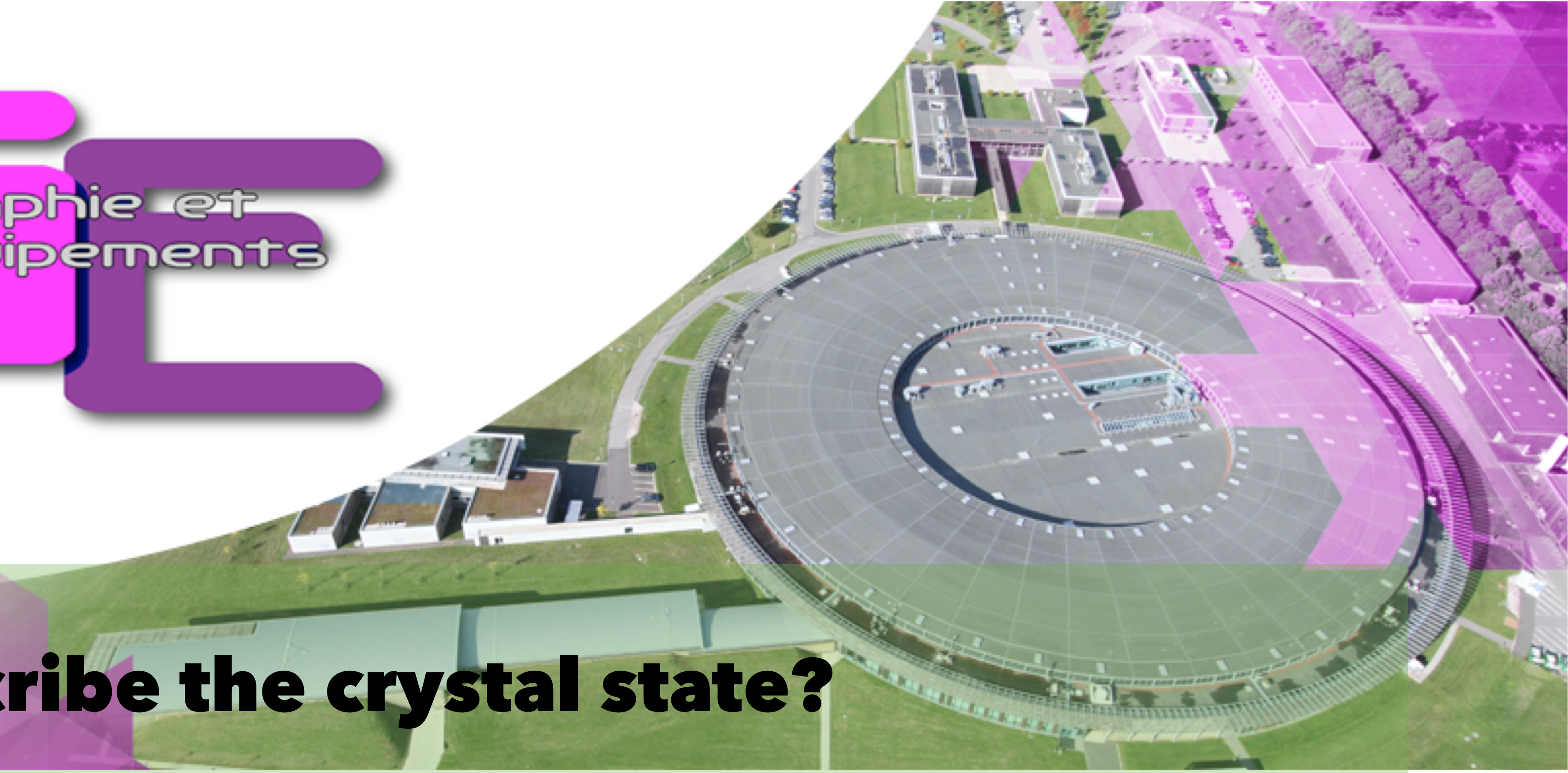
CGE
Cristallographie et Grands Equipements

School of Crystallography 2024



How to describe the crystal state?

Geometric Crystallography, & symmetries

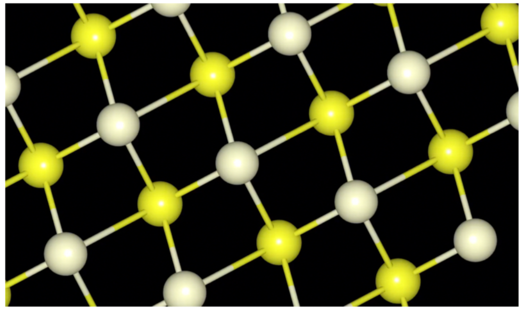
Delphine Cabaret, IMPMC

delphine.cabaret@sorbonne-universite.fr

SCIENCES SORBONNE UNIVERSITÉ

Introduction: what is a crystal?

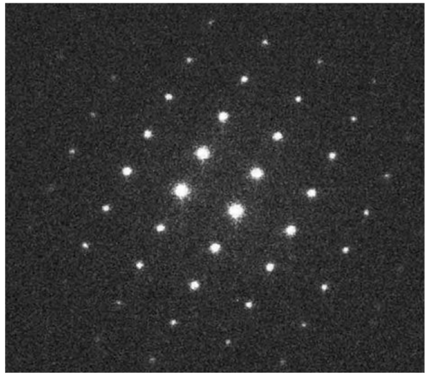
A crystal is a solid composed of atoms arranged in a motif (or a *pattern*) that is periodic in 3 dimensions.



Since 1992 (IUCR) :

« A material is a crystal if it has ***essentially a sharp diffraction pattern »***

➔ All solids with long range order
(translation symmetry in spaces of **dimension ≥ 3**)



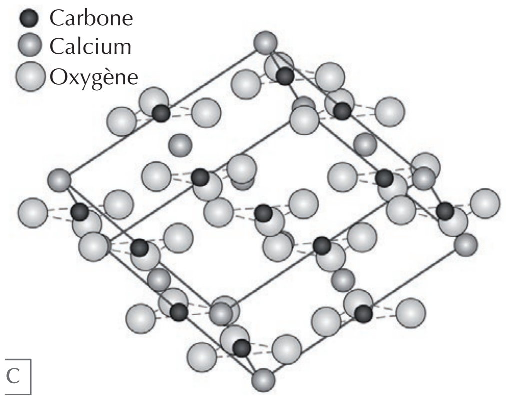
Nature Materials 10, 890–896 (2011)

cf. article de B. Toudic, Reflets de la Physique 2015, vol 44-45

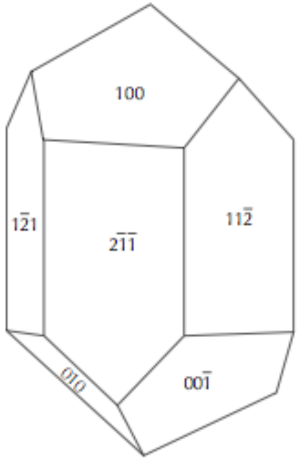
Introduction: the periodic crystals

translation symmetry

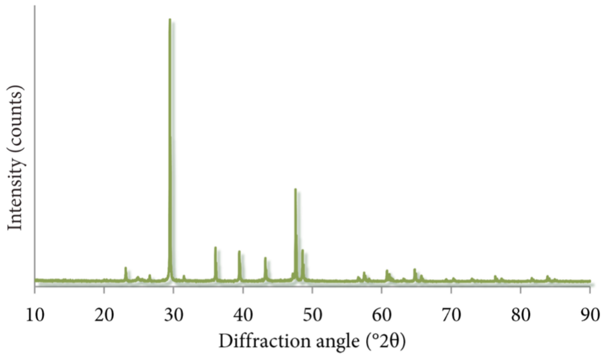
ex: $CaCO_3$ (calcite)

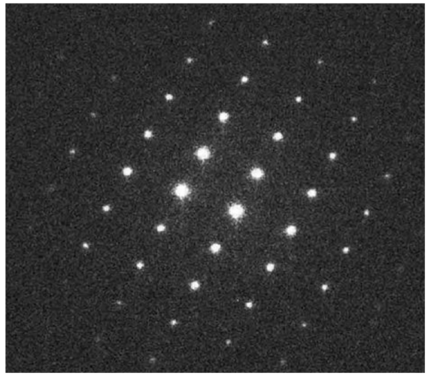


B. Toudic, Reflets de la Physique 2015, vol 44-45



law of rational indices





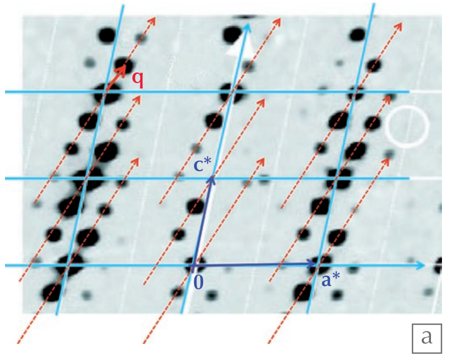
Nature Materials 10, 890–896 (2011)

Introduction: aperiodic crystals

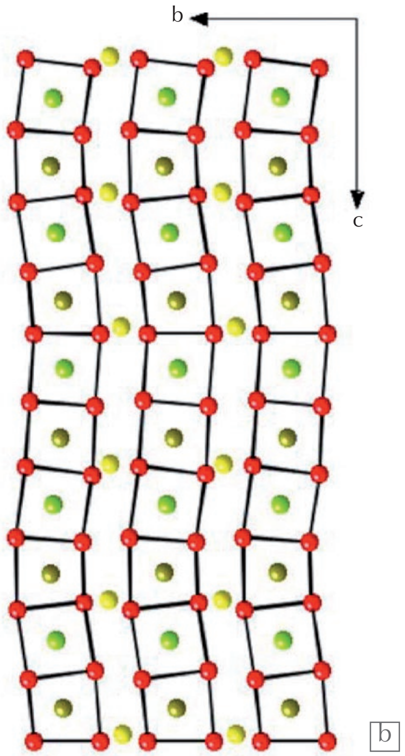
No translation symmetry in the **3D space**

incommensurate crystals, modulated phases

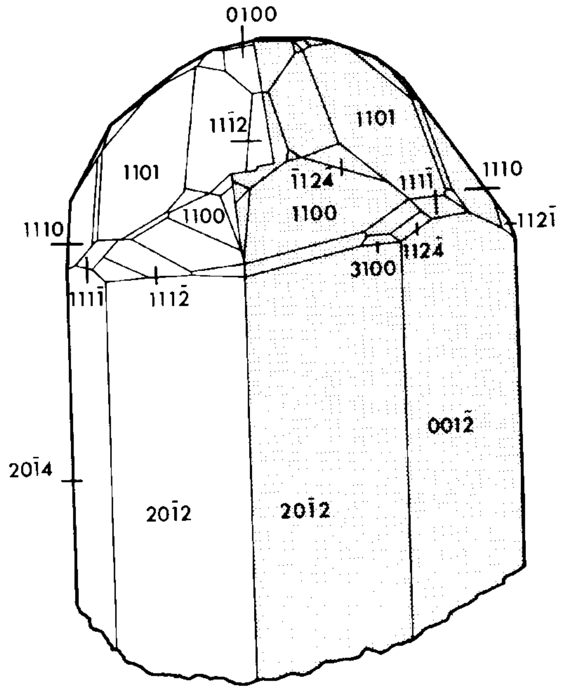
Periodicity (order at infinite) cannot be described in a 3D space



3. Structure incommensurable modulée du carbonate de sodium γ-Na_2CO_3.
(a) Plan de diffraction (a^*, c^*) du réseau réciproque de γ-Na_2CO_3. Il est constitué de pics de Bragg, preuve d'un ordre à grande distance, mais requiert pour son indexation complète un vecteur de base complémentaire, $\mathbf{q} = \alpha\, \mathbf{a}^* + \gamma\, \mathbf{c}^*$. On observe les pics de Bragg du réseau périodique moyen (aux sommets des parallélogrammes bleus), et les pics satellites alignés le long des flèches rouges (parallèles à **q**).
(b) La solution structurale modulée, projetée selon **a** (atomes d'oxygène en rouge, atomes de sodium en jaune et vert, les atomes de carbone sont omis). Une onde statique de déplacements transversaux (parallèles à **b**) apparaît dans la direction **c**. La longueur d'onde de la modulation est $2\pi/q$.



B. Toudic, Reflets de la Physique 2015, vol 44-45



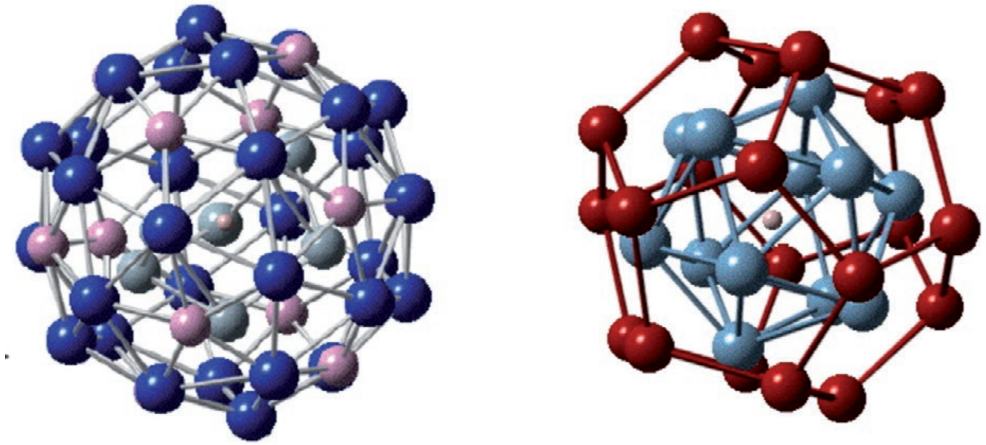
calaverite $Au_{1-x}Ag_xTe$

Introduction: aperiodic crystals

No translation symmetry in the **3D space**

quasicrystals (1982, Nobel prize in chemistry in 2011)

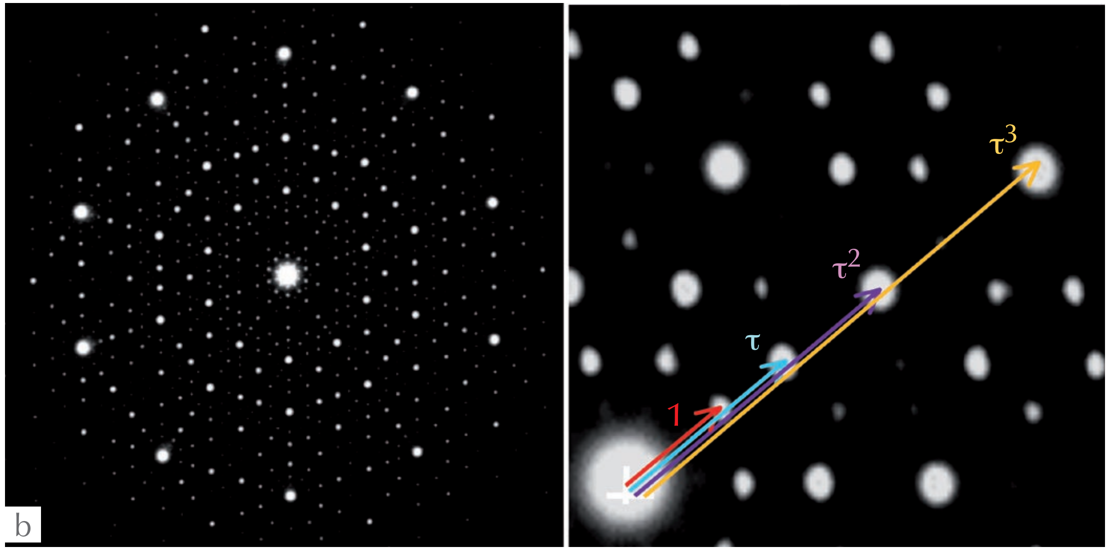
ex : alloy AlPdMn



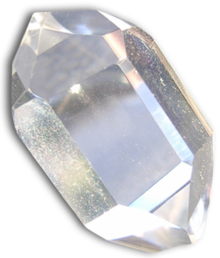
9. Amas atomiques dont est constitué principalement un alliage quasicristallin de type AlMnPd. À gauche, amas de type Mackay (51 atomes) ; à droite, amas de type Bergman (33 atomes).

