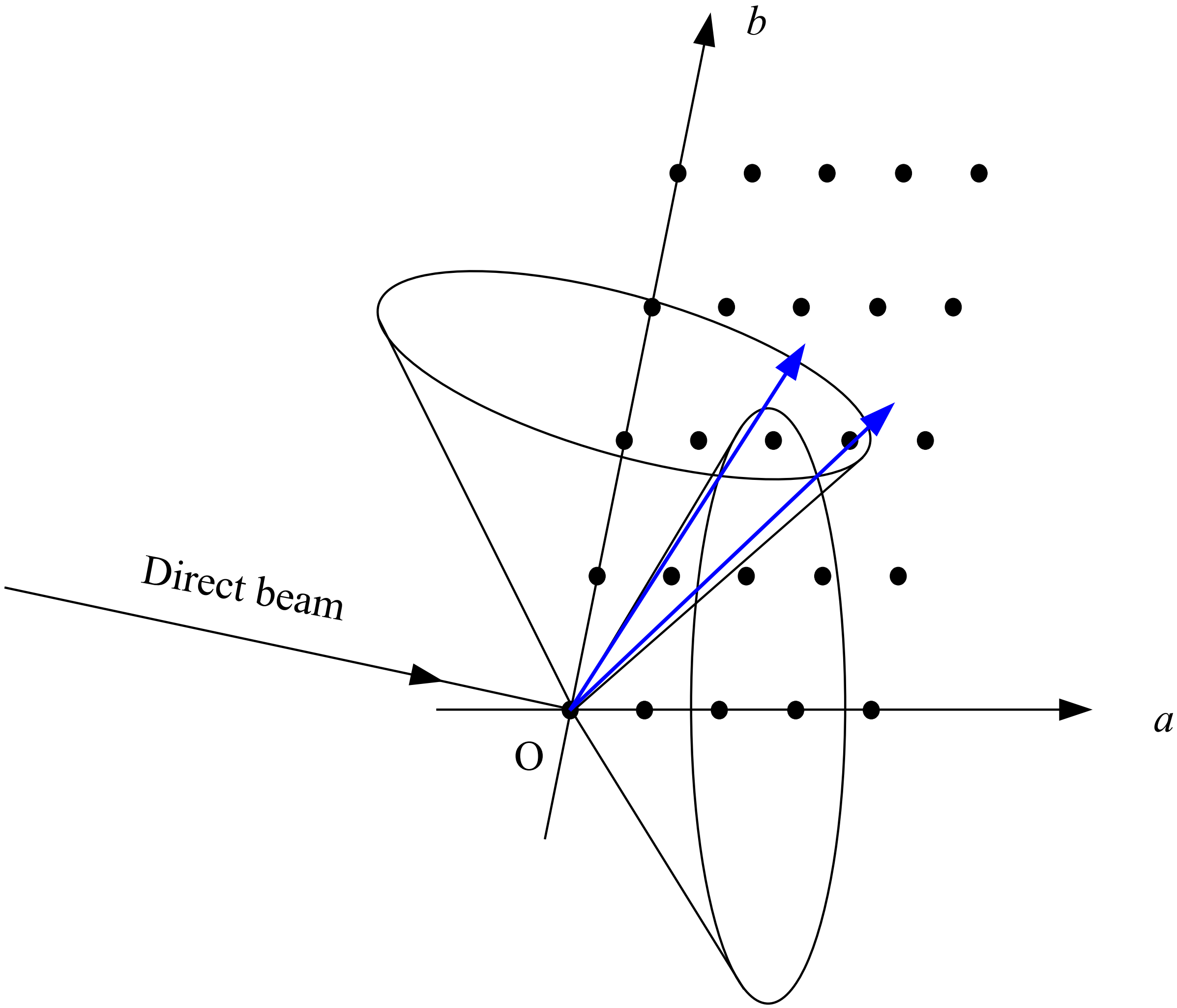
# One-dimensional diffraction



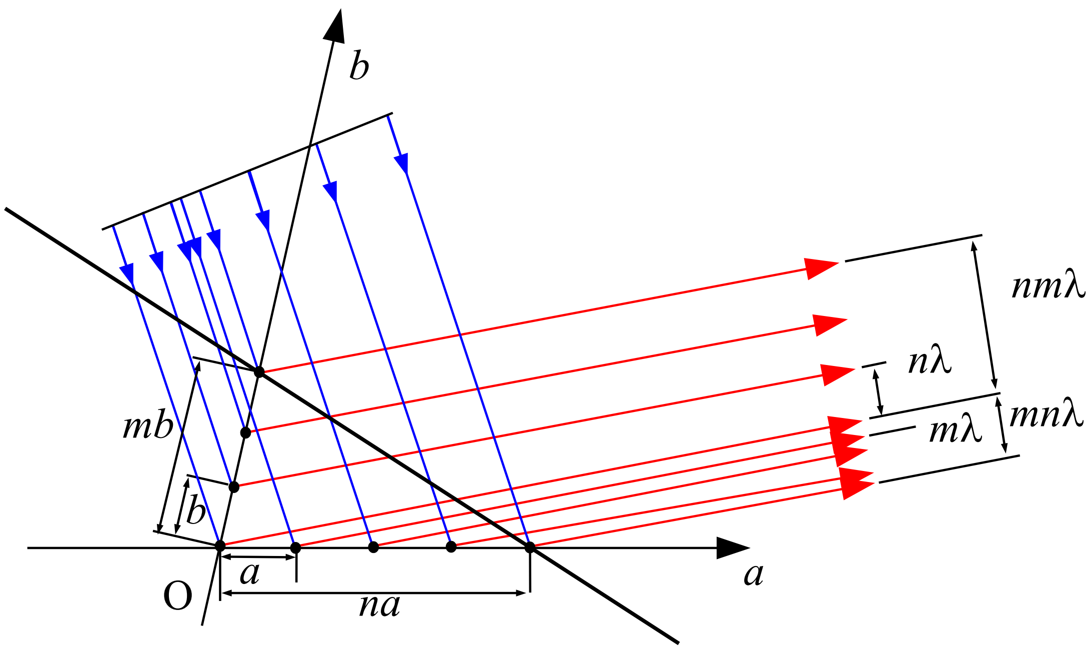

From M..J. Burger, *X-ray crystallography*

