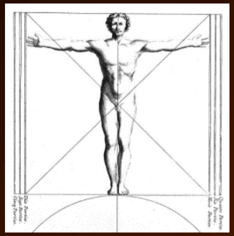
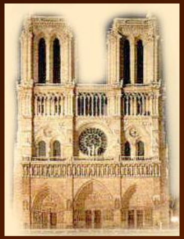
Basics symmetry in condensed matter physics

Sylvain Ravy
Laboratoire de physique des solides
CNRS, Université Paris-Saclay

- Symmetry:
  - From greak (sun) "with" (metron) "measure"
  - Same etymology as "commensurate"
  - Until mid-XIX: only mirror symmetry





- Transformation, Group
  - Évariste Galois 1811, 1832.

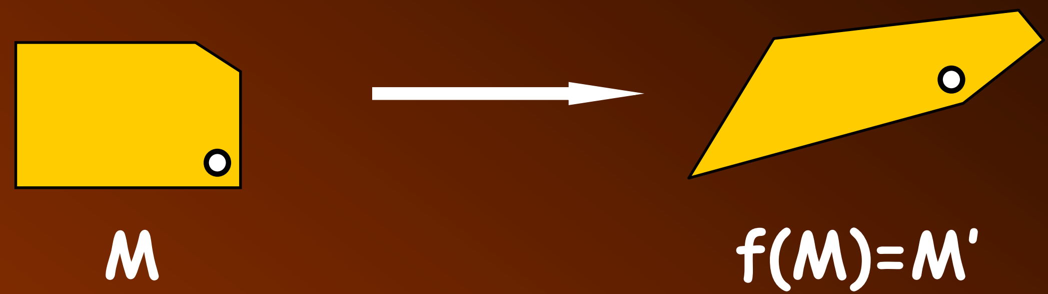
Definitions

Symmetry:

Property of invariance of an objet under a space transformation

Transformation

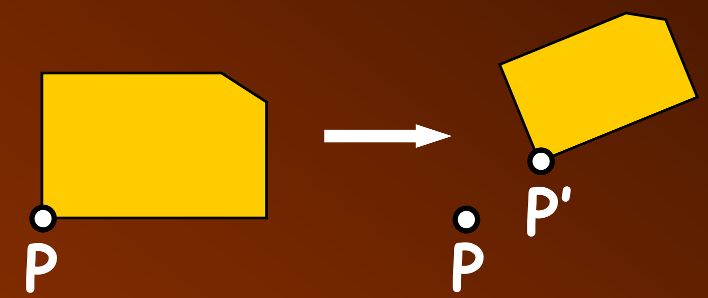
- **Bijection which** maps a geometric set in itself



- **Affine transformation** maps two points P and P' such that:

$$f(M) = P' + O(\overrightarrow{PM})$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \begin{pmatrix} t_{xx} & t_{yx} & t_{zx} \\ t_{xy} & t_{yy} & t_{zy} \\ t_{xz} & t_{yz} & t_{zz} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



f : positions

O : vectors

Isometries

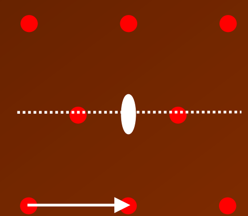
$f(M) = P' + O(\overrightarrow{PM})$

- Isometry $||O(u)||=||u||$

distance-preserving map

- Two types of isometry:
  - Affine isometry: $f(M)$
    - Transforms points – space groups
    - Microscopic properties of crystals (electronic structure)

- Translation
- Rotations
- Reflections

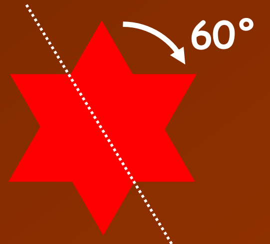


- Helix of pitch P

$(\alpha,\ P\alpha\ /2\pi)$

  - Linear isometry $O(\overrightarrow{PM})$
    - Transforms vectors (directions) – point groups
    - Macroscopic properties of crystals (response functions)

- Rotations
- Reflections

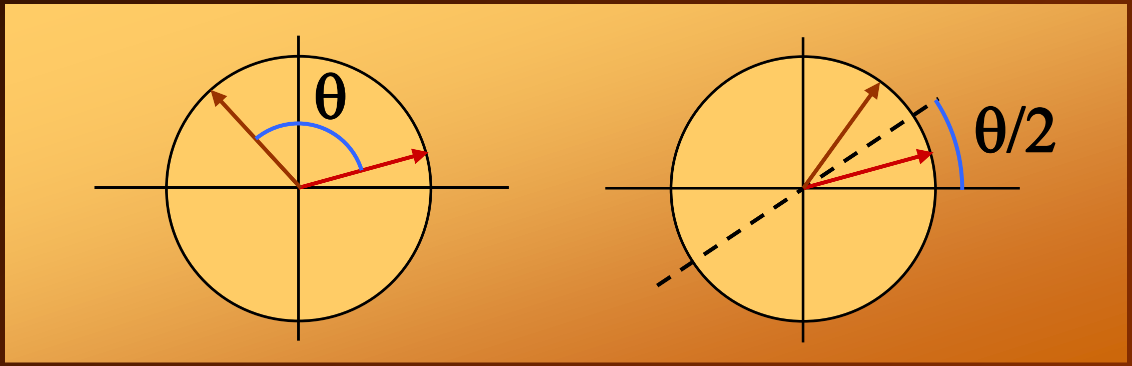


Linear isometry- 2D

$||O(u)|| = ||u||$

- In the plane (2D)

  - Rotations
  - Reflections (reflections through an axis)



$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

- Determinant +1
- Eigenvalues $e^{i\theta}$, $e^{-i\theta}$

$$\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

- Determinant -1
- Eigenvalues -1, 1

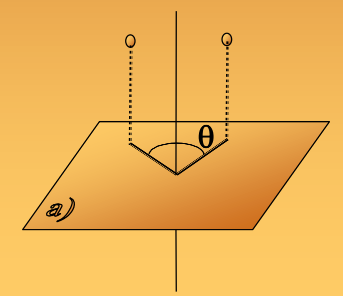
Linear isometry - 3D

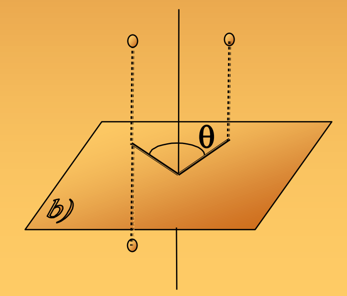
- $||O(u)|| = |\lambda|\,||u||$
  Eigenvalues $|\lambda| = 1$

- λ : 3rd degree equation (real coefficients)
  ± 1, $e^{i\theta}$, $e^{-i\theta}$ (det. = ± 1)

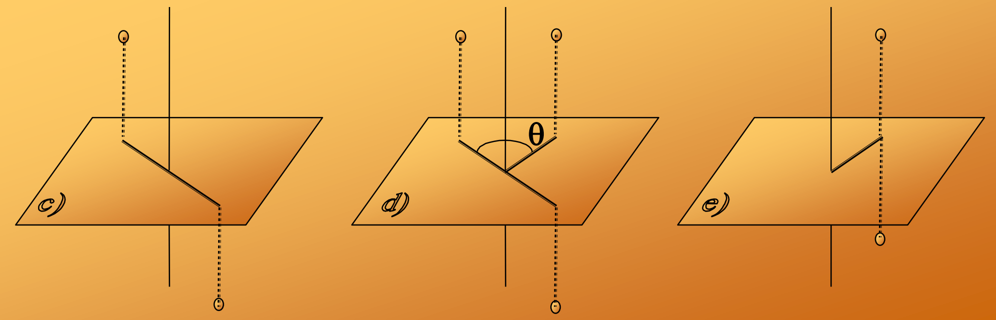
• In space (3D) :

• det. = 1 • Direct symmetry	• det. = -1 • Indirect symmetry
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}$
Rotations	Rotoreflections