B. Toudic, Reflets de la Physique 2015, vol 44-45

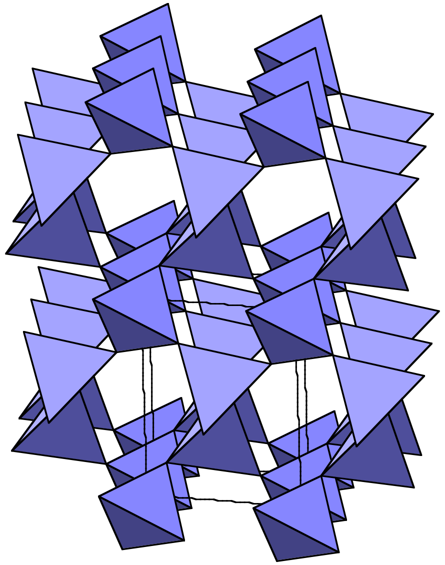
$$\tau = 2\cos(2\pi/10)$$

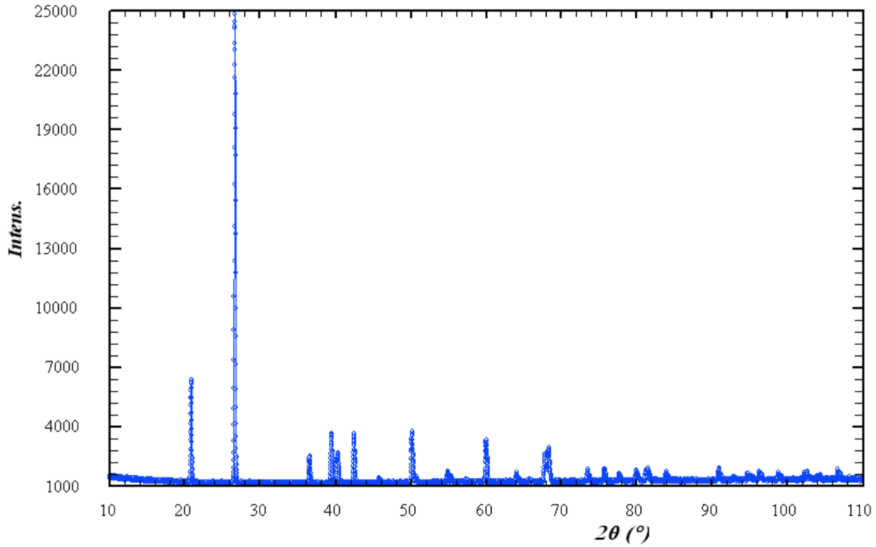


Introduction: what is a crystal?

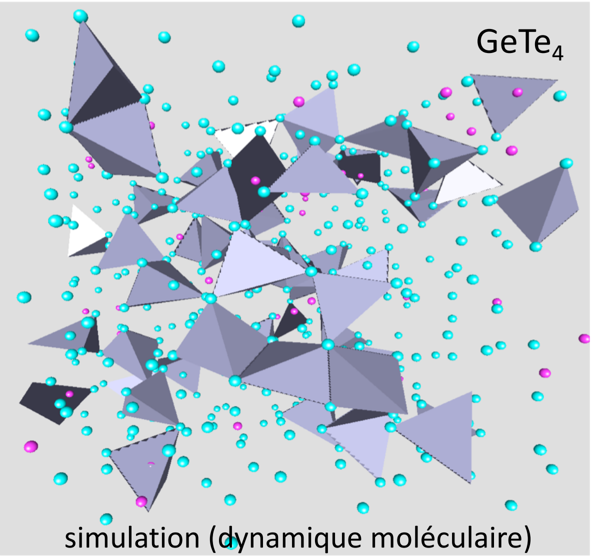


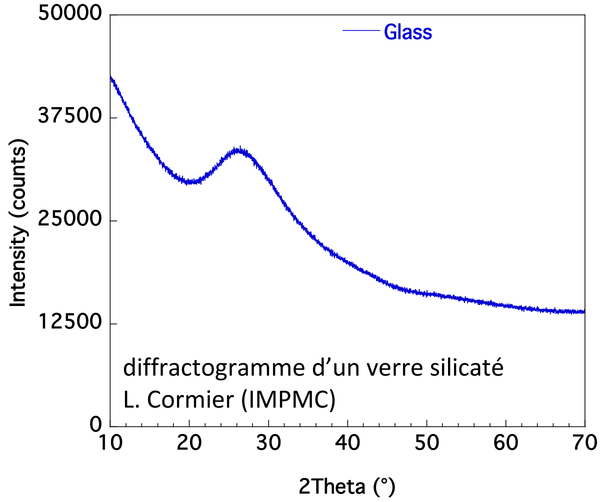
quartz





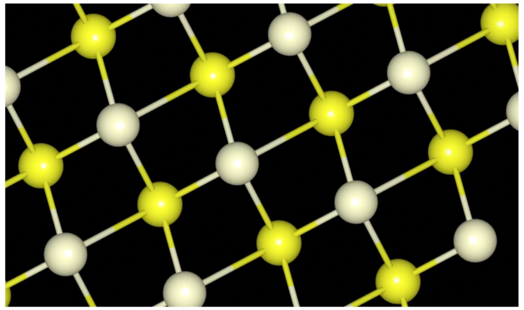
crystal ≠ glass





Introduction: what is a crystal?

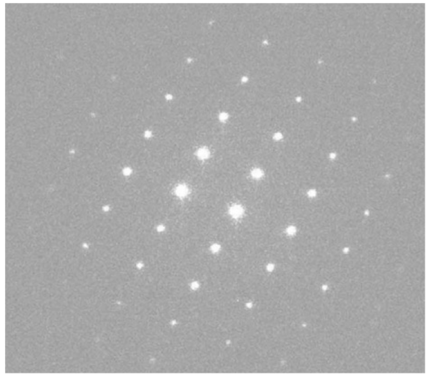
A crystal is a solid composed of atoms arranged in a motif (or a *pattern*) that is periodic in 3 dimensions.



Since 1992 (IUCR) :

« A material is a crystal if it has ***essentially a sharp diffraction pattern*** *»*

➔ All solids with long range order
(translation symmetry in spaces of **dimension ≥ 3**)



Nature Materials 10, 890–896 (2011)

cf. article de B. Toudic, Reflets de la Physique 2015, vol 44-45

Objectives: *what you should know at the end of the course*

example 1

Inorganic Chemistry
Article
pubs.acs.org/IC

Crystal Structures of $Li_6B_4O_9$ and $Li_3B_{11}O_{18}$ and Application of the Dimensional Reduction Formalism to Lithium Borates

Gwenaëlle Rousse,*,†,‡ Benoît Baptiste,† and Gérald Lelong*,†

†Institut de Minéralogie, de Physique des Matériaux, et de Cosmochimie (IMPMC), Sorbonne Universités-UPMC Univ Paris 06, UMR CNRS 7590, Muséum National d'Histoire Naturelle, IRD UMR 206, 4 Place Jussieu, F-75005 Paris, France

‡FRE 3677, Chimie du Solide et Energie, Collège de France, 11 Place Marcelin Berthelot, and Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, 75231 Paris Cedex 05, France

?

$Li_3B_{11}O_{18}$ crystallizes in the *P*2$_1$/*c* space group with lattice parameters *a* = 17.7607(8) Å, *b* = 7.7737(4) Å, *c* = 9.6731(4) Å, and *β* = 100.906(4)°. The lithium, boron, and oxygen atoms are distributed in the general 4*e* Wyckoff site (see Table 4 for the complete list of atomic positions). The

?

Objectives: *what you should know at the end of the course*

example 2

PHYSICAL REVIEW B **89**, 064305 (2014)

Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations

Lianhua He,[1] Fang Liu,[2] Geoffroy Hautier,[3,4] Micael J. T. Oliveira,[3,5] Miguel A. L. Marques,[3,6] Fernando D. Vila,[7] J. J. Rehr,[7] G.-M. Rignanese,[3,4] and Aihui Zhou[1]

The unit cell of α-quartz is trigonal (space group $P3_221$). It contains nine atoms: the Si atoms are located at $(u,0,0)$ on the $3a$ Wyckoff sites, while the O atoms are located at (x,y,z) on the $6c$ Wyckoff sites. Hence, four internal coordinates u, x, y, z are required, besides the two lattice constants a and c, in order to completely determine the structure. The theoretical value

α-quartz = α-SiO_2

Periclase = MgO

The space group of periclase is $Fm\bar{3}m$. The O atom occupies the $4a$ Wyckoff site $(0,0,0)$ and the Mg atom is located at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ occupying the $4b$ Wyckoff sites. In Table II,

Objectives: *what you should know at the end of the course*

example 3

PHYSICAL REVIEW B **78**, 195103 (2008)

X-ray linear dichroism in cubic compounds: The case of Cr^{3+} in $MgAl_2O_4$

Amélie Juhin,[1,*] Christian Brouder,[1] Marie-Anne Arrio,[1] Delphine Cabaret,[1] Philippe Sainctavit,[1] Etienne Balan,[1,2] Amélie Bordage,[1] Ari P. Seitsonen,[1] Georges Calas,[1] Sigrid G. Eeckhout,[3] and Pieter Glatzel[3]

mechanical properties.[13] In $MgAl_2O_4$ spinel ($Fd\bar{3}m$ space-group symmetry), Al^{3+} cations occur at octahedral sites, which exhibit D_{3d} (or $\bar{3}m$) symmetry and build chains aligned along the six twofold axis of the cubic structure.[14]

The number of equivalent octahedral sites in the unit cell is four, denoted hereafter as sites A, B, C, and D, depending on their direction of distortion, either $[\bar{1}11]$, $[11\bar{1}]$, $[111]$, or $[1\bar{1}1]$, respectively (Fig. 1 and Table. I). During the Al to Cr

?

?

?

Objectives: *what you should know at the end of the course*

example 3

Extract of the space-group table of spinel

$Fd\bar{3}m$	O_h^7	$m\bar{3}m$	Cubic
No. 227	$F\ 4_1/d\ \bar{3}\ 2/m$		Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 2

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

Coordinates: $(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions: h,k,l permutable

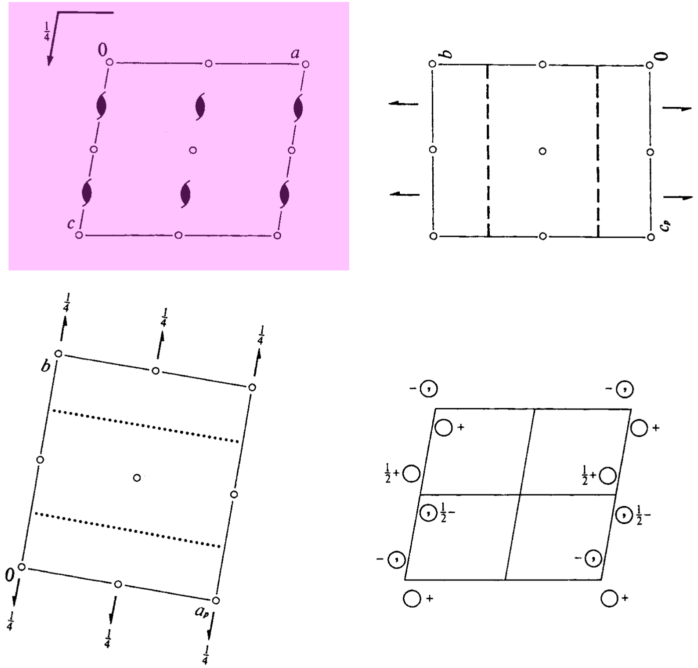
Multiplicity	Wyckoff letter	Site symmetry	Coordinates	Reflection conditions
192	i	1	(1) x,y,z (2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$ (3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$ (4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$ (5) z,x,y (6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$ (7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$ (8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$ (9) y,z,x (10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$ (11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$ (12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$ (13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$ (14) $\bar{y},\bar{x},\bar{z}$ (15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$ (16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$ (17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$ (19) $\bar{x},\bar{z},\bar{y}$ (20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$ (21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$ (22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$ (23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$ (24) $\bar{z},\bar{y},\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$ (27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$ (28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$ (29) $\bar{z},\bar{x},\bar{y}$ (30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$ (31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$ (32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$ (33) $\bar{y},\bar{z},\bar{x}$ (34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$ (35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$ (36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$ (37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$ (38) y,x,z (39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$ (40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$ (41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$ (42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$ (43) x,z,y (44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$ (45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$ (46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$ (47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$ (48) z,y,x	General: hkl : $h+k=2n$ and $h+l,k+l=2n$ $0kl$: $k+l=4n$ and $k,l=2n$ hhl : $h+l=2n$ $h00$: $h=4n$
				Special: as above, plus
96	h	..2	$0,y,\bar{y}$ $\frac{3}{4},\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2}$ $\frac{1}{4},y+\frac{1}{2},y+\frac{3}{4}$ $\frac{1}{2},\bar{y}+\frac{3}{4},y+\frac{1}{4}$ $\bar{y},0,y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{4}$ $y+\frac{3}{4},\frac{1}{4},y+\frac{1}{2}$ $y+\frac{1}{4},\frac{1}{2},\bar{y}+\frac{3}{4}$ $y,\bar{y},0$ $\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y+\frac{1}{2},y+\frac{3}{4},\frac{1}{4}$ $\bar{y}+\frac{3}{4},y+\frac{1}{4},\frac{1}{2}$ $0,\bar{y},y$ $\frac{1}{4},y+\frac{3}{4},y+\frac{1}{2}$ $\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4}$ $\frac{1}{2},y+\frac{1}{4},\bar{y}+\frac{3}{4}$ $y,0,\bar{y}$ $y+\frac{1}{2},\frac{1}{4},y+\frac{3}{4}$ $\bar{y}+\frac{1}{4},\frac{3}{4},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{3}{4},\frac{1}{2},y+\frac{1}{4}$ $\bar{y},y,0$ $y+\frac{3}{4},y+\frac{1}{2},\frac{1}{4}$ $\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{4}$ $y+\frac{1}{4},\bar{y}+\frac{3}{4},\frac{1}{2}$	no extra conditions
96	g	..m	x,x,z $\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{2}$ $\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{z}+\frac{3}{4}$ $x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4}$ z,x,x $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$ $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$ $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$ x,z,x $\bar{x}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$ $x+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$ $\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$ $x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$ $\bar{x},\bar{x},\bar{z}$ $x+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$ $\bar{x}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$ $x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$ $\bar{x},\bar{z},\bar{x}$ $x+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$ $z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$ $z+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$ $\bar{z}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$ $\bar{z},\bar{x},\bar{x}$	no extra conditions
48	f	2.mm	$x,\frac{1}{8},\frac{1}{8}$ $\bar{x}+\frac{3}{4},\frac{1}{8},\frac{5}{8}$ $\frac{1}{8},x,\frac{1}{8}$ $\frac{5}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},x$ $\frac{1}{8},\frac{5}{8},\bar{x}+\frac{3}{4}$ $\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$ $\frac{7}{8},\bar{x},\frac{7}{8}$ $x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$ $\bar{x}+\frac{1}{2},\frac{7}{8},\frac{3}{8}$ $\frac{7}{8},\frac{3}{8},\bar{x}+\frac{1}{2}$ $\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
32	e	.3m	x,x,x $\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$ $\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$ $x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$ $x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$ $\bar{x},\bar{x},\bar{x}$ $x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$ $\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	no extra conditions
16	d	$.\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},0$ $\frac{3}{4},0,\frac{1}{4}$ $0,\frac{1}{4},\frac{3}{4}$	hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$ (for d and c)
16	c	$.\bar{3}m$	$0,0,0$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$ $\frac{1}{4},\frac{1}{2},\frac{3}{4}$ $\frac{1}{2},\frac{3}{4},\frac{1}{4}$	
8	b	$\bar{4}3m$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$ $\frac{1}{8},\frac{5}{8},\frac{1}{8}$	hkl : $h=2n+1$ or $h+k+l=4n$ (for b and a)
8	a	$\bar{4}3m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{7}{8},\frac{3}{8},\frac{3}{8}$	