# Two-dimensional diffraction




From M..J. Burger, *X-ray crystallography*

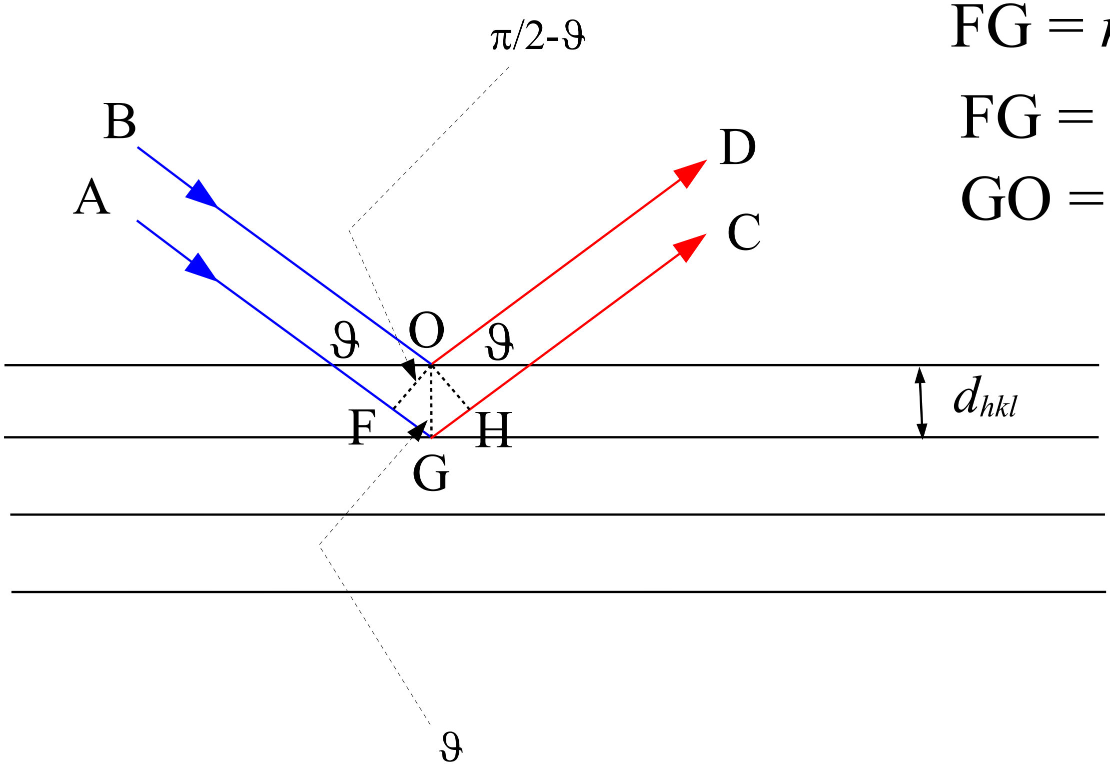
# Interpreting diffraction as “reflection”