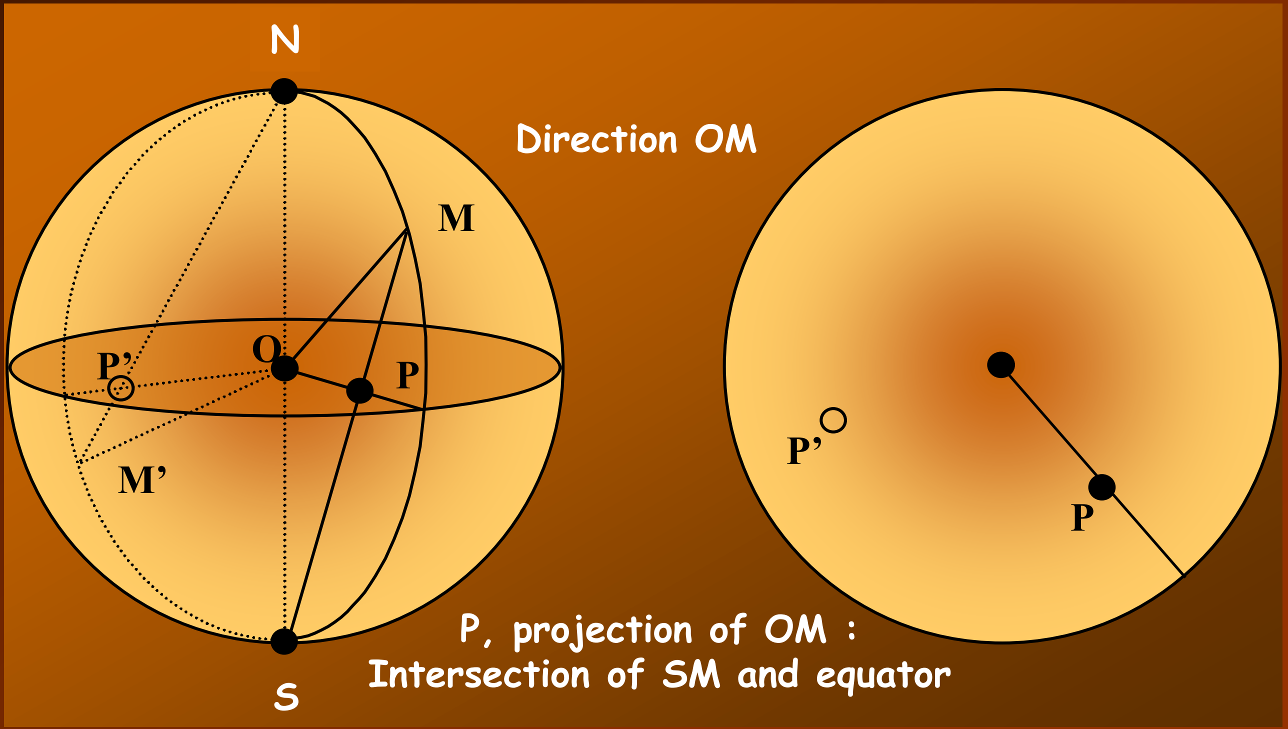
a) Rotation by angle θ
b) Roto-reflection θ
Improper rotation



c) Inversion (π)
d) Roto-inversion (π+θ)
c) Reflection (0)

Stereographic projection

- To represent directions
  preserves angles on the sphere

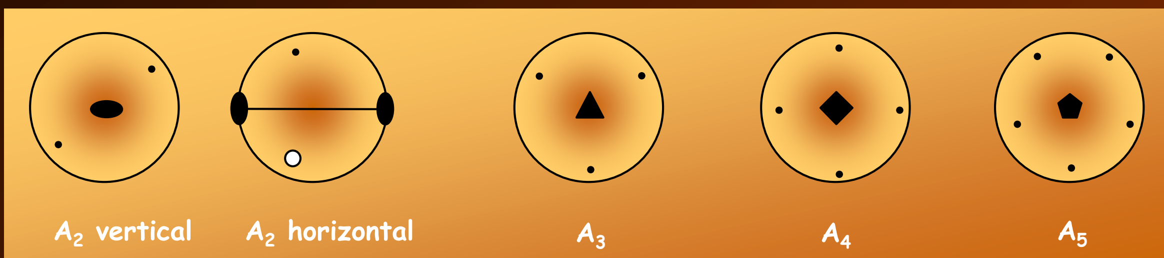


- Conform transformation (preserves angles locally) but **not affine**

Main symmetry operations

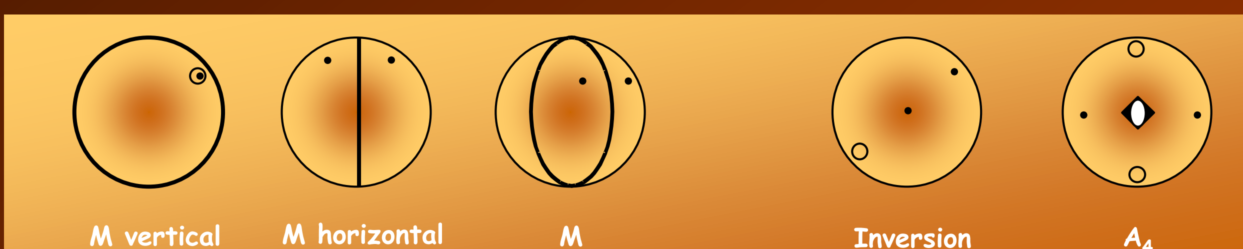
- Conventionally
  - Rotations (A_n)
  - Reflections (M)
  - Inversion (C)
  - Rotoinversion ($\bar{A}_n$)

- Direct
  - n-fold rotation A_n ($2\pi/n$)
  - Represented by a polygon of same symmetry.



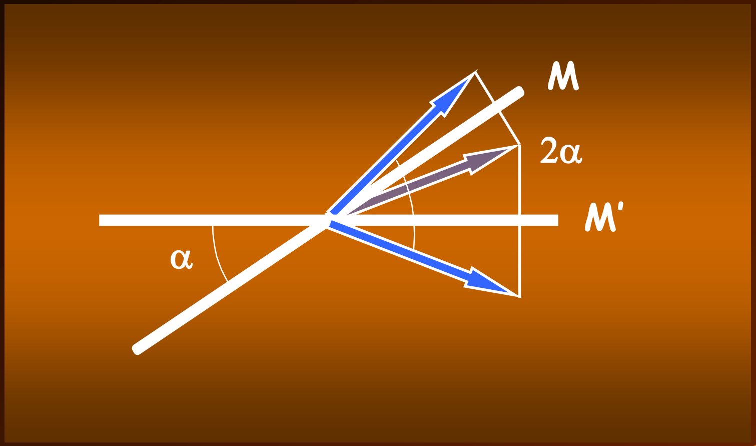
- Indirect
  - Rotoreflections ($\tilde{A}_n$)
  - Reflection (M)
  - Inversion (C)
  - Rotoinversions ($\bar{A}_n$)