Objectives: *what you should know at the end of the course*

Space-group table of the Li-borate

$P2_1/c$	C_{2h}^5	$2/m$	Monoclinic
No. 14	$P1\,2_1/c\,1$		Patterson symmetry $P1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

CONTINUED No. 14 $P2_1/c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 14)

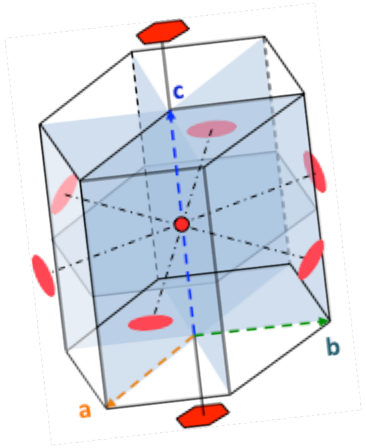
Minimal non-isomorphic supergroups

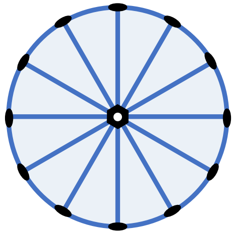
I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

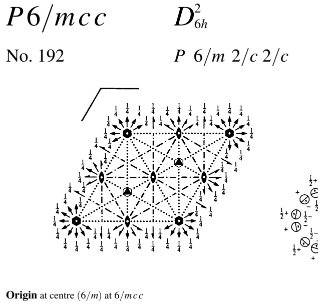
Course outline

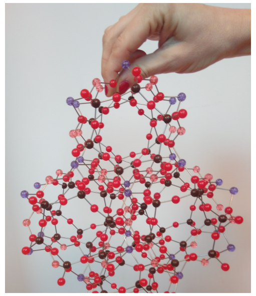
1- Symmetry observation in natural crystals
2- Internal cause of the natural crystal shape
3 – Crystal lattice, cell, motif
4 – Lattice direction and planes
5 – Reciprocal lattice
6 – Crystal lattice & symmetries
7 – Conventional cell (unit cell)
8 – Stereographic projection
9 – Roto-inversions
10 – The 32 crystallographic point groups
11 – The 7 crystal systems
12 – The 14 Bravais lattices
13 – The 230 space-groups





$\frac{6}{m}$mm





Plan du cours

1- Observation des symétries des cristaux naturels

2- Cause interne de la forme des cristaux naturels

3 - Réseau, maille, motif

4 – Rangées et plans réticulaires

5 – Réseau réciproque

6 - Réseau et symétries

7 - Maille conventionnelle

8 – Projection stéréographique

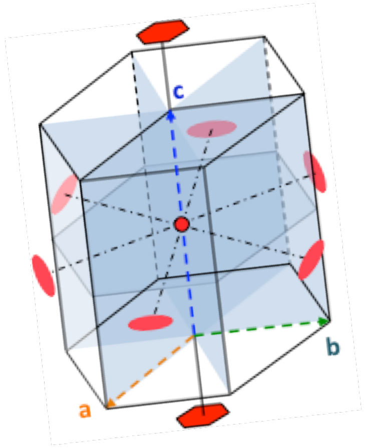
9 – Roto-inversions

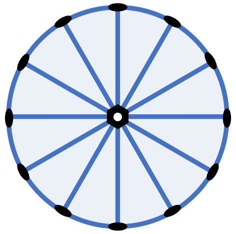
10 – Les 32 groupes ponctuels cristallographiques

11 – Les 7 systèmes cristallins

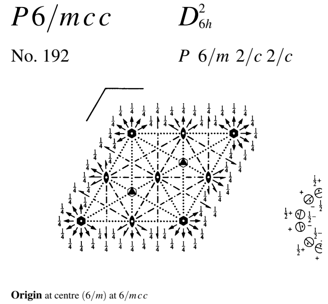
12 – Les 14 réseaux de Bravais

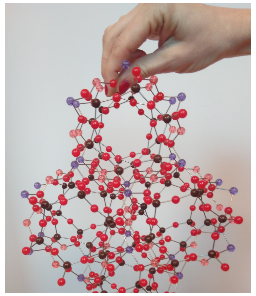
13 – Les 230 groupes d'espace





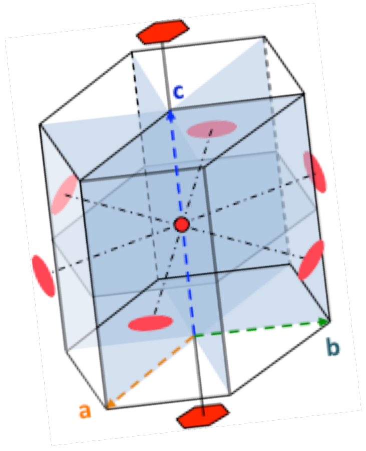
$\frac{6}{m}mm$

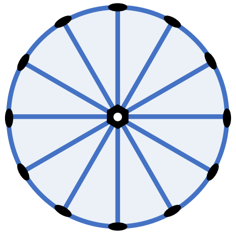




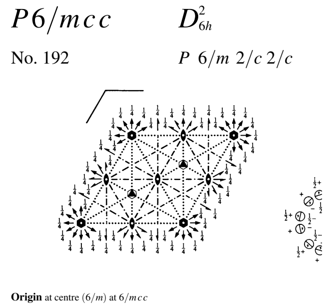
Course outline

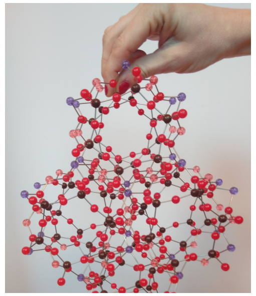
1- Symmetry observation in natural crystals
2- Internal cause of the natural crystal shape
3 – Crystal lattice, cell, motif
4 – Lattice direction and planes
5 – Reciprocal lattice
6 – Crystal lattice & symmetries
7 – Conventional cell (unit cell)
8 – Stereographic projection
9 – Roto-inversions
10 – The 32 crystallographic point groups
11 – The 7 crystal systems
12 – The 14 Bravais lattices
13 – The 230 space-groups



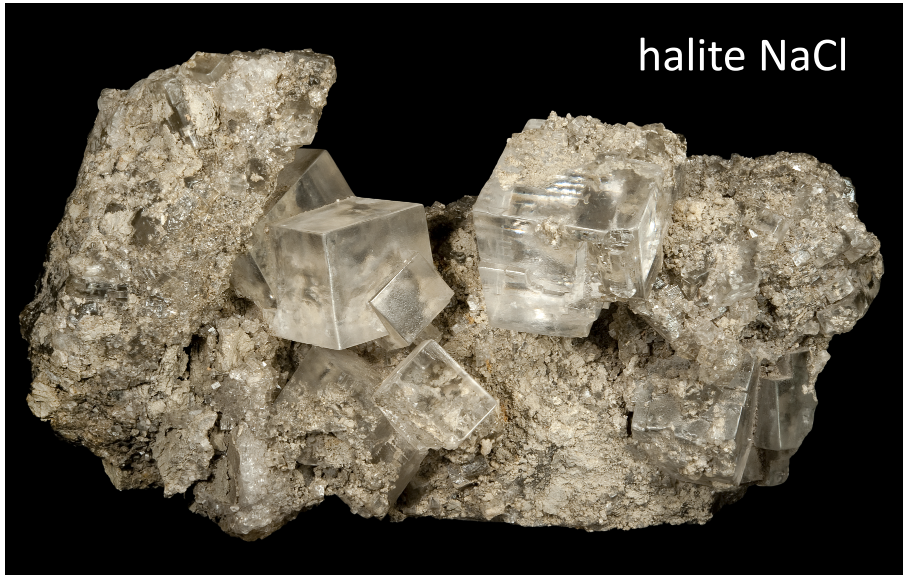


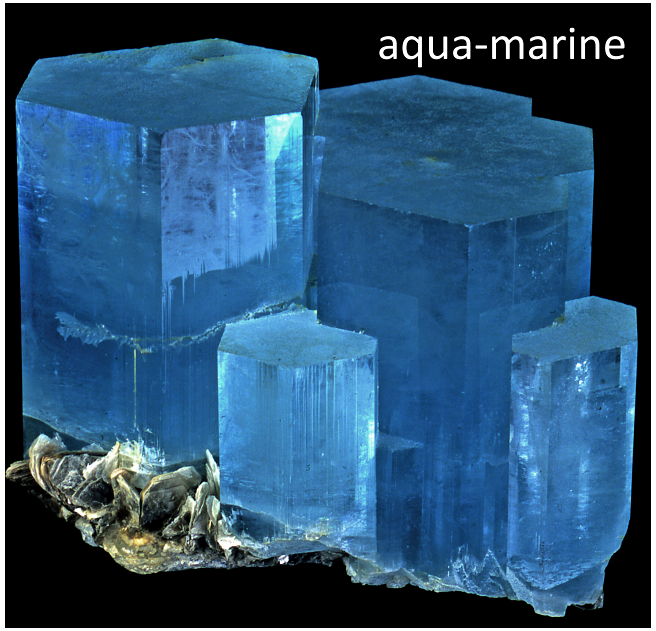
$\frac{6}{m}mm$

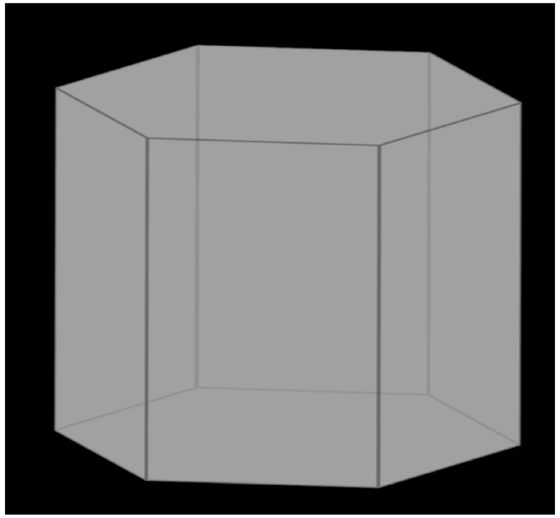


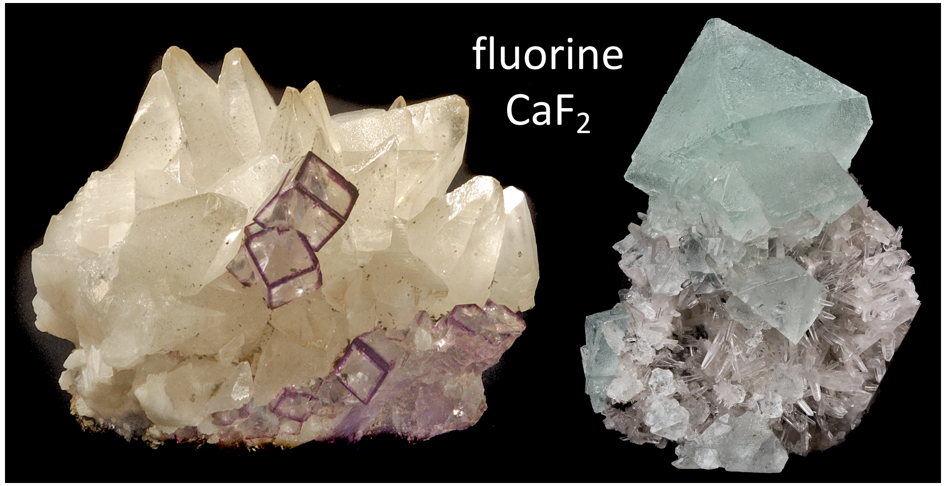


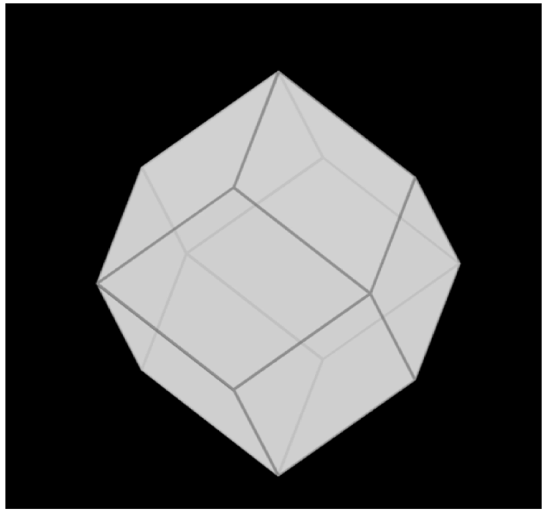
1- Symmetry observation in natural crystals