From M.J. Burger, *X-ray crystallography*

# Bragg's law

Path difference of BD and AC: FGH




Condition for positive interference

FGH = $n\lambda$

FG = $n\lambda/2$

FG = GO$\sin\vartheta$

GO = $d_{hkl}$

$$n\lambda/2 = d_{hkl}\sin\vartheta_{hkl}$$

$$\boldsymbol{n\lambda = 2d_{hkl}\sin\vartheta_{hkl}}$$

**Bragg's law**

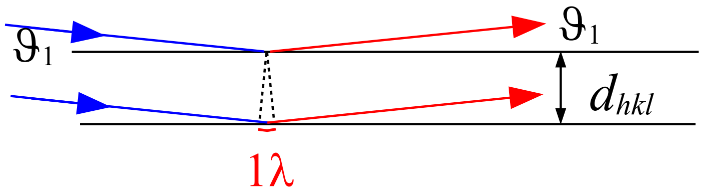
*n*-th diffraction order

From M..J. Burger, *X-ray crystallography*

# Diffraction order (interpreted as “reflection”)

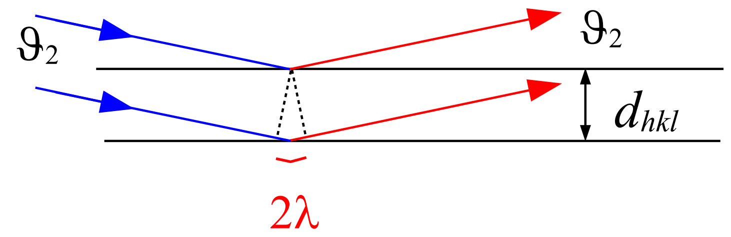
## First order

$\vartheta_1 = \sin^{-1}(\lambda/2d_{hkl})$



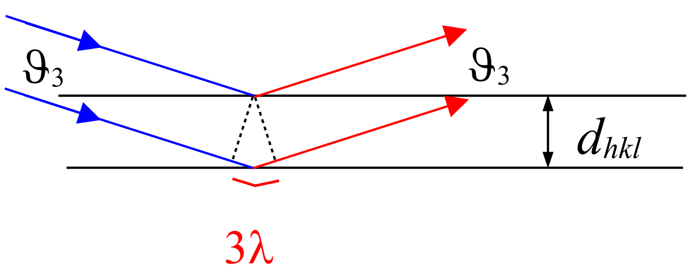

## Second order

$\vartheta_2 = \sin^{-1}(2\lambda/2d_{hkl})$



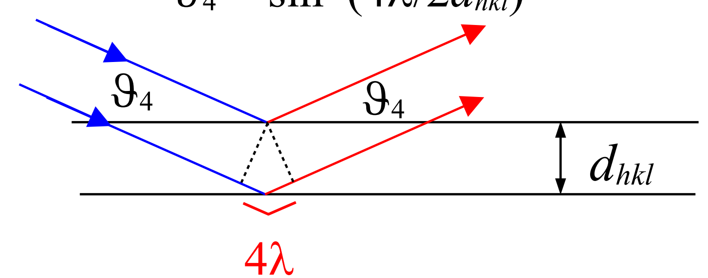

## Third order

$\vartheta_3 = \sin^{-1}(3\lambda/2d_{hkl})$




## Fourth order

$\vartheta_4 = \sin^{-1}(4\lambda/2d_{hkl})$




**Physical limit**

**$|\sin(\vartheta)| \leq 1$**

# Diffraction order: the output from a black-box software

| $h$ | $k$ | $l$ | $n$ | $d$(Å) | \|F\| | 2ϑ | | $h$ | $k$ | $l$ | $n$ | $d$(Å) | \|F\| | 2ϑ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 7.675267 | 21.6095 | 5.29693 | | 1 | -1 | 0 | 1 | 5.957833 | 0.455688 | 6.82546 |