- Symmetry element
  - Locus of invariant points



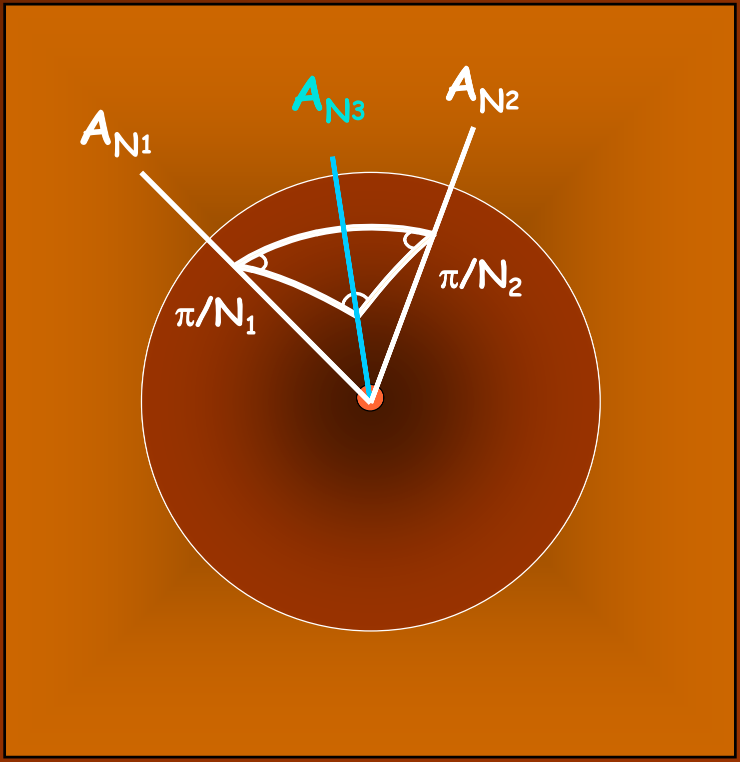
Composition of symmetries

- Two reflections with angle α = rotation 2α



$$M'M = A$$

- Euler construction



Composition of two rotations = rotation

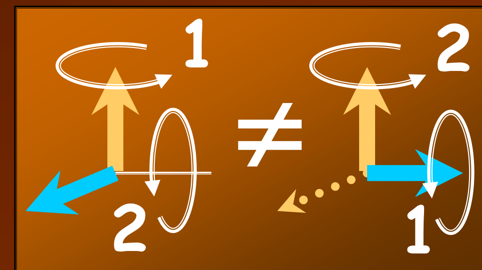
$$A_{N2}A_{N1} = A_{N3}$$

- No relation between N_1, N_2 et N_3

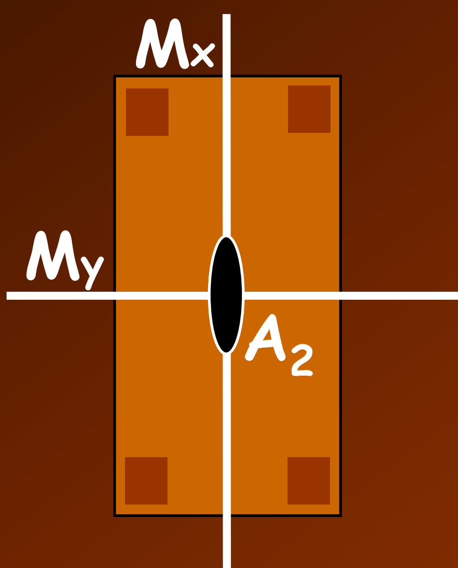
Point group: definition

- The set of symmetries of an object forms a group G : point group

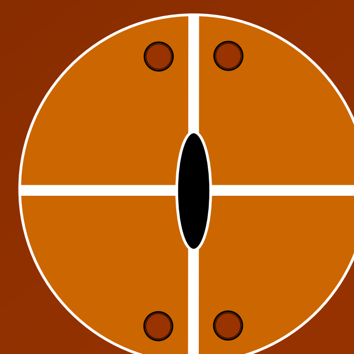
  - A and B $\subset$ G, AB $\subset$ G (closure)
  - Associativity (AB)C=A(BC)
  - Identity element E (1-fold rotation)
  - Invertibility A, A^{-1}
  - No commutativity in general (rotation 3D)



- Example: point group of a rectangular table (2mm)



*	E	Mx	My	A2
E	E	Mx	My	A2
Mx	Mx	E	A2	My
My	My	A2	E	Mx
A2	A2	My	Mx	E

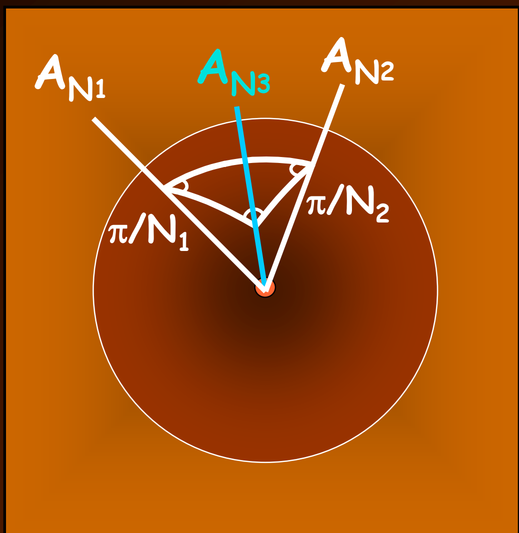


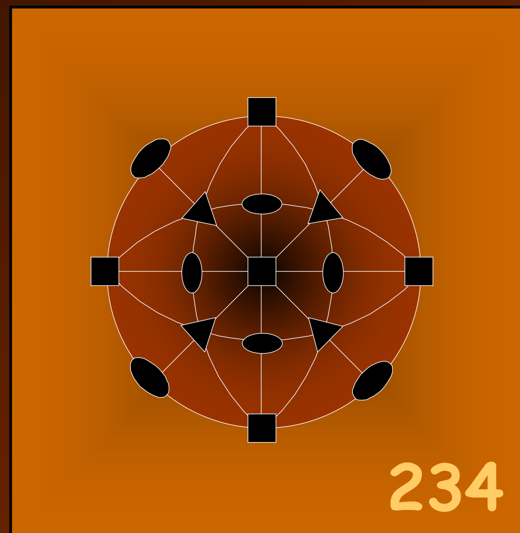
2mm

- Multiplicity: number of elements

Composition of rotations

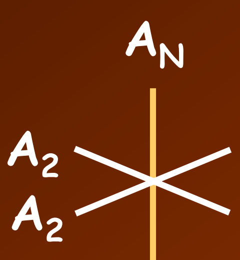
Constraints





Spherical triangle, angles verifies:

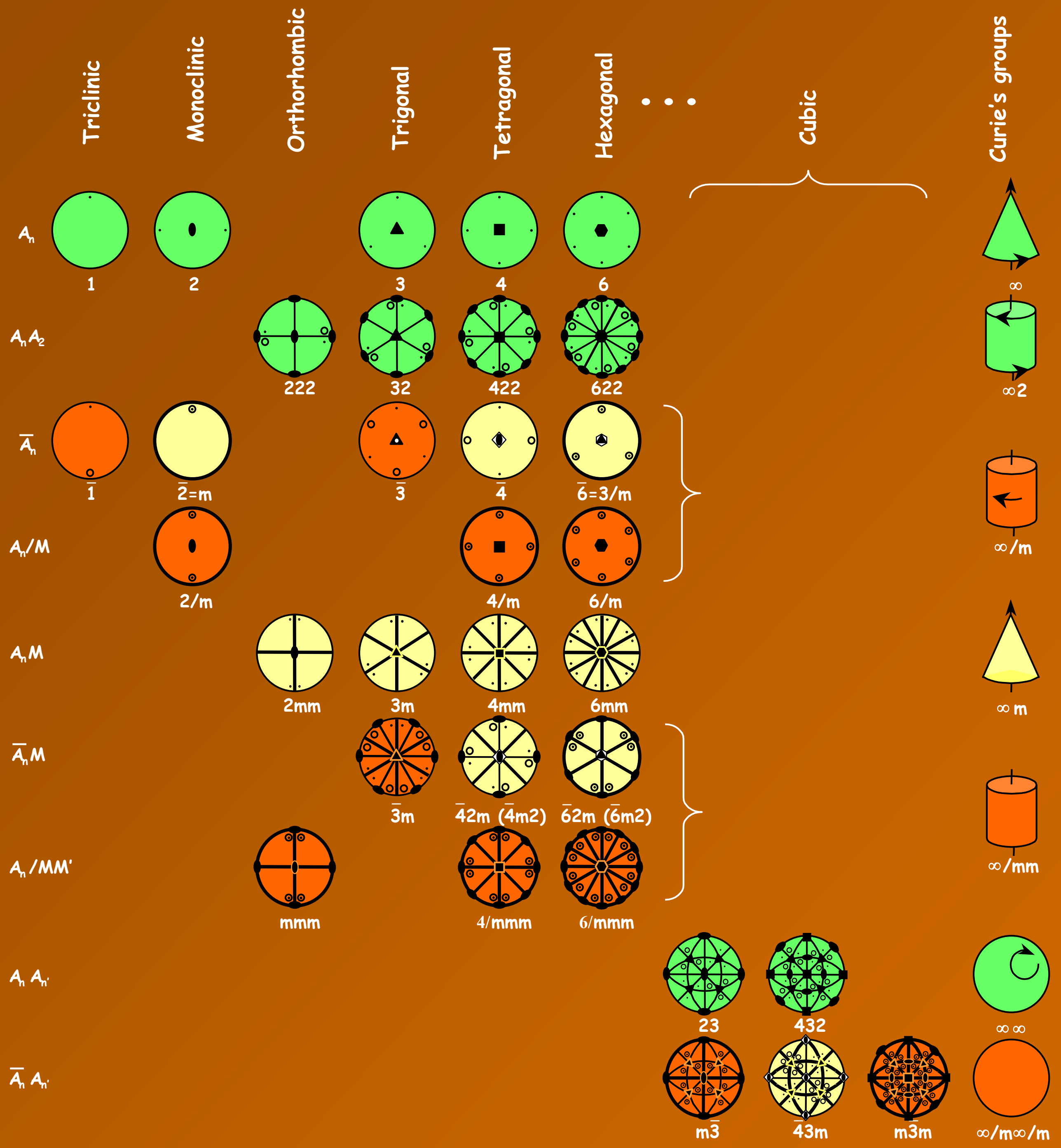
$$\frac{\pi}{N_1}+\frac{\pi}{N_2}+\frac{\pi}{N_3}>\pi \qquad \frac{1}{N_1}+\frac{1}{N_2}+\frac{1}{N_3}>1$$