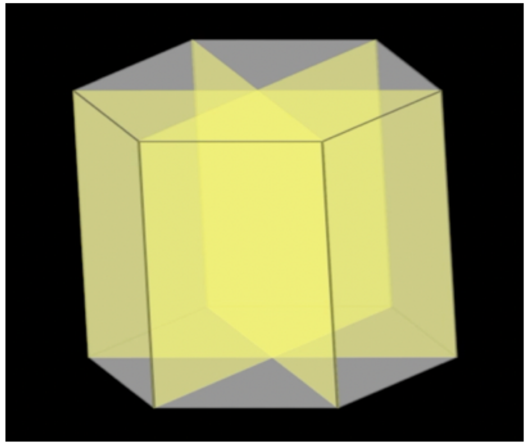




Crédits photos : Collection de Minéraux de Sorbonne Université

1- Symmetry observation in natural crystals

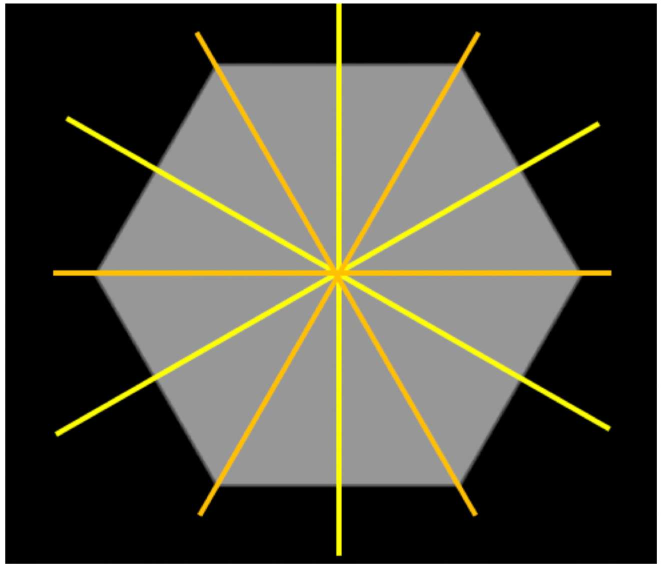
Highlighting mirror planes



aquamarine model:
hexagonal-based straight prism

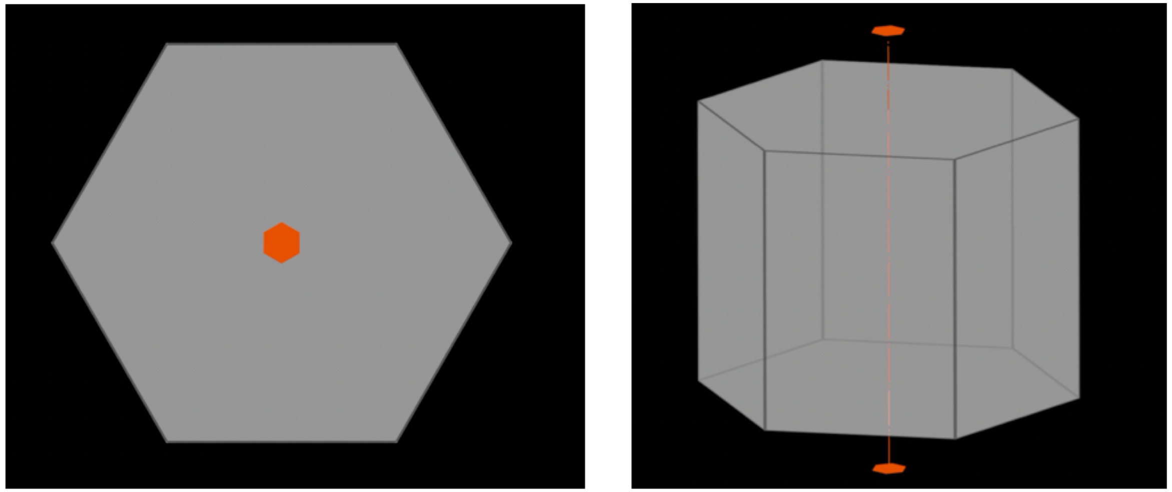
- **3 mirror planes**
  parallel to vertical edges
  and cutting the edges of the
  hexagonal base in the middle

- **3 mirror planes**
  parallel to the vertical edges and
  joining two corners opposite
  in the hexagonal base



1- Symmetry observation in natural crystals

Highlighting 6-fold rotation axis



axis A_6 or 6

$\varphi = 60° = \frac{2\pi}{6}$

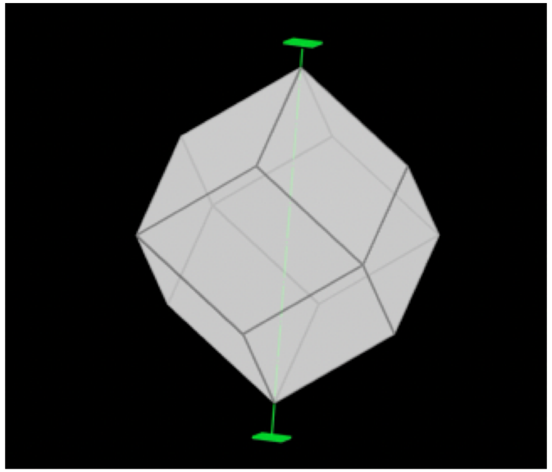
1- Symmetry observation in natural crystals

Highlighting 4-fold, 3-fold and 2-fold rotation axes

rhombododecahedron

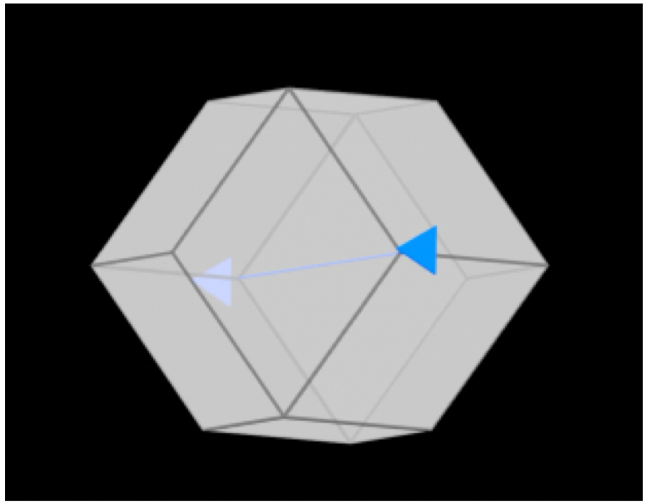
(12-face polyhedron)

Highlighting 4-fold, 3-fold and 2-fold rotation axes



axis A_4 or 4

$$\varphi = 90° = \frac{2\pi}{4}$$

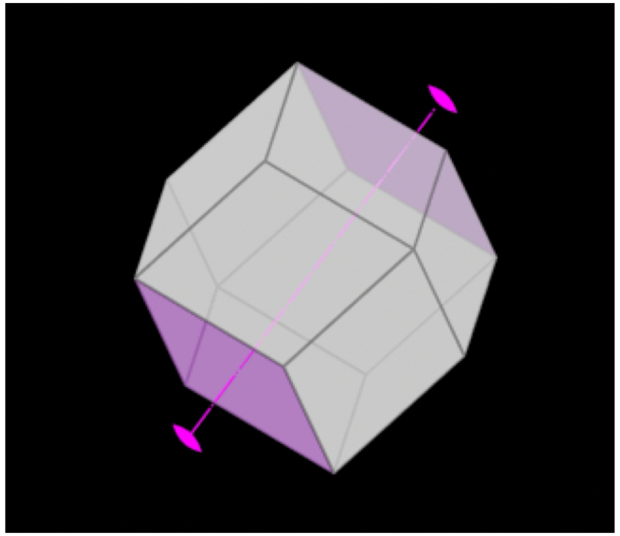


axis A_3 or 3

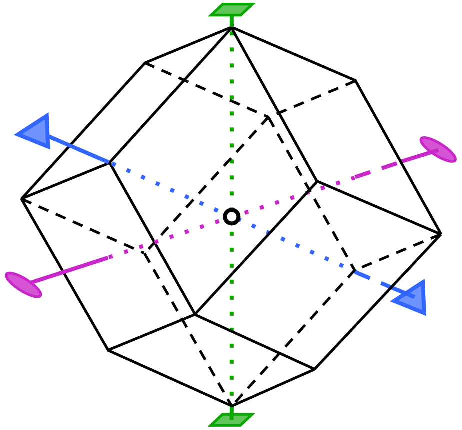
$$\varphi = 120° = \frac{2\pi}{3}$$

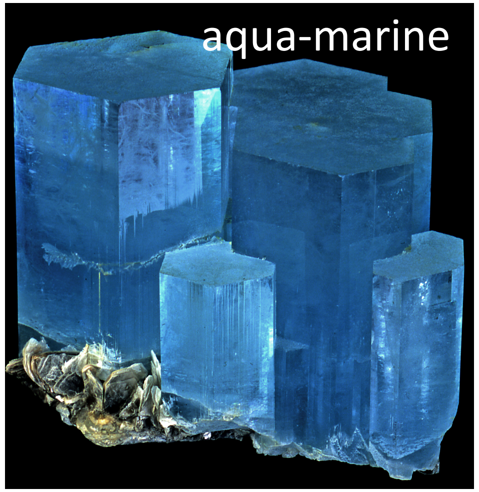
axis A_2 or 2

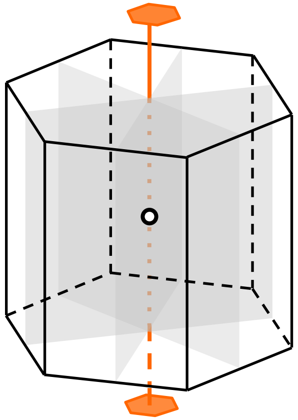
$$\varphi = 180° = \frac{2\pi}{2}$$



1- Symmetry observation in natural crystals







rotations

A_2 A_3 A_4 A_6

mirror

M

centre of symmetry

C

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

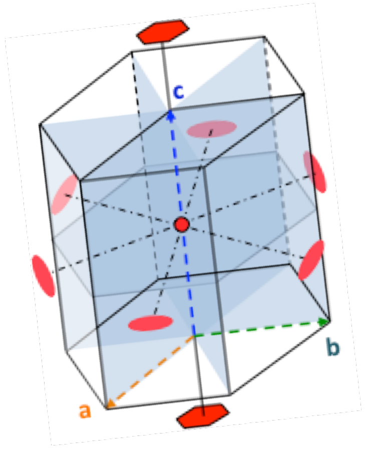
9 – Roto-inversions

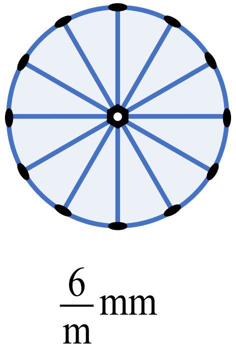
10 – The 32 crystallographic point groups

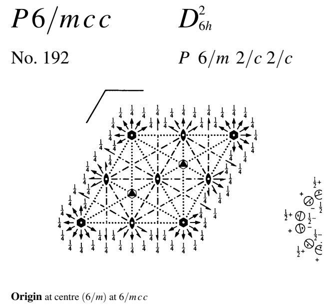
11 – The 7 crystal systems

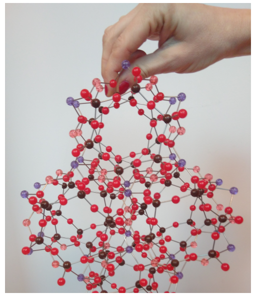
12 – The 14 Bravais lattices

13 – The 230 space-groups



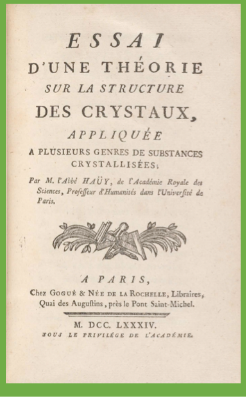






2- Internal cause of the natural crystal shape

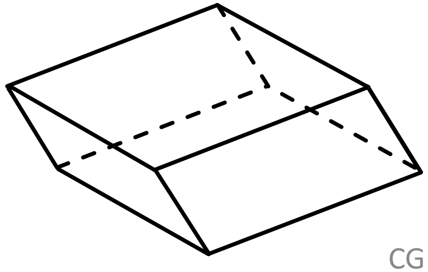
René Just Haüy
(1784)


ESSAI
D'UNE THÉORIE
SUR LA STRUCTURE
DES CRYSTAUX,
APPLIQUÉE
A PLUSIEURS GENRES DE SUBSTANCES CRYSTALLISÉES;
Par M. l'Abbé HAÜY, de l'Académie Royale des Sciences, Professeur d'Humanités dans l'Université de Paris.

A PARIS,
Chez GOGUÉ & NÉE DE LA ROCHELLE, Libraires, Quai des Augustins, près le Pont Saint-Michel.
M. DCC. LXXXIV.
SOUS LE PRIVILÉGE DE L'ACADÉMIE.

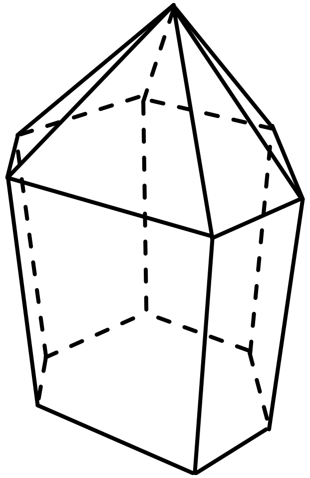
Torbern Bergman

Rhombohedron

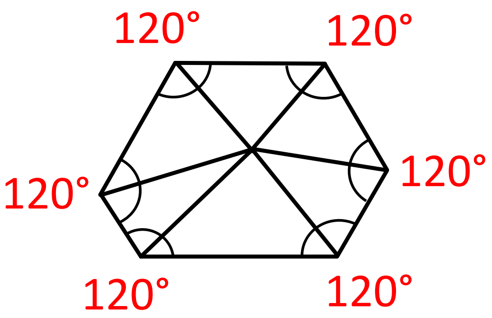


Jean-Baptiste
Romé de l'Isle

Law of constancy of interfacial angles

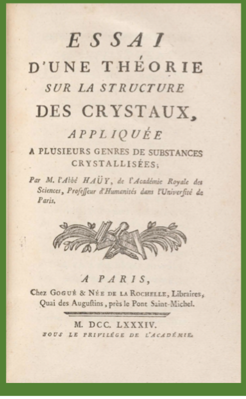


crystal of quartz



2- Internal cause of the natural crystal shape

René Just Haüy (1784)



ESSAI
D'UNE THÉORIE
SUR LA STRUCTURE
DES CRYSTAUX,
APPLIQUÉE
A PLUSIEURS GENRES DE SUBSTANCES CRYSTALLISÉES;
Par M. l'Abbé HAÜY, de l'Académie Royale des Sciences, Professeur d'Humanités dans l'Université de Paris.

A PARIS,
Chez GOGUÉ & NÉE DE LA ROCHELLE, Libraires, Quai des Augustins, près le Pont Saint-Michel.
M. DCC. LXXXIV.
SOUS LE PRIVILÈGE DE L'ACADÉMIE.