| 2 | 0 | 0 | 2 | ~~3.837633~~ | 64.8796 | 10.60522 | | 2 | -2 | 0 | 2 | ~~2.978916~~ | 152.06 | 13.67528 |
| 3 | 0 | 0 | 3 | ~~2.558422~~ | 60.0323 | 15.93645 | | 3 | -3 | 0 | 3 | ~~1.985944~~ | 2.03328 | 20.57463 |
| 4 | 0 | 0 | 4 | ~~1.918817~~ | 55.7276 | 21.30267 | | 2 | 0 | -1 | 1 | 3.510011 | 27.4588 | 11.59836 |
| 0 | 1 | 0 | 1 | 7.118295 | 1.97581 | 5.71172 | | 4 | 0 | -2 | 2 | ~~1.755005~~ | 11.4148 | 23.31771 |
| 0 | 2 | 0 | 2 | ~~3.559147~~ | 5.59593 | 11.43769 | | 1 | 0 | -1 | 1 | 5.446232 | 12.3383 | 7.46748 |
| 0 | 3 | 0 | 3 | ~~2.372765~~ | 1.38733 | 17.19250 | | 2 | 0 | -2 | 2 | ~~2.723116~~ | 52.8763 | 14.96692 |
| 0 | 4 | 0 | 4 | ~~1.779574~~ | 14.1963 | 22.99137 | | 3 | 0 | -3 | 3 | ~~1.815411~~ | 7.99568 | 22.53150 |
| 0 | 0 | 1 | 1 | 7.034205 | 5.31933 | 5.78006 | | 0 | 1 | -1 | 1 | 5.061394 | 3.24668 | 8.03617 |
| 0 | 0 | 2 | 2 | ~~3.517102~~ | 80.2575 | 11.57489 | | 0 | 2 | -2 | 2 | ~~2.530697~~ | 32.8314 | 16.11220 |
| 0 | 0 | 3 | 3 | ~~2.344735~~ | 52.062 | 17.39961 | | 0 | 3 | -3 | 3 | ~~1.687131~~ | 5.77121 | 24.26978 |
| 0 | 0 | 4 | 4 | ~~1.758551~~ | 109.986 | 23.27004 | | | | | | | | |