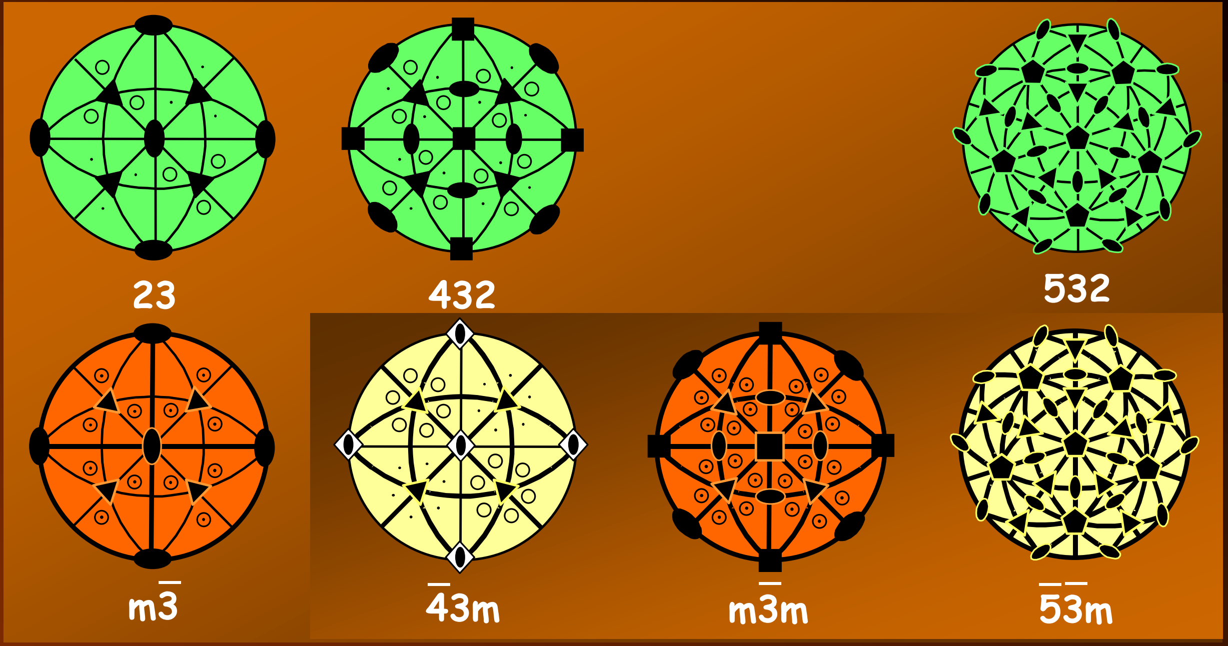
22N (N>2), 233, 234, 235

Dihedral groups — Multiaxial groups

Points groups



- Sorted by Symmetry degree
- Curie's limiting groups
- Chiral, propers
- Impropers
- Centrosymmetric



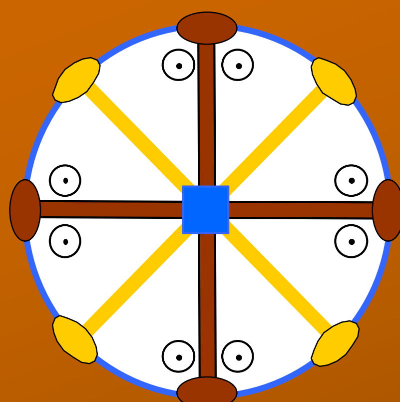
Multiaxial groups

Platonic solid

Points group: Notations

- Hermann-Mauguin (International notation - 1935)
  - Generators (not minimum)
  - Symmetry directions
  - Reflection (-): defined by the normal to the plane

Primary Direction: higher-order symmetry



Secondary directions : lower-order

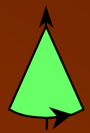
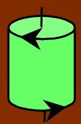
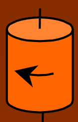
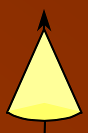
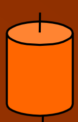
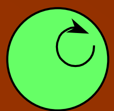
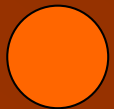
$$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$$

Notation réduite $\frac{4}{m}mm$

Tertiary directions : lowest-order

- Schönflies : C_n, D_n, D_{nh} (D_{4h})

The 7 limiting point groups (Curie's Groups)

	∞	Rotating cone	Axial + polar vector (SO(2))
	$\infty 2$	Twisted cylinder	Axial tensor (optical gyration)
	∞/m	Rotating cylinder	Axial vector (H)
	∞m	Cone	Polar vector (E, F) (O(2))
	∞/mm	Cylinder	Polar tensor (Compressive stress)
	$\infty\infty$	Rotating sphere	Axial scalar (chirality) (SO(3))
	$\infty/m\infty/m$	Sphere	Polar scalar (pressure, mass) (O(3))

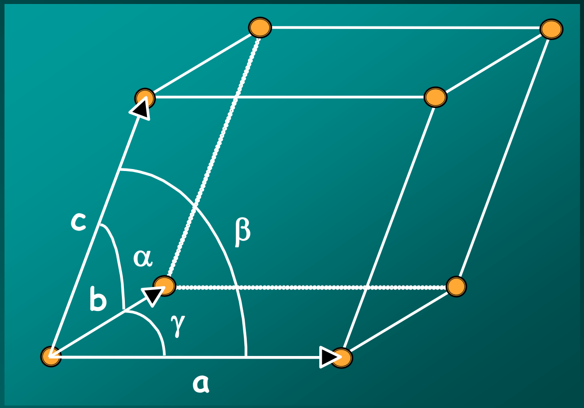
Symmetry of position: periodic order

• Lattice :

• Set of points (nodes):

$R_{uvw} = u\,a + v\,b + w\,c$

(a, b, c) basis, (u, v, w) integers.

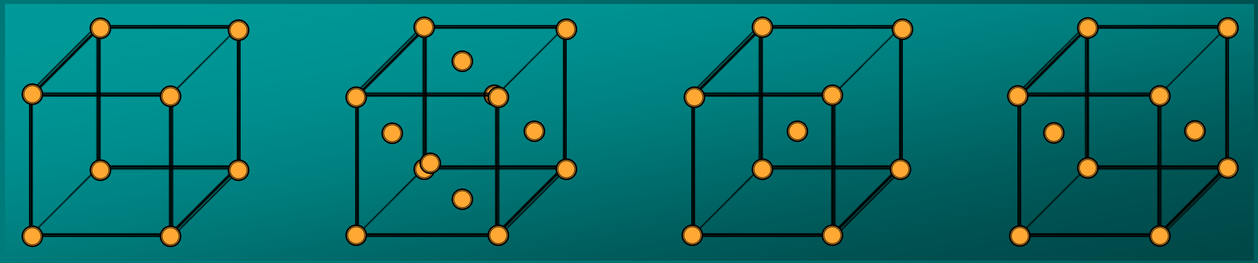


• Unit cell :

• Volume with no gaps or overlaps, g[al] parallelepipedic (a,b,c)

• Primitive (one node), multiple (symmetry) : elementary (unit cell)

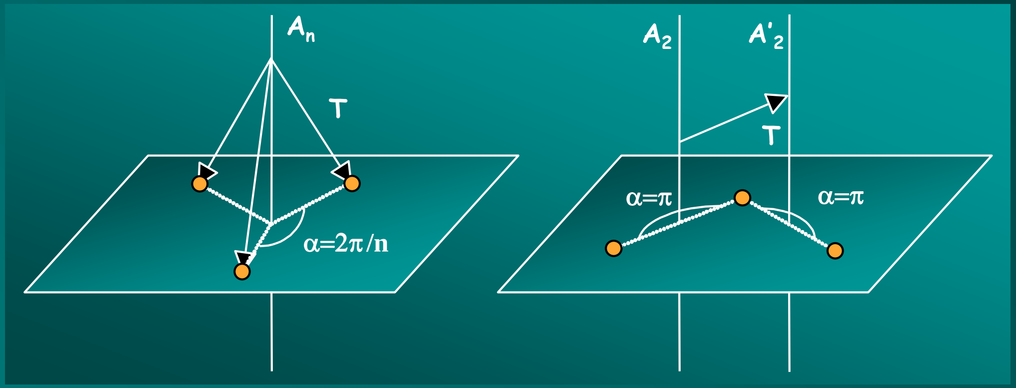
• Conventionnal unit cells :



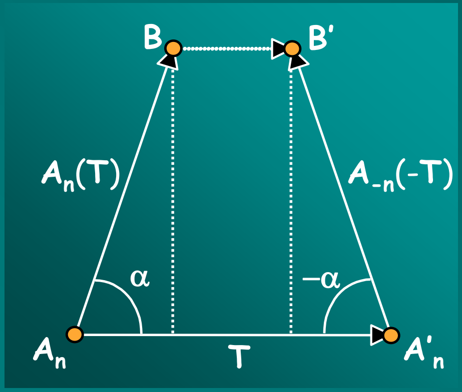
P : Primitive F : Face-centred I : Body-centred A,B,C : Base-centred

Point symmetry of lattices

- **Only 1-, 2-, 3- 4-, 6-fold symmetries are compatible with periodicity**
  - Every symmetry axe A_n is normal to a lattice plane



- Symmetry of this plane A_n



- BB' lattice vector
- $BB' = T - 2T\cos\alpha = mT$

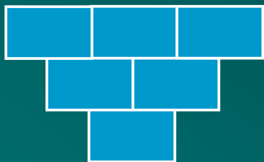
$\cos\alpha = p/2$

p	cos α	α	n=2π/α	BB'
-2	-1	π	2	3T
-1	-0.5	2π/3	3	2T
0	0	π/2	4	T
1	0.5	π/3	6	0
2	1	0	1	0