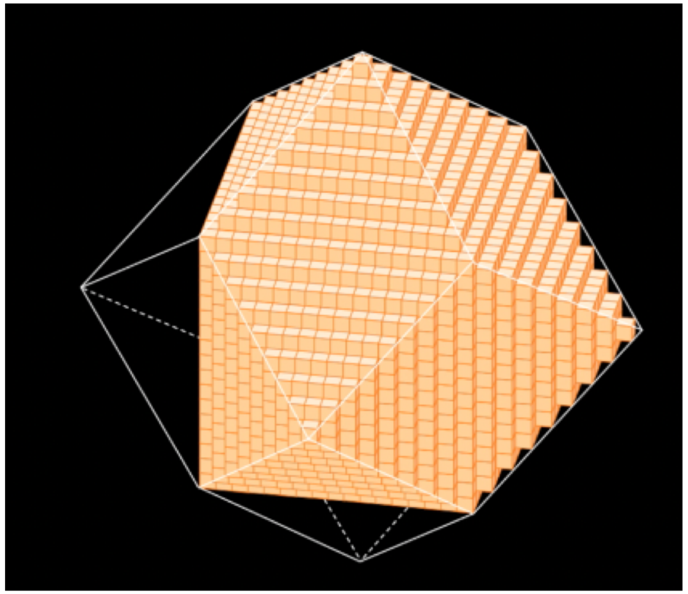
primitive solid

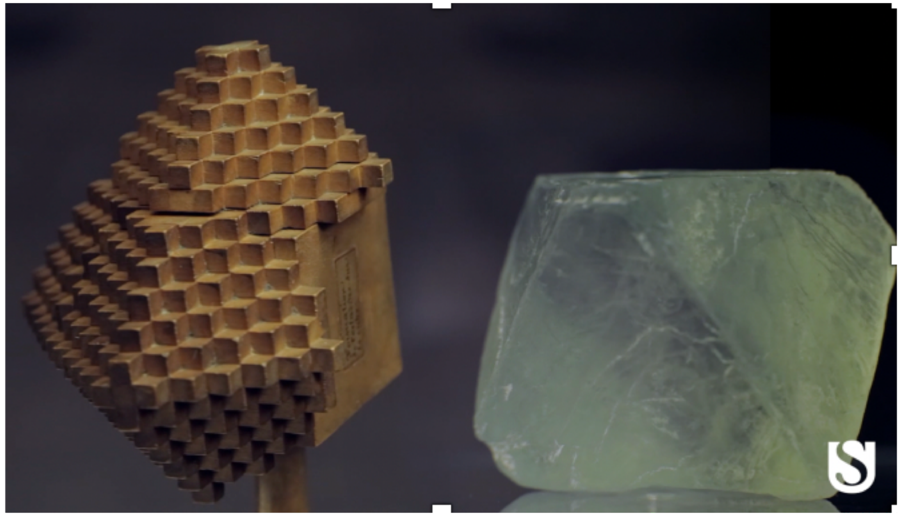
↓

"molécule intégrante"

↓

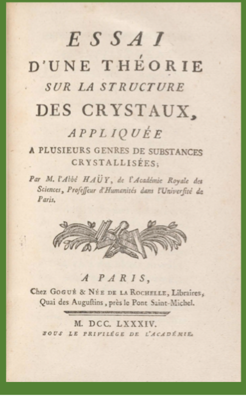
law of rational decrements





2- Internal cause of the natural crystal shape

René Just Haüy
(1784)


ESSAI
D'UNE THÉORIE
SUR LA STRUCTURE
DES CRYSTAUX,
APPLIQUÉE
A PLUSIEURS GENRES DE SUBSTANCES
CRYSTALLISÉES;
Par M. l'Abbé HAÜY, de l'Académie Royale des Sciences, Professeur d'Humanités dans l'Université de Paris.

A PARIS,
Chez GOGUÉ & NÉE DE LA ROCHELLE, Libraires, Quai des Augustins, près le Pont Saint-Michel.
M. DCC. LXXXIV.
SOUS LE PRIVILÉGE DE L'ACADÉMIE.

primitive solid

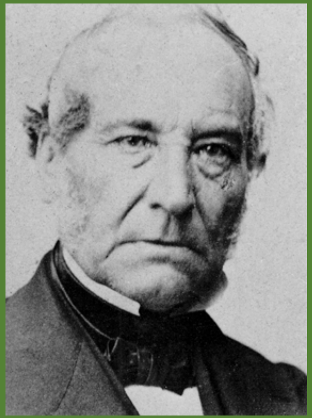
↓

"molécule intégrante"

↓

law of rational decrements

Gabriel Delafosse



cell

lattice

motif

Auguste Bravais
(1848)

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

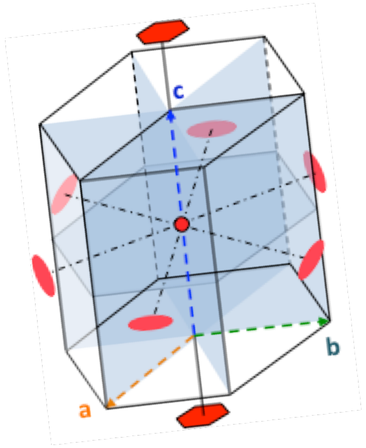
9 – Roto-inversions

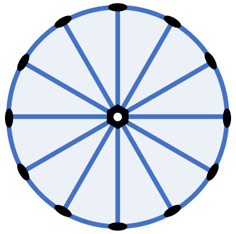
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

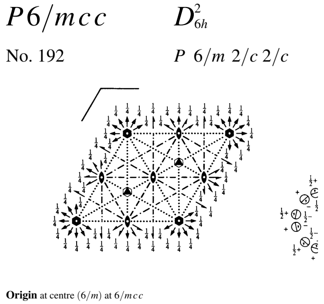
12 – The 14 Bravais lattices

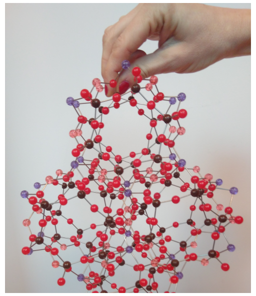
13 – The 230 space-groups





$\frac{6}{m}mm$

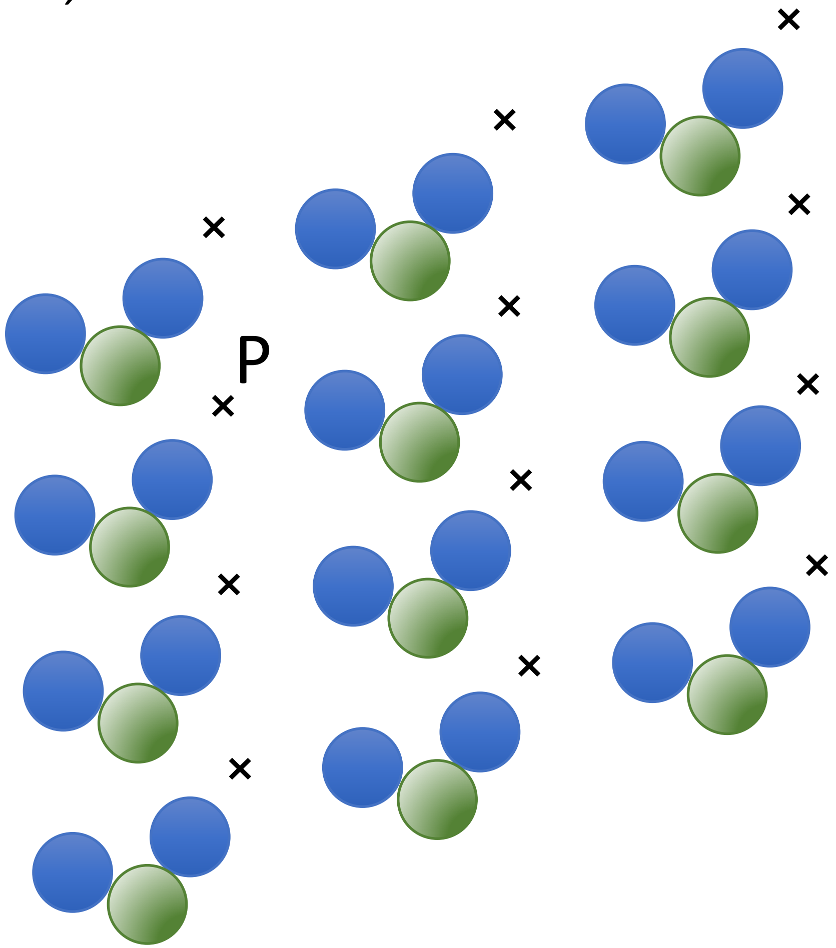




3 – Crystal lattice, cell, motif

The Bravais postulate

"Given any P point in a crystal, there is in the medium, ***a discrete, unlimited in the 3 directions of space, number of points*** *around which the arrangement of atoms is the same, with the same orientation, as around point P."*



All the points define a **lattice**.
The points are called **lattice points**.

NB: The **lattice points** do not correspond to any physical entity.
There should be no confusion between the lattice points and atoms.

3 – Crystal lattice, cell, motif

lattice → basis vectors

The lattice is defined, in 3D, by **3 basis vecteurs** $\vec{a}$, $\vec{b}$ and $\vec{c}$ that are non colinear.

All the lattice points are obtained by linear combinaison :

$$\vec{t} = \mathrm{u}\,\vec{a} + \mathrm{v}\,\vec{b} + \mathrm{w}\,\vec{c}$$

u, v , w: relative integers

lattice translation

lattice → how to identify a lattice point

$\vec{t} = \vec{a} + \vec{b} + \vec{c}$

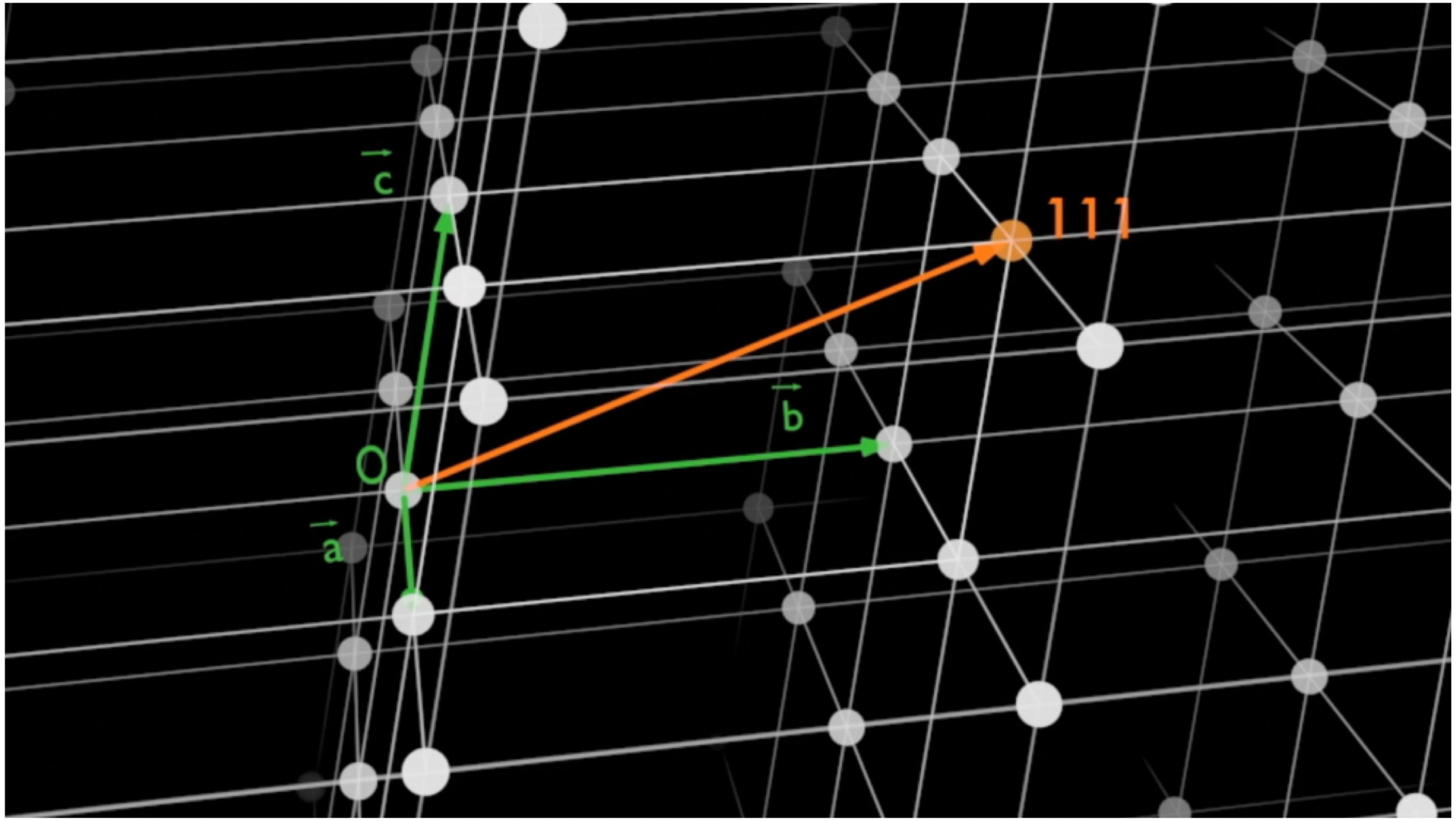
→ lattice point 111

$\vec{t} = -\vec{a} + 2\vec{b}$

→ lattice point $\bar{1}20$

$\vec{t} = \vec{a} - \vec{b} + 2\vec{c}$

→ lattice point $1\bar{1}2$



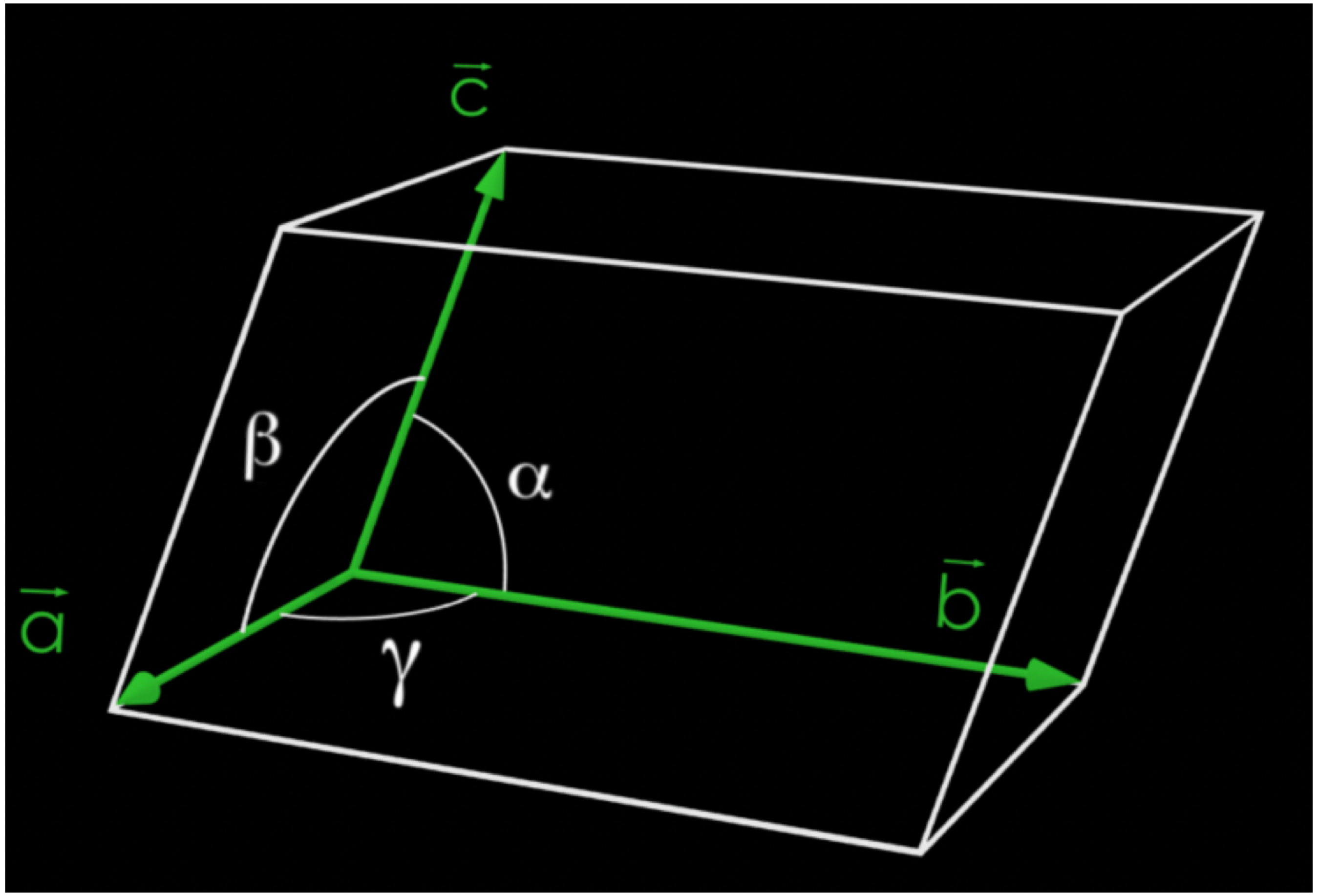
basis vectors → cell

3 basis vectors: $\vec{a}$, $\vec{b}$ and $\vec{c}$

6 parameters:
- 3 lengths a, b, c
- 3 angles α, β et γ

volume:

$$V = (\vec{a}, \vec{b}, \vec{c}) = \vec{a} \cdot (\vec{b} \times \vec{c})$$



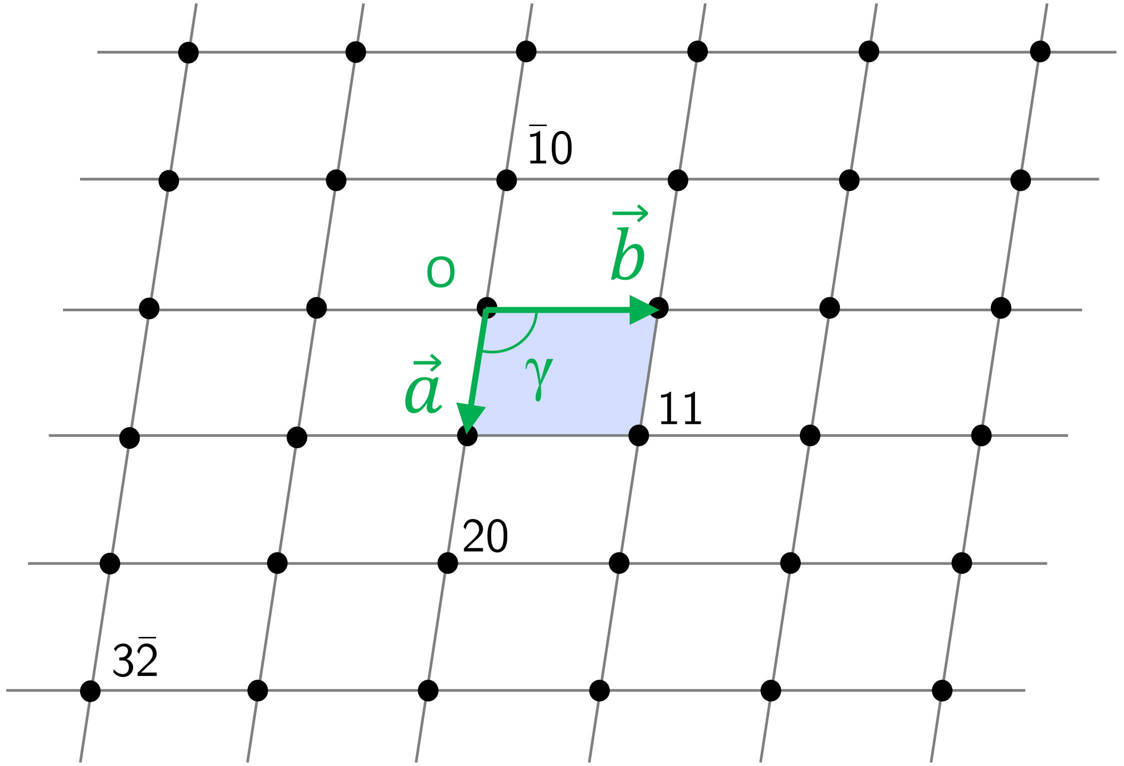
2D cell

2 basis vectors: $\vec{a}$ and $\vec{b}$

3 parameters:
- 2 lengths a, b
- 1 angle $\gamma \geq 90°$

surface:

$$S = |\vec{a} \times \vec{b}|$$

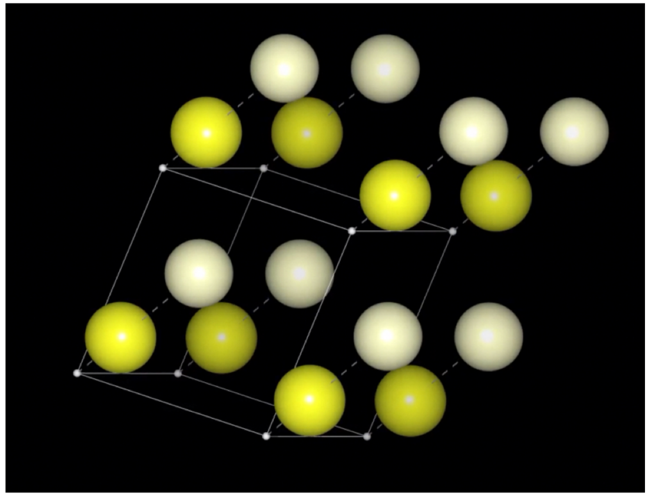


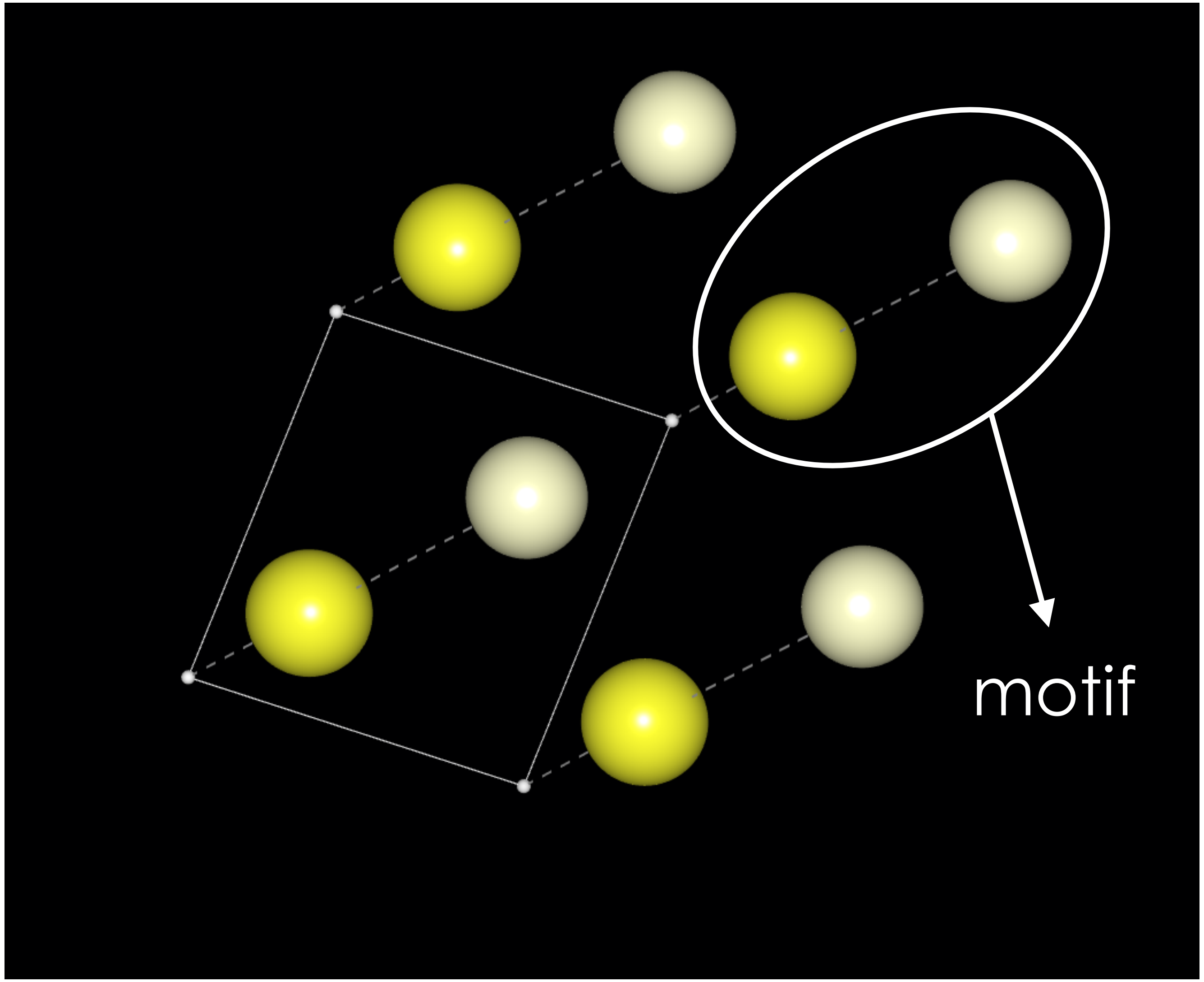
3 – Crystal lattice, cell, motif

motif

primitive-cell content

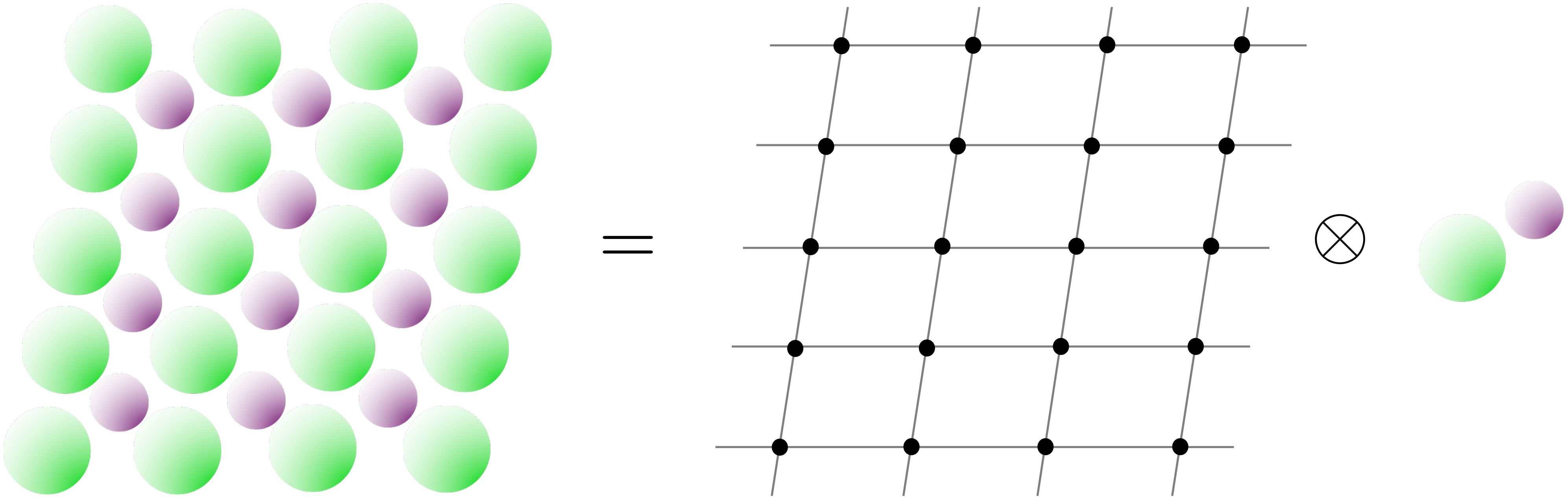
one atom
or a set of atoms
attached to each lattice point





3 - Réseau, maille, motif

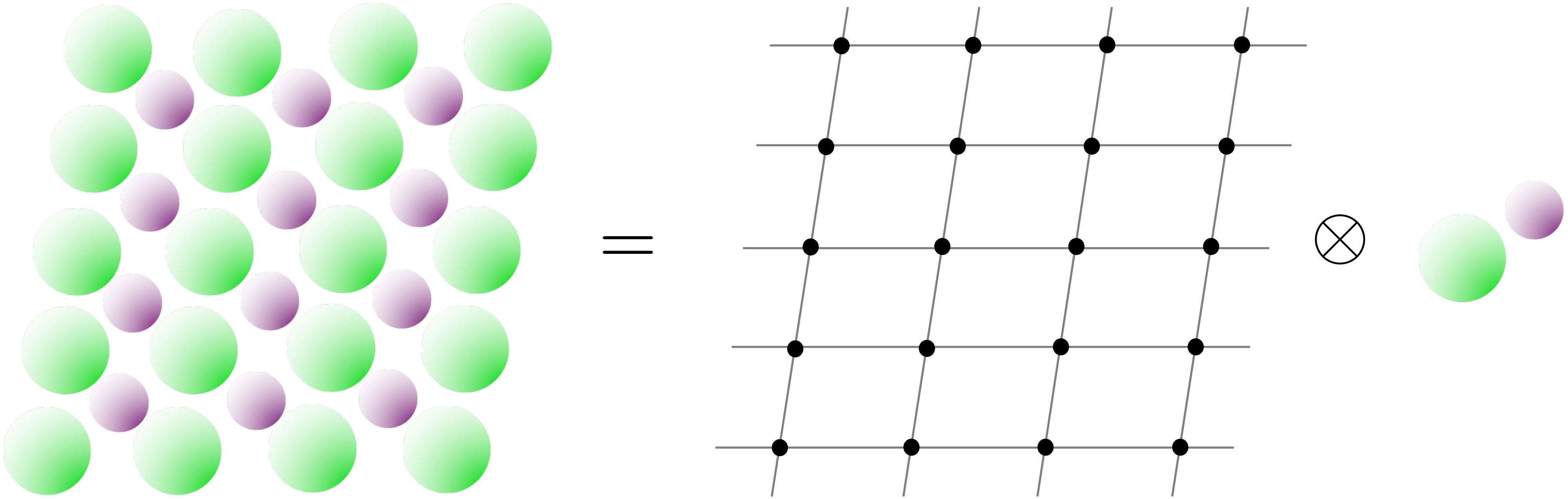
cristal



cristal = réseau ⊗ motif

3 – Crystal lattice, cell, motif

crystal



crystal $=$ lattice $\otimes$ motif

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

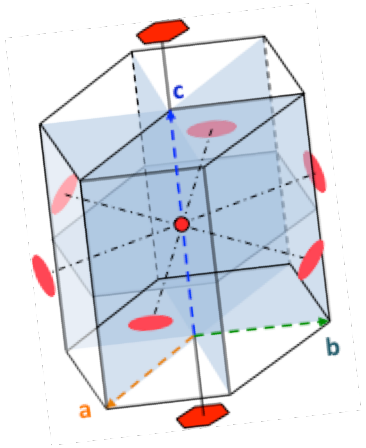
9 – Roto-inversions

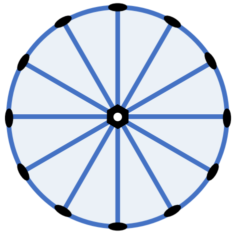
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