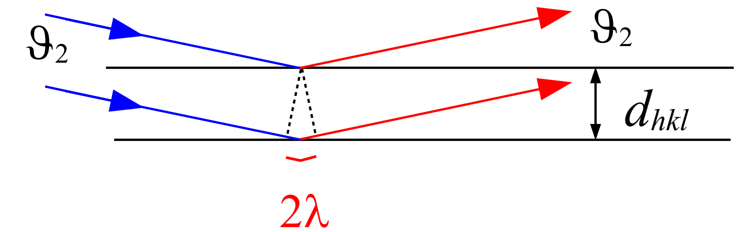
$$\vartheta_n = \sin^{-1}\left(\frac{n\lambda}{2d_{hkl}}\right) = \sin^{-1}\left(\frac{\lambda}{2\frac{d_{hkl}}{n}}\right) = \sin^{-1}\left(\frac{\lambda}{2d_{nhnknl}}\right)$$

Non-existing ($nh$,$nk$,$nl$) family of planes

# Higher-order diffraction reas as first-order diffraction for a non-reticular plane

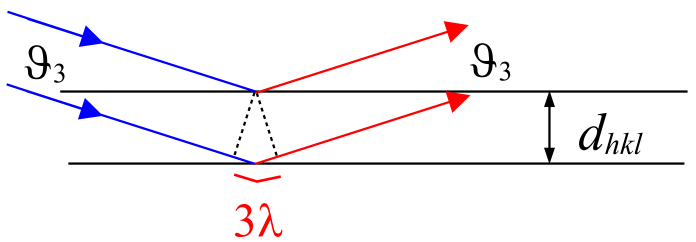
Second order diffraction from the family (*hkl*)

$\vartheta_2 = \sin^{-1}(2\lambda/2d_{hkl})$



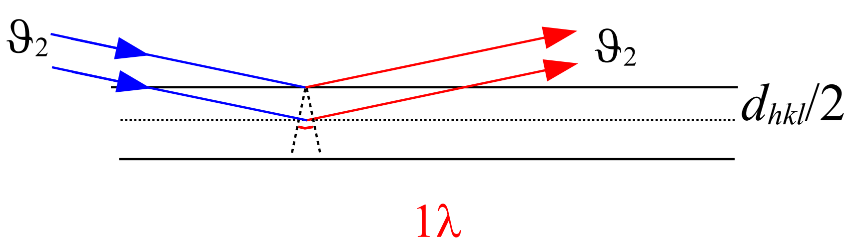

Third order diffraction from the family (*hkl*)