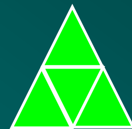
• Tilings

• No gaps or overlaps

Only symmetry **compatible** with translation : 1, 2, 3, 4, 6

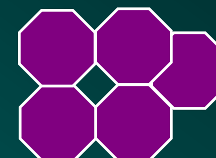


2

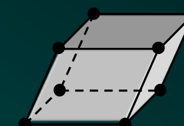


3

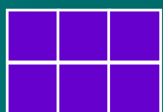
5



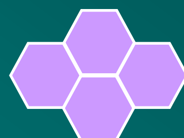
8



1

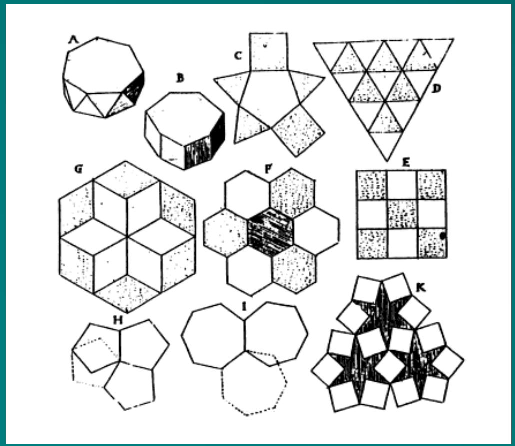


4

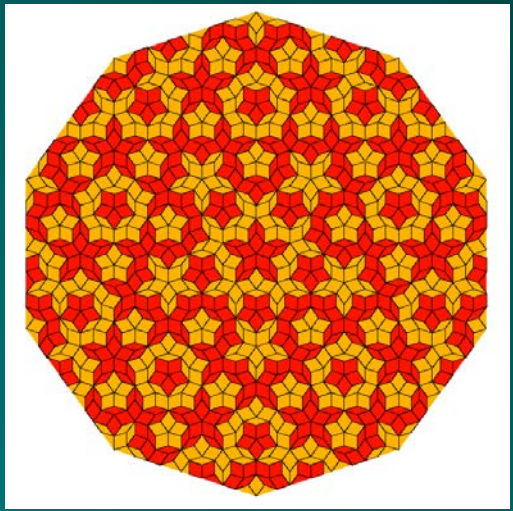


6

• Kepler (1571-1630) in 1619 : « Harmonices Mundi »