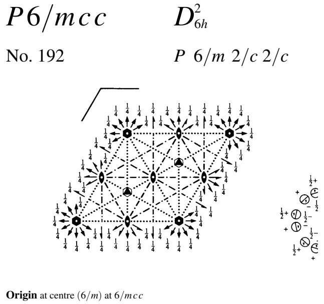
12 – The 14 Bravais lattices

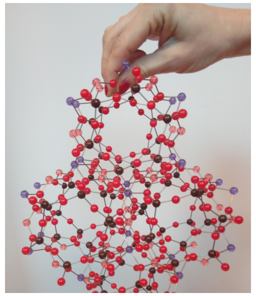
13 – The 230 space-groups





$\frac{6}{m}$mm





A line passing through two lattice points corresponds to a Lattice direction

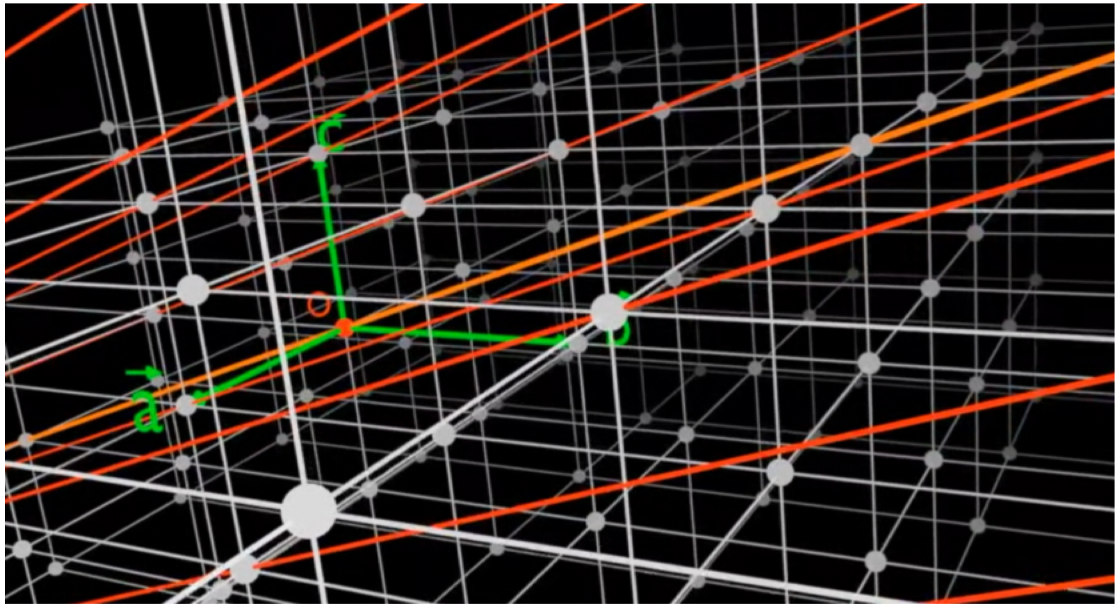
→ It contains an infinity of lattice points

Indexing directions:

Any line is parallel to a particular line passing through the origin (which is a lattice point) and through another lattice point of coordinates (u, v, w).

→ lattice direction [uvw]

lattice direction

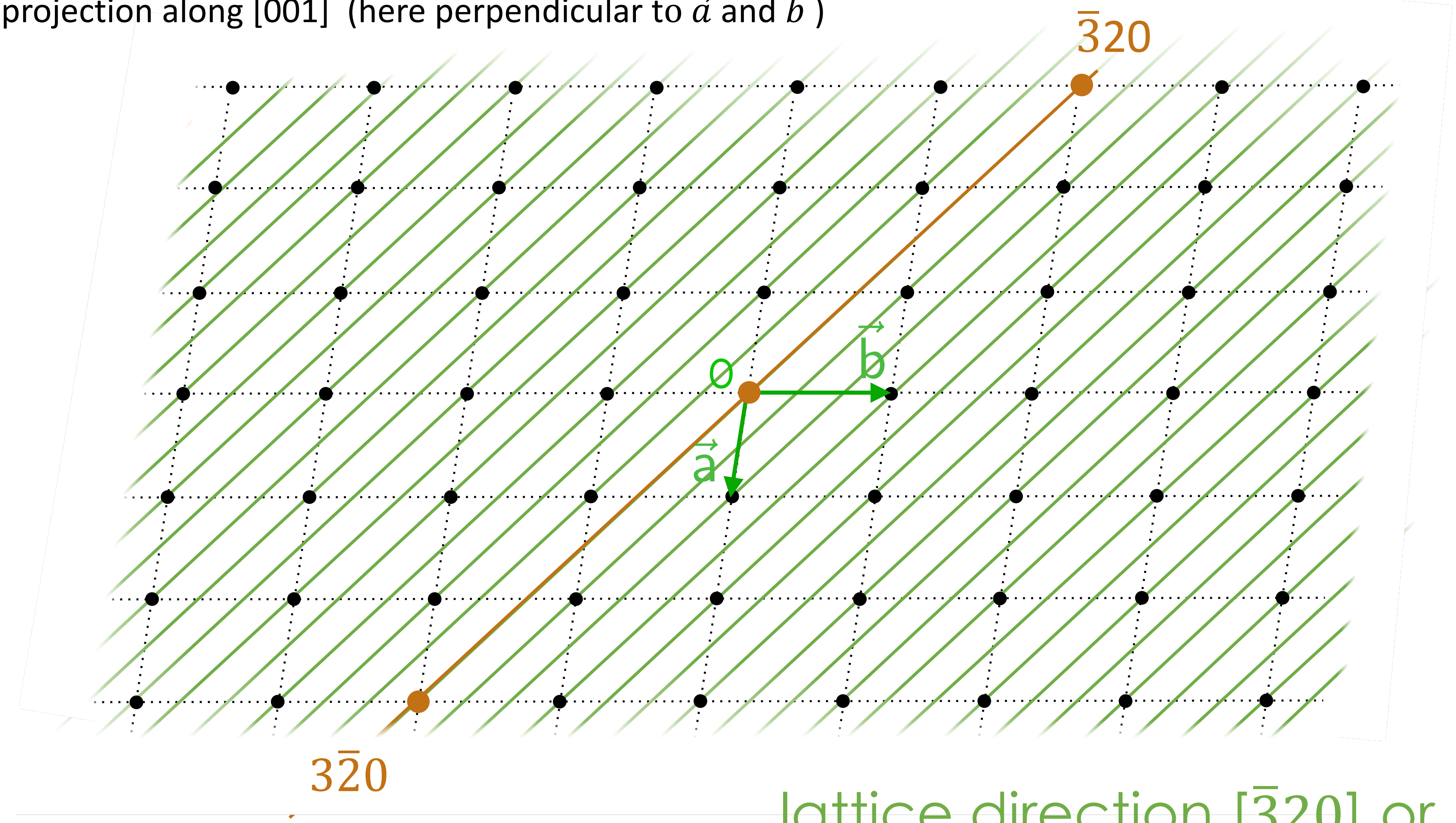


lattice direction [021]

4 – Lattice direction and planes

lattice direction

in projection along [001] (here perpendicular to $\vec{a}$ and $\vec{b}$)

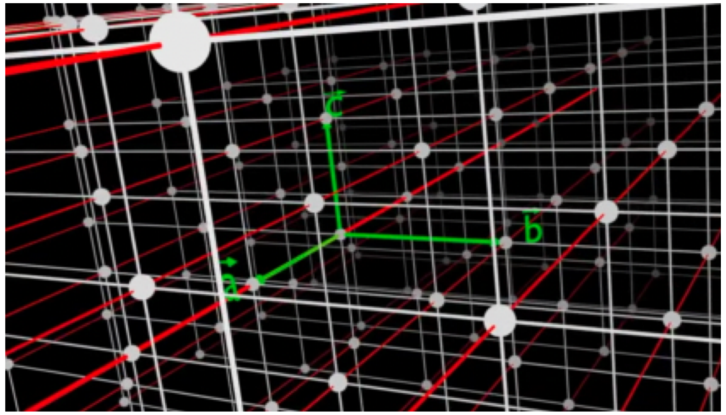


lattice direction [$\bar{3}20$] or [$3\bar{2}0$]

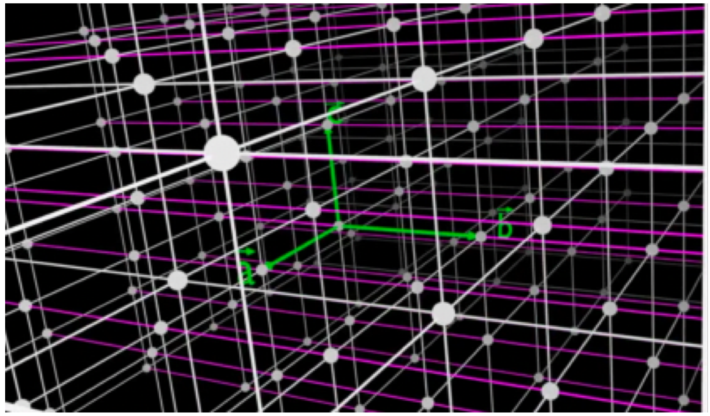
4 – Lattice direction and planes

lattice direction

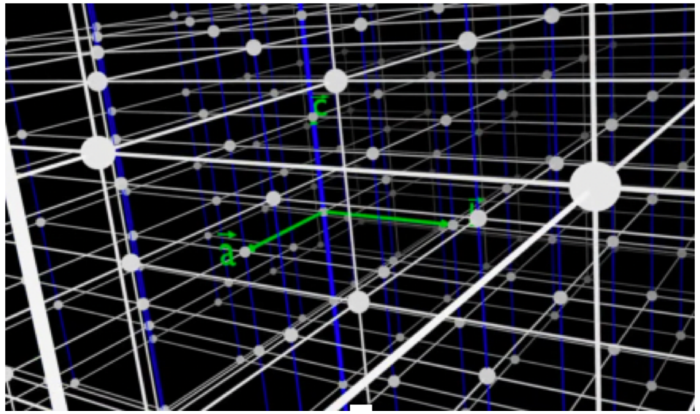
[100]



[010]



[001]

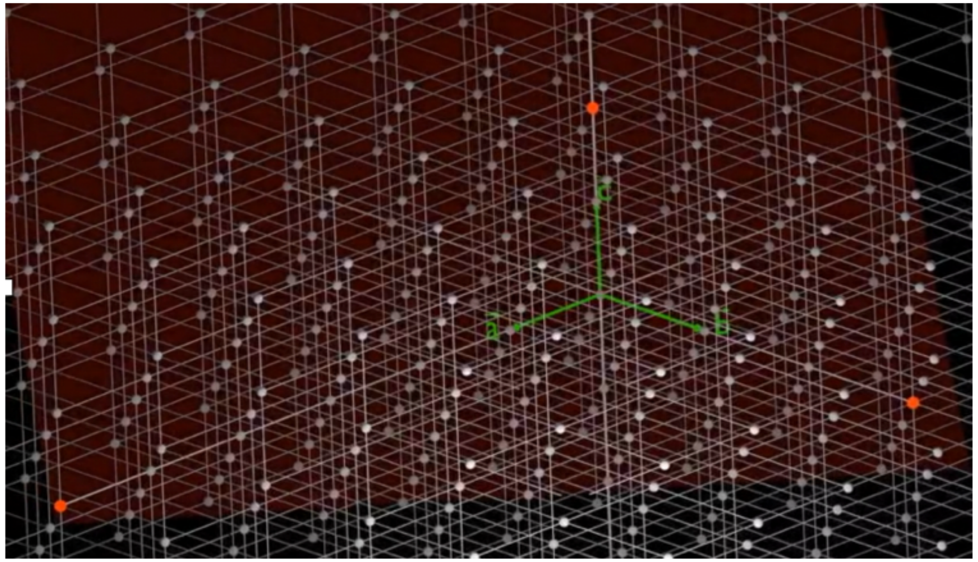


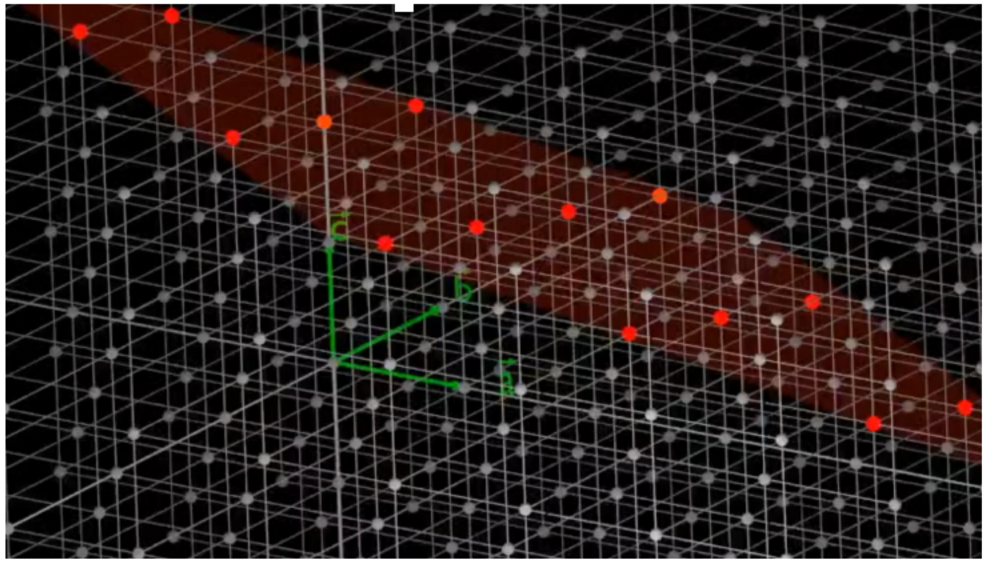
4 – Lattice direction and planes

lattice planes

Lattice plane: any plane passing through 3 non colinear lattice points

→ A lattice plane contains an infinity of lattice points and forms a 2D lattice.

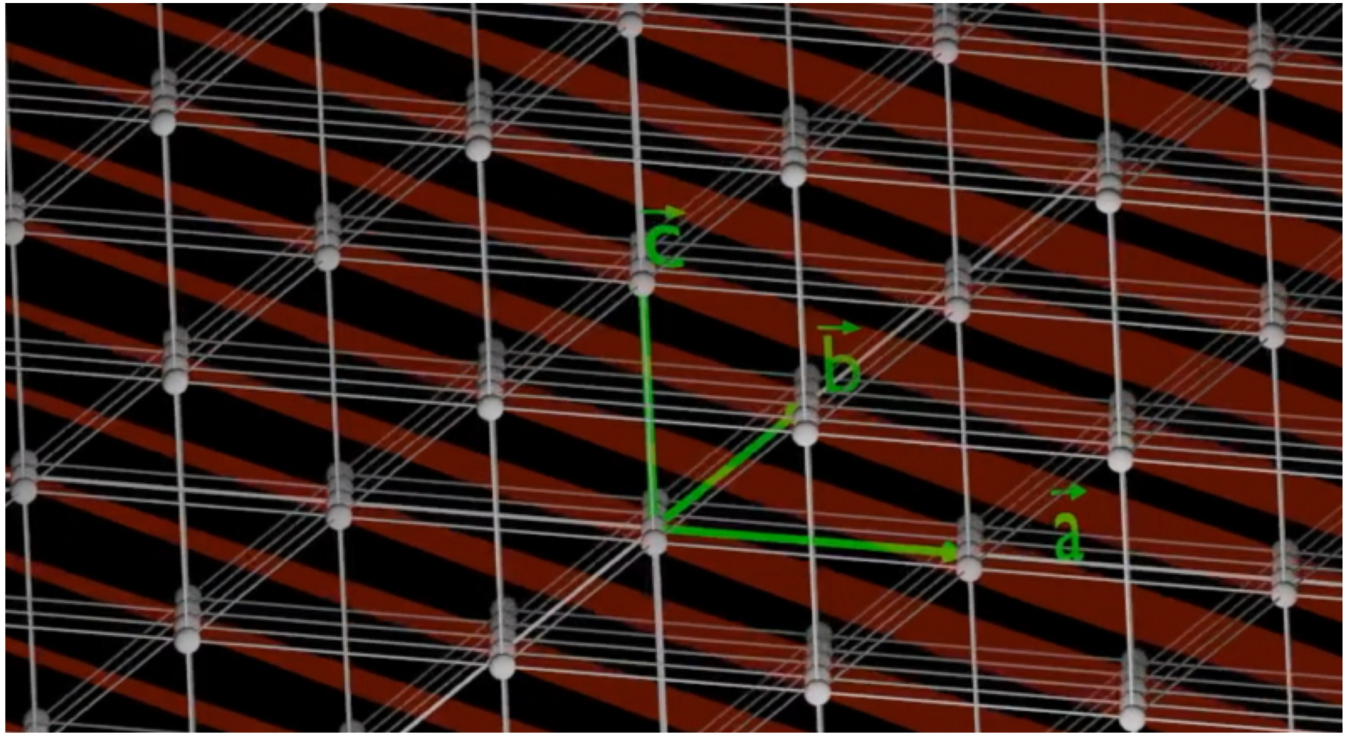




lattice-plane family

Lattice-plane family: infinity of equidistant and parallel lattice planes.