$\vartheta_3 = \sin^{-1}(3\lambda/2d_{hkl})$



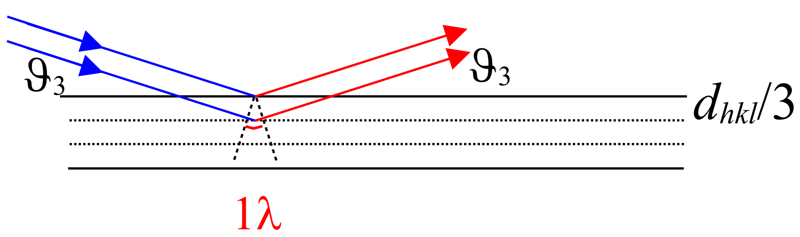

First order diffraction from a non-existing (2*h*2*k*2*l*) family

$\vartheta_2 = \sin^{-1}[\lambda/(2d_{hkl}/2)]$

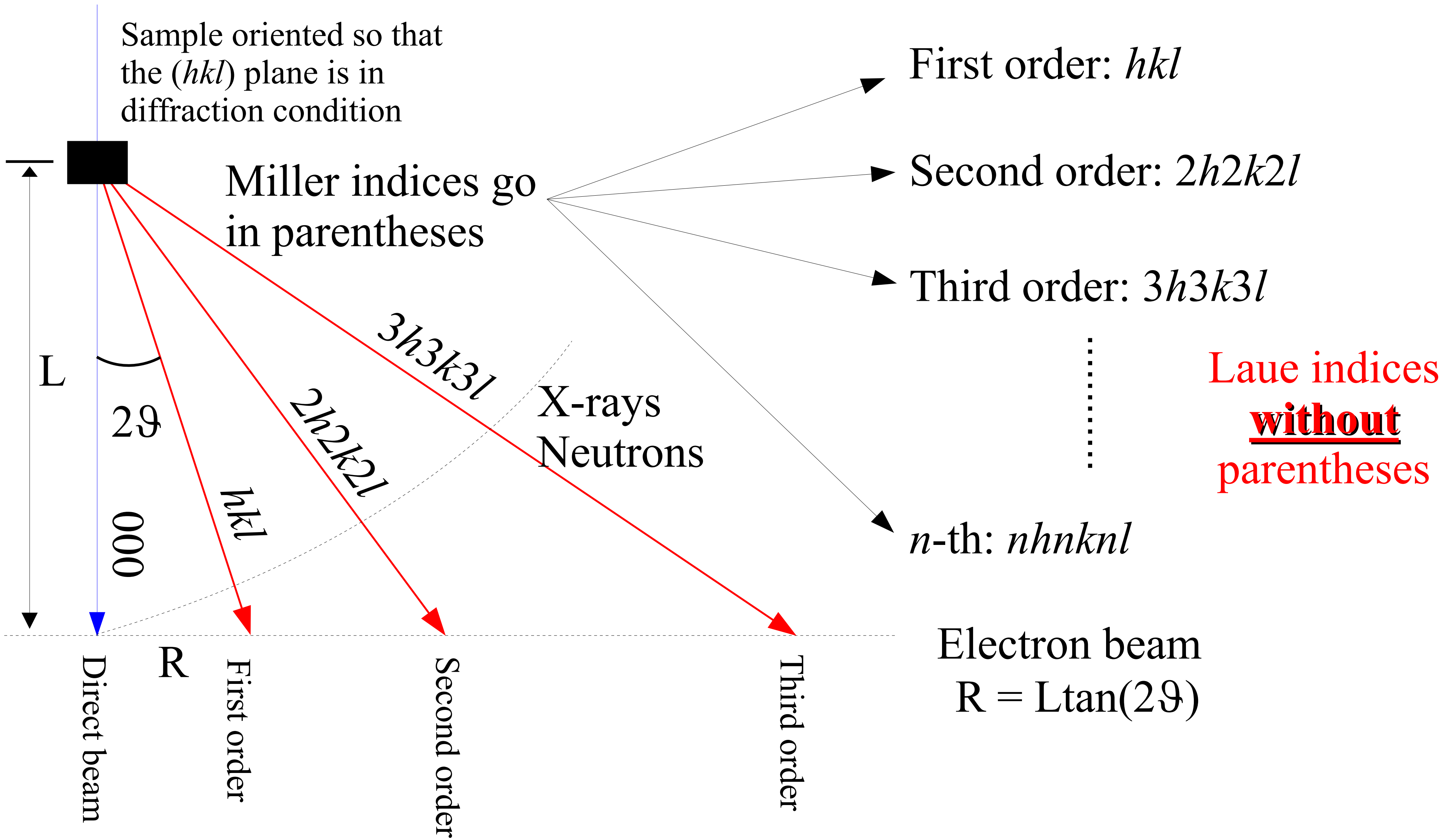



First order diffraction from a non-existing (3h3*k*3*l*) family

$\vartheta_3 = \sin^{-1}[\lambda/(2d_{hkl}/3)]$



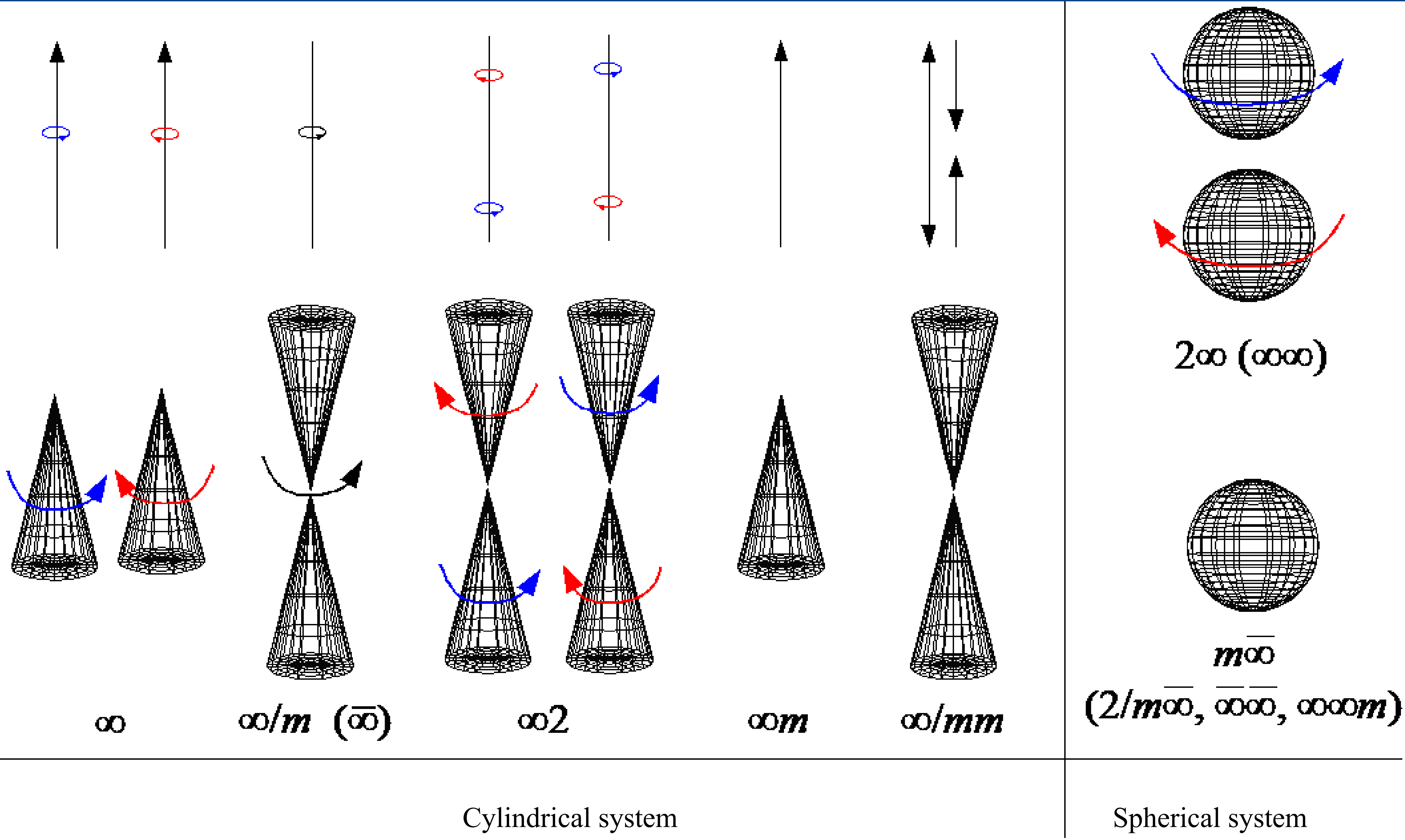
# Miller vs. Laue indices




**Warning**: Miller indices are relatively prime ONLY if a primitive cell is used!

# Curie’s law applied to crystals

# Curie groups



# 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

$$\mathbf{G \supseteq K \cap F}$$

# Pyrolectric effect

Change of polarization in a dielectric undergoing a change of temperature

$\mathrm{F} = m\overline{\infty}$ $\longrightarrow$ $\mathrm{K} \cap \mathrm{F} = \mathrm{K}$

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

Necessary condition for the phenomenon to occur

$$\mathbf{K} \subset \infty \boldsymbol{m}$$

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

$F = \infty/mm = \infty/m2/m$ G (point group of the electric field) : $\infty m$

Necessary condition for the phenomenon to occur

$$\mathbf{K \cap \infty/\mathit{m}2/\mathit{m} \subset \infty \mathit{m}}$$

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.