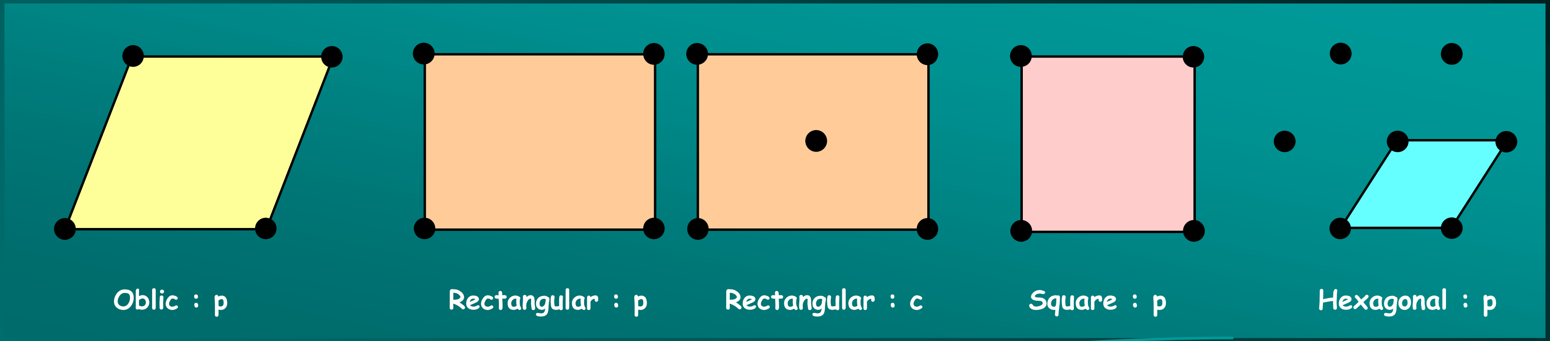
Towards Penrose tilling



2D lattices

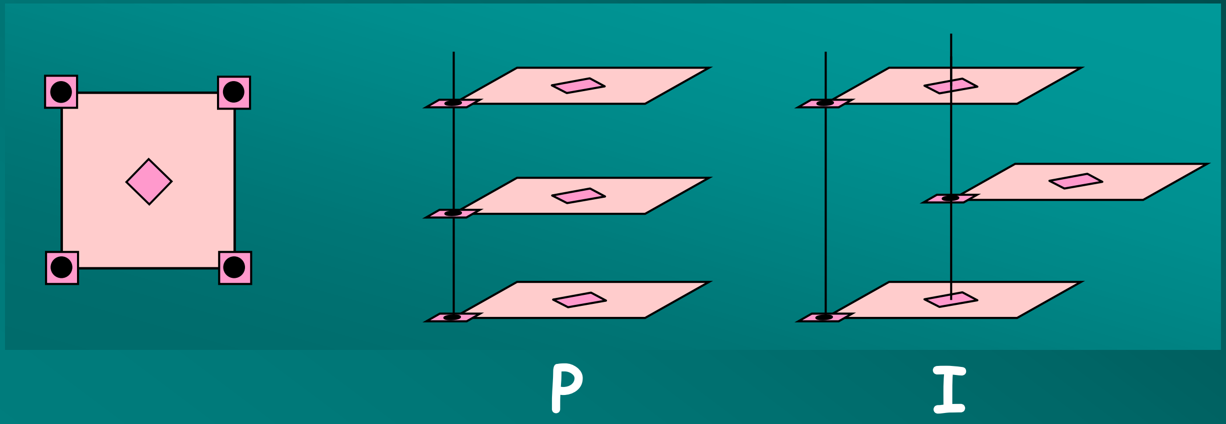
•In 2D

- 4 systems (systems)
- 5 latttice modes

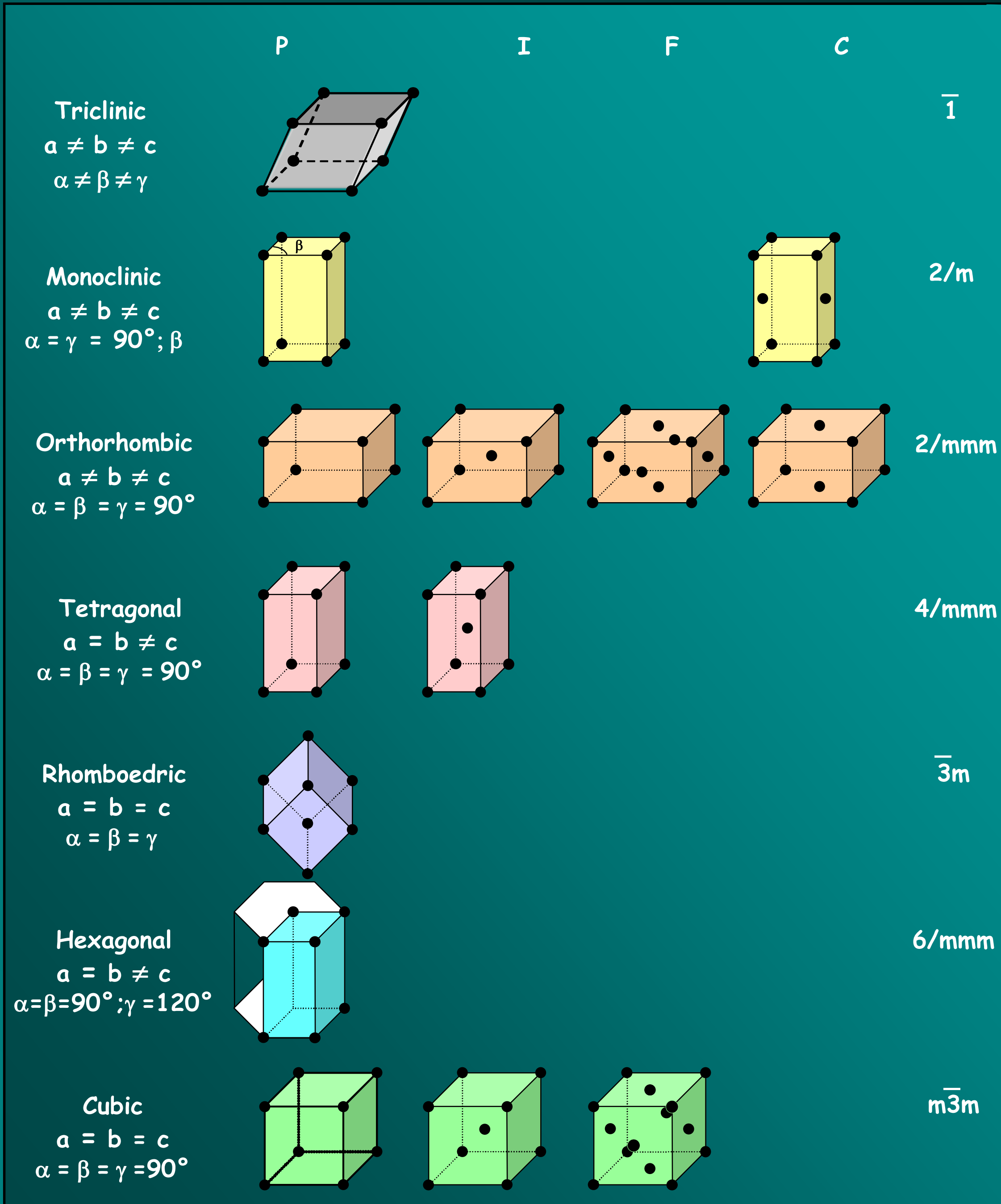


•In 3D

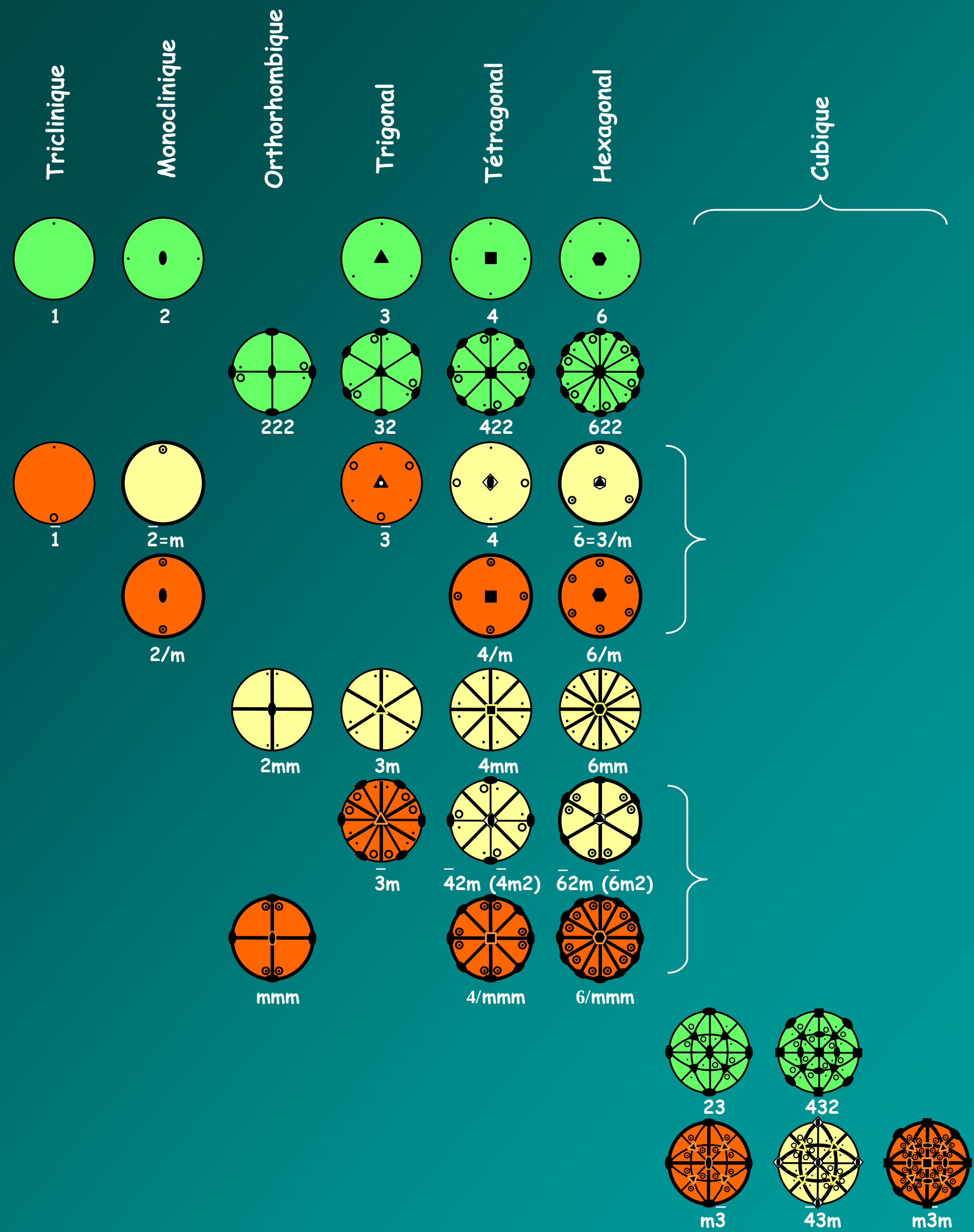
- Stacking of 2D lattices preserving symmetry (Ex. square)



Bravais lattices



- **In 3D**
  - 7 systems (symmetry)
  - 14 lattice modes



32 crystal classes

- Crystallographic point groups

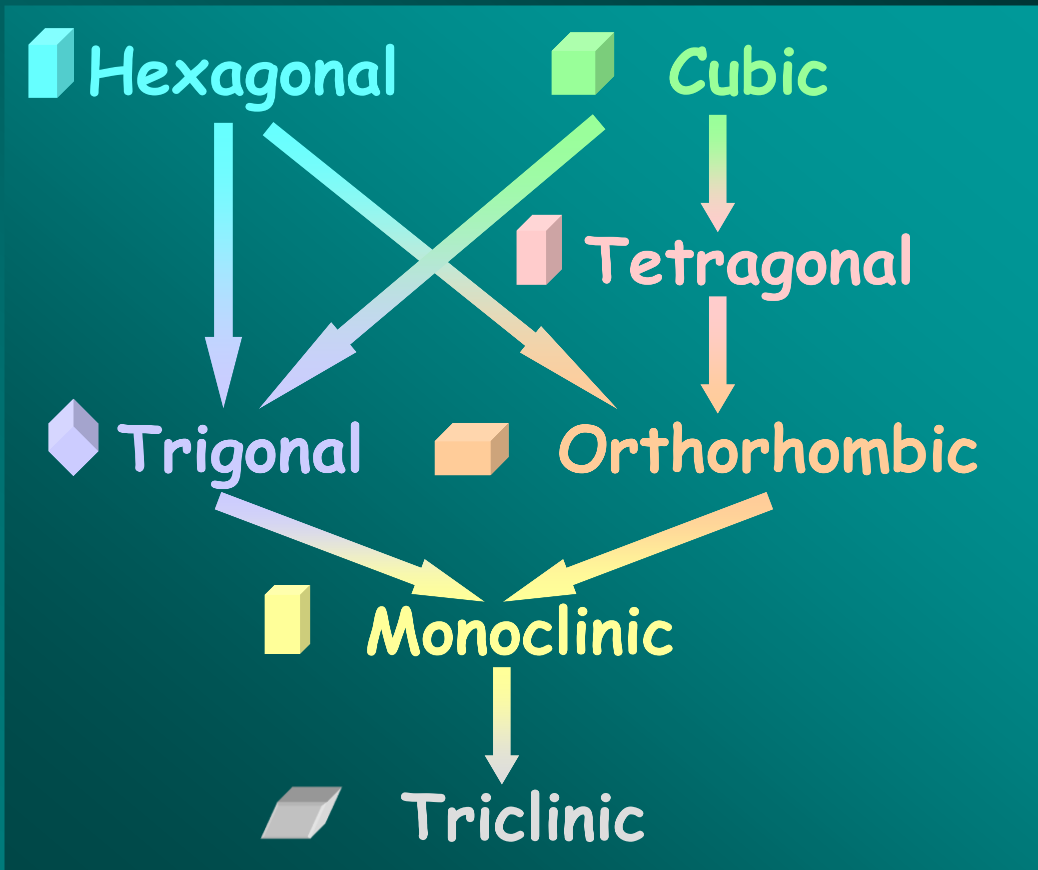
- 7 crystal systems

- Holohedral : with the lattice symmetry Ex : Tétragonal (4/mmm)

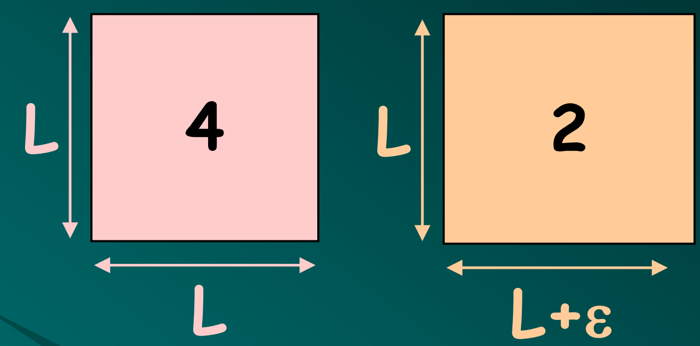
... hemihedral, tetarto-hedral

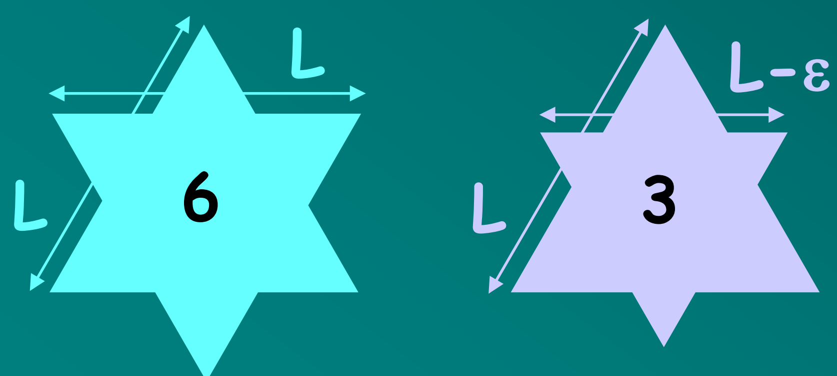
Chiral groups (Direct sym)
Centrosym groups (Laue class)
Improper groups (ind sym.- inv)

Relations between the 7 systems

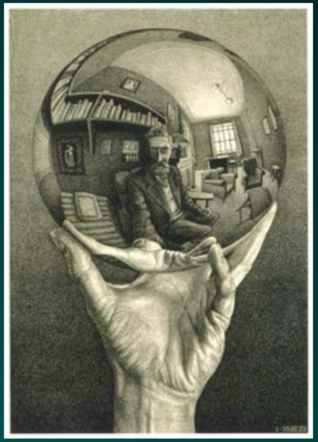


- Group/subgroup
  - Symmetry breaking
  - Phase transitions





Space groups

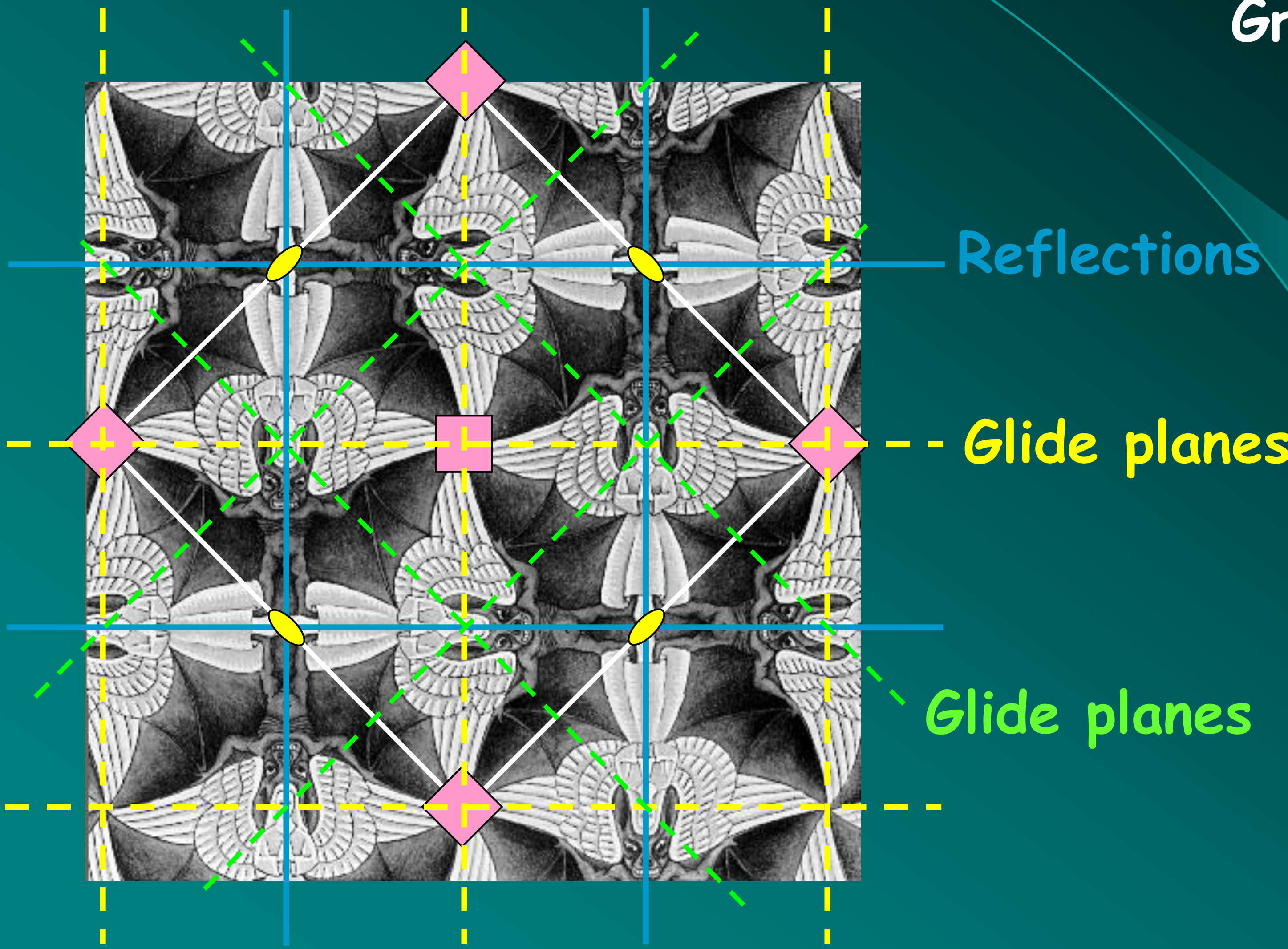


- Mauritz Cornelis Escher
  - Dutch graphic artist (1898-1972)

Groupe P4 (chiral)

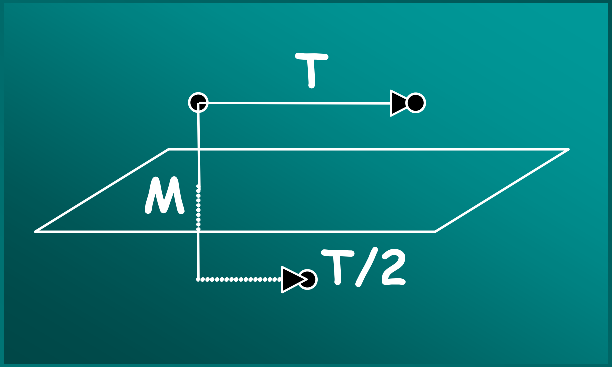
New symmetries

Groupe P4gm



New symmetries 3D

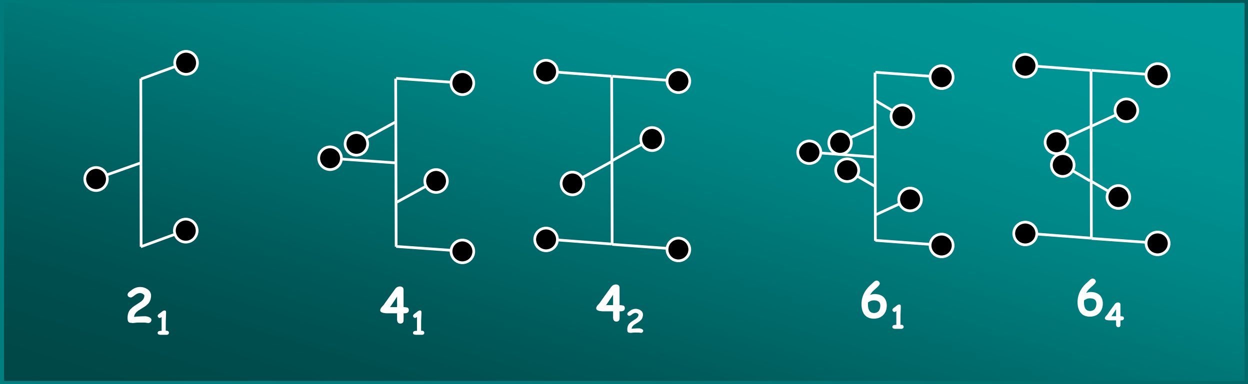
- **Glide plane (M,t)**
  - After two reflections M, periodicity T
  - t=T/2



- Notation :
  a, b, c, n, d, g

- **Combination (O, t)**
  O : Rotation, Reflection
  T : translation

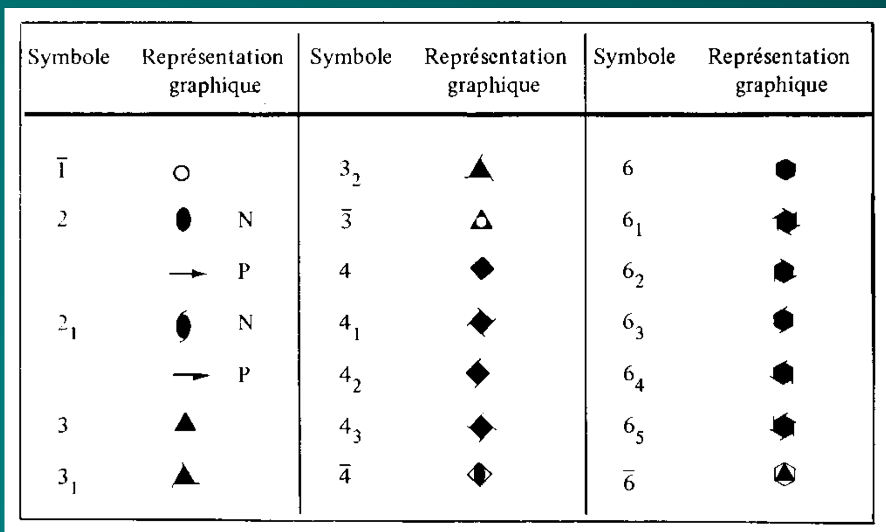
- **Screw axis (A_N, t)**
  - After N translations t periodicity: mc
  - t = mc/N



- Notation :
  N_m
  (A_N, mc/N)

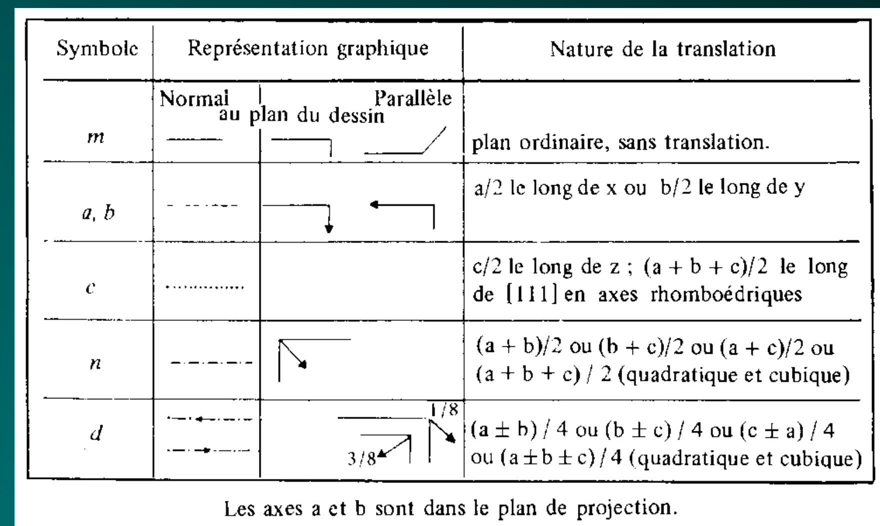
Symmetry operations

- Rotations
- Roto-reflections
- Screw axis



Symbole	Représentation graphique	Symbole	Représentation graphique	Symbole	Représentation graphique
$\bar{1}$		3_2		6	
2	N	$\bar{3}$		6_1	
	P	4		6_2	
2_1	N	4_1		6_3	
	P	4_2		6_4	
3		4_3		6_5	
3_1		$\bar{4}$		$\bar{6}$	

- Reflection
- Glide plane



Symbole	Représentation graphique (Normal / Parallèle au plan du dessin)	Nature de la translation
m		plan ordinaire, sans translation.
a, *b*		a/2 le long de x ou b/2 le long de y
c		c/2 le long de z ; (a + b + c)/2 le long de [111] en axes rhomboédriques
n		(a + b)/2 ou (b + c)/2 ou (a + c)/2 ou (a + b + c) / 2 (quadratique et cubique)
d	1/8, 3/8	(a ± b) / 4 ou (b ± c) / 4 ou (c ± a) / 4 ou (a ± b ± c) / 4 (quadratique et cubique)

Les axes a et b sont dans le plan de projection.

Space groups

- 230 space groups
  - 7 crystalline systems
- Notations
  - Directions (primary, etc.)
  - Lattice mode
  - Generators

Tetragonal
Body centered

$$I4_1/amd$$

- Point Group
  - Without translation

$$\frac{4}{m}mm$$

Symmetry

• Linear Symmetry

• Rotations
• Roto-reflections

• Conventionnally

• Rotations (A_n)
• Reflections (M)
• Inversion (C)
• Roto-inversions ($\bar{A}_n$)

• Symmetry of position

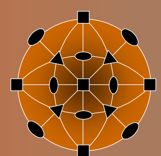
• Translations
• T= u a + v b + w c

• Symmetry allowed
• 1, 2, 3, 4, 6 ($\bar{3}$, $\bar{4}$, $\bar{6}$)
• M, C

• 14 Bravais lattices

• Translations
• Rotations
• Roto-reflections
+
• Screw axis
• Glide plane

Point groups



32 Crystal classes

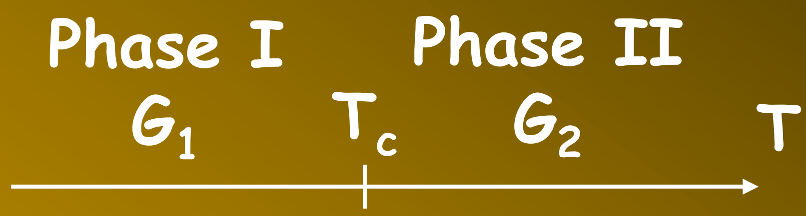
230 Space group

(7 systems)

• 7 Curie

• 7 crystal systems

Phase Transitions

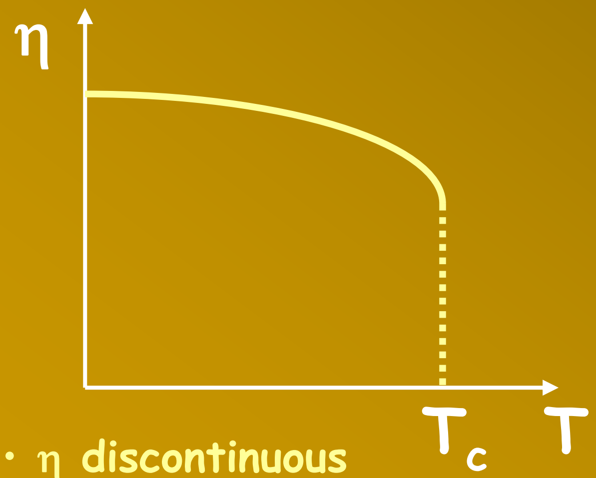


·Landau theory :

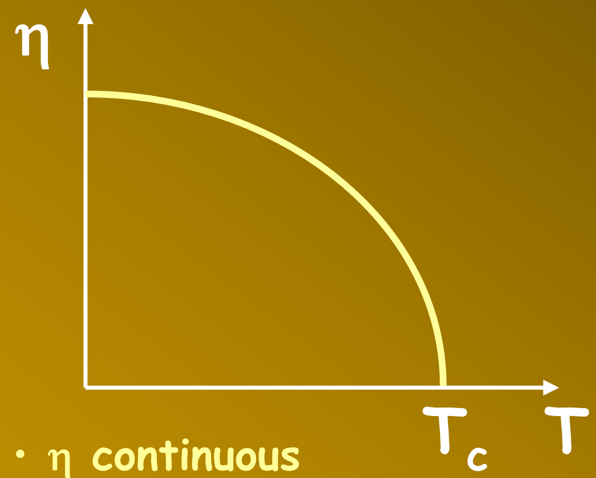
- G_1 and G_2 have no relation group/sub-group : 1st order transition (sulfur $\alpha \leftrightarrow$ sulfur β)

- G_1 sub-group of G_2 ($G_1 \subset G_2$)

An order parameter η can be defined, zero in the symmetrical phase



- η discontinuous
- 1st order transition
- Hysteresis, latent heat



- η continuous
- 2nd order transition
- Coexistence at critical point

$BaTiO_3$

Order parameter:
polarization

• Ferroelectric

- Perovskite ABO_3

- T > 120 °C, Cubic $Pm\bar{3}m$, paraelectric
- 0°C < T < 120 °C, Tetragonal $P4mm$, ferroelectric
  $P4mm \subset Pm\bar{3}m$, 1st order transition (domains).
- -90°C < T < 0 °C, Orthorhombic $Cmm2$
  $Cmm2 \not\subset P4mm$, 1st order transition .
- T < -90 °C, Rhombohedral $R3m$
  $R3m \not\subset Cmm2$, 1st order transition .

Ba^{2+}, Ti^{4+}, O^{2-}