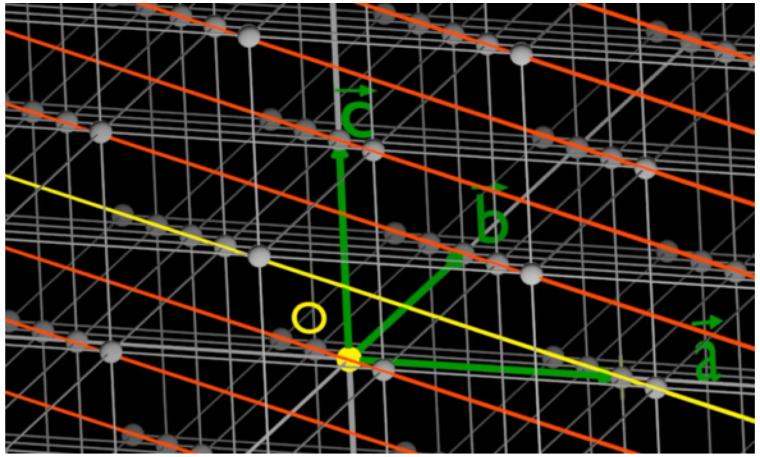
→ A lattice-plane family contains all the lattice points of the 3D lattice.

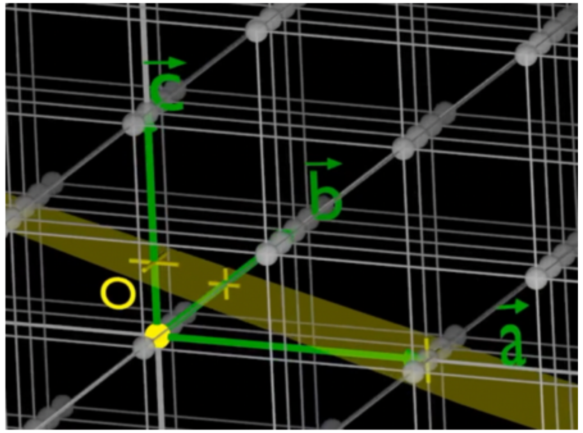


lattice-plane family

A **lattice-plane family** is labeled **(hkl)**

h, k and l are Miller indices, which are relative prime integer numbers.





axis [100] cut in a/1
axis [010] cut in b/2
axis [001] cut in c/3

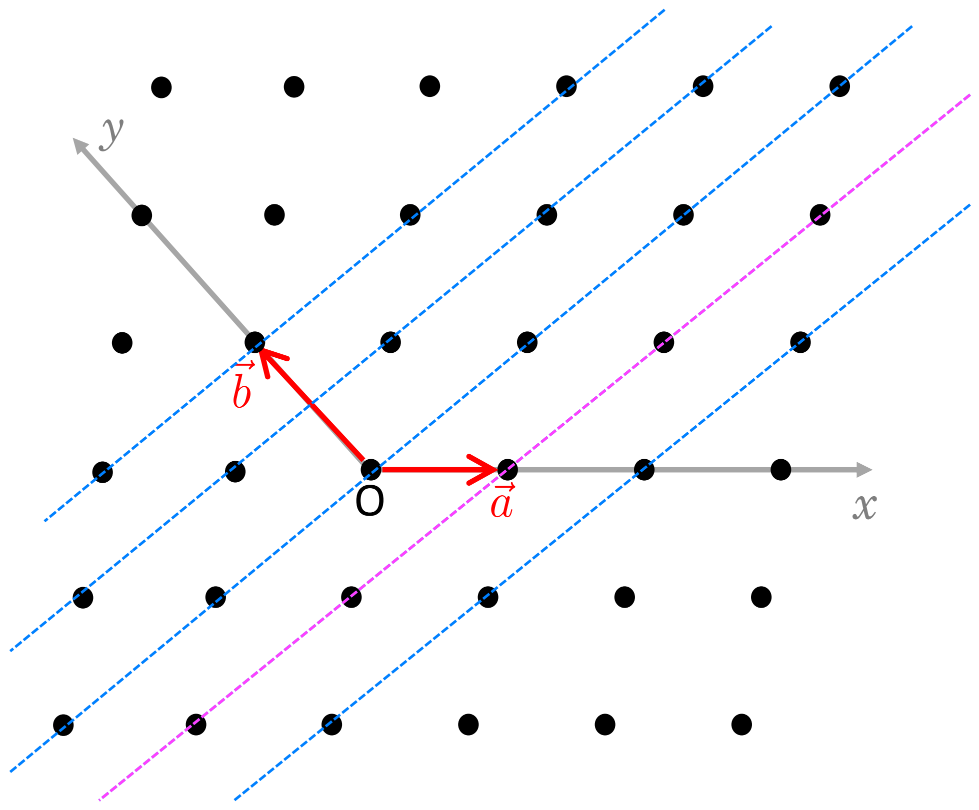
➔ lattice-plane family (123)

lattice-plane family

A **lattice-plane family** is labeled **(hkl)**

(hkl) refers to as the lattice-plane family such as the plane of the family that is the closest to the lattice-origin point, cuts (O*x*) axis in *a*/$\boldsymbol{h}$, (O*y*) axis in *b*/$\boldsymbol{k}$ and (O*z*) axis in *c*/$\boldsymbol{l}$.

here $h = 1$, $k = -2$ et $l = 0$
→ lattice plane family $(1\bar{2}0)$



projection in plane (***a***,***b***)

lattice-plane family

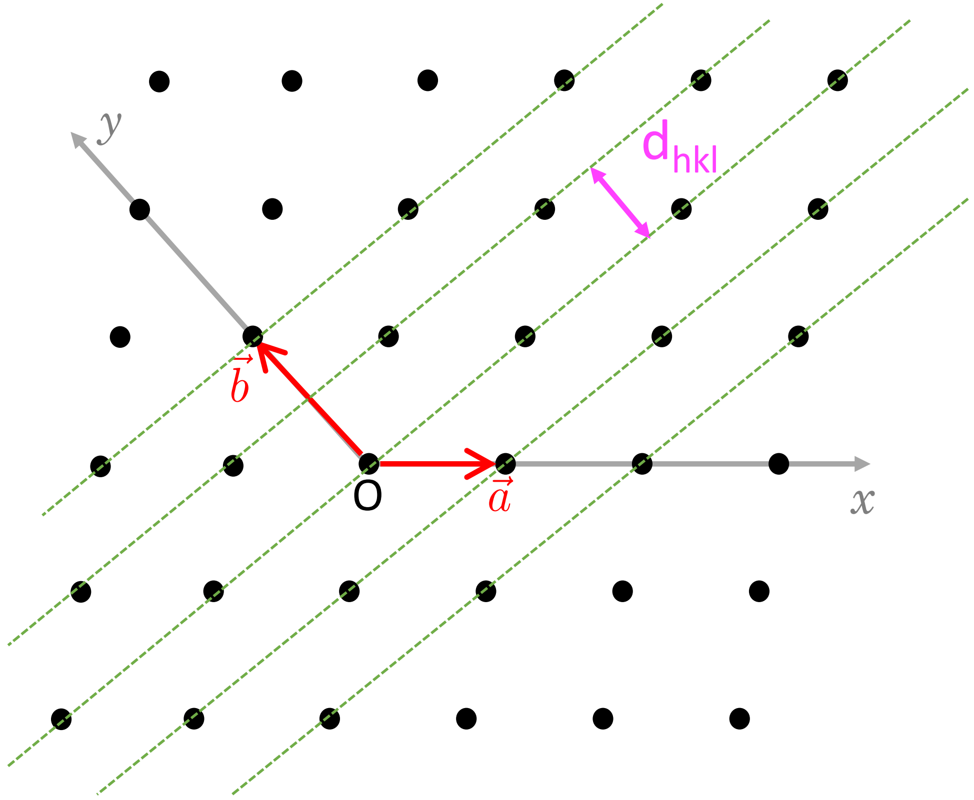
d-spacing:

distance between

two consecutive planes belonging to

the same (hkl) family,

noted d_{hkl}.



projection in plane (***a***,***b***)

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

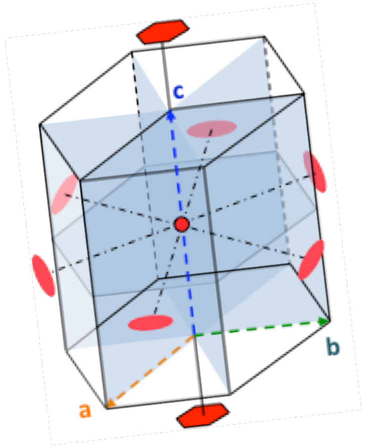
9 – Roto-inversions

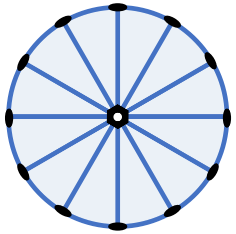
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

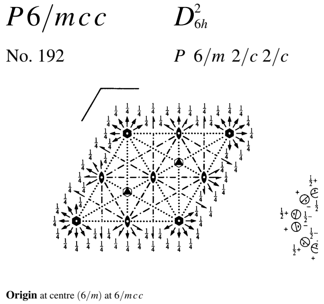
12 – The 14 Bravais lattices

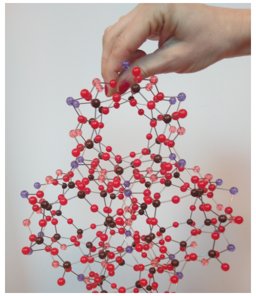
13 – The 230 space-groups





$\frac{6}{m}mm$

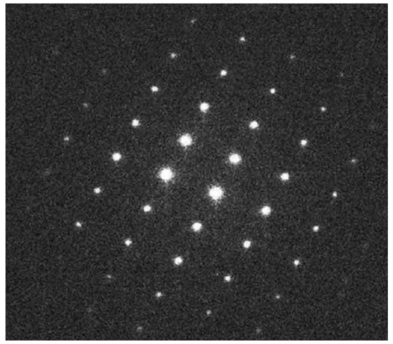




5 – Reciprocal lattice

- makes easier some crystallographic calculations
- naturally derived from the diffraction theory

for any radiation (X, neutrons, electrons)



Nature Materials 10, 890–896 (2011)

Définition

Given a direct lattice with basis vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$.
The corresponding reciprocal lattice is defined by $\vec{a}^\star$, $\vec{b}^\star$ and $\vec{c}^\star$ such that:

$$\vec{a}\cdot\vec{a}^\star = \sigma \qquad \vec{a}\cdot\vec{b}^\star = 0 \qquad \vec{a}\cdot\vec{c}^\star = 0$$
$$\vec{b}\cdot\vec{a}^\star = 0 \qquad \vec{b}\cdot\vec{b}^\star = \sigma \qquad \vec{b}\cdot\vec{c}^\star = 0$$
$$\vec{c}\cdot\vec{a}^\star = 0 \qquad \vec{c}\cdot\vec{b}^\star = 0 \qquad \vec{c}\cdot\vec{c}^\star = \sigma$$

In crystallography: $\sigma = 1$

In solid-state physics: $\sigma = 2\pi$

5 – Reciprocal lattice

$$\vec{b} \cdot \vec{a}^{\star} = 0 \quad \Longrightarrow \vec{a}^{\star} \perp \vec{b}$$

$$\vec{c} \cdot \vec{a}^{\star} = 0 \quad \Longrightarrow \vec{a}^{\star} \perp \vec{c}$$

so $\vec{a}^{\star} = \alpha' \, \vec{b} \times \vec{c}$ where α' is a constant

then $\vec{a} \cdot \vec{a}^{\star} = \alpha' \, \underbrace{\vec{a} \cdot \left(\vec{b} \times \vec{c}\right)}_{V}$

we know that $\vec{a} \cdot \vec{a}^{\star} = 1$

thus $\alpha' = \dfrac{1}{V}$

Hence

$$\vec{a}^{\star} = \frac{\vec{b} \times \vec{c}}{V}$$

And in the same way:

$$\vec{b}^{\star} = \frac{\vec{c} \times \vec{a}}{V} \qquad \vec{c}^{\star} = \frac{\vec{a} \times \vec{b}}{V}$$

Unité de longueur : $Å^{-1}$ ou nm^{-1}

relationship with the direct lattice

- We can show[1]:

$$V\,V^{\star} = 1$$

[1] *To do so, we express V as a function of a, b and c. Then, we use the following formula of the 3-vector product:* $\mathbf{A}\times(\mathbf{B}\times\mathbf{C})=(\mathbf{A}.\mathbf{C})\mathbf{B}-(\mathbf{A}.\mathbf{B})\mathbf{C}$

- We can show:

Any plane of the direct lattice belonging to the family (hkl) corresponds to a direction of the reciprocal lattice of the same indices, [hkl]*, which is perpendicular to (hkl).

$$[hkl]^{\star} \perp (hkl)$$

relationship with the direct lattice

$$[hkl]^\star \perp (hkl)$$

examples

Reciprocal space			Direct space	
$\vec{a}^\star$	// $[100]^\star$	$\perp$	$(\vec{b}, \vec{c})$	= (100)
$\vec{b}^\star$	// $[010]^\star$	$\perp$	$(\vec{c}, \vec{a})$	= (010)
$\vec{c}^\star$	// $[001]^\star$	$\perp$	$(\vec{a}, \vec{b})$	= (001)

relationship with the direct lattice

- d-spacing calculation:

$$d_{hkl} \;\| \vec{t}^{\star}_{hkl} \| = 1$$

where $\vec{t}^{\star}_{hkl} \parallel [hkl]^{\star}$ and $\vec{t}^{\star}_{hkl} = h\vec{a}^{\star} + k\vec{b}^{\star} + l\vec{c}^{\star}$

In a cubic lattice: $$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

relationship with the direct lattice

- Condition to have (hkl) **parallel** to [uvw]:

$\vec{t}^{\star}_{hkl} \perp \vec{t}_{uvw}$ ➔ scalar product equal to zero

with $\vec{t}^{\star}_{hkl} = h\vec{a}^{\star} + k\vec{b}^{\star} + l\vec{c}^{\star}$

and $\vec{t}_{uvw} = u\,\vec{a} + v\,\vec{b} + w\,\vec{c}$

thus $$h\,u + k\,v + l\,w = 0$$

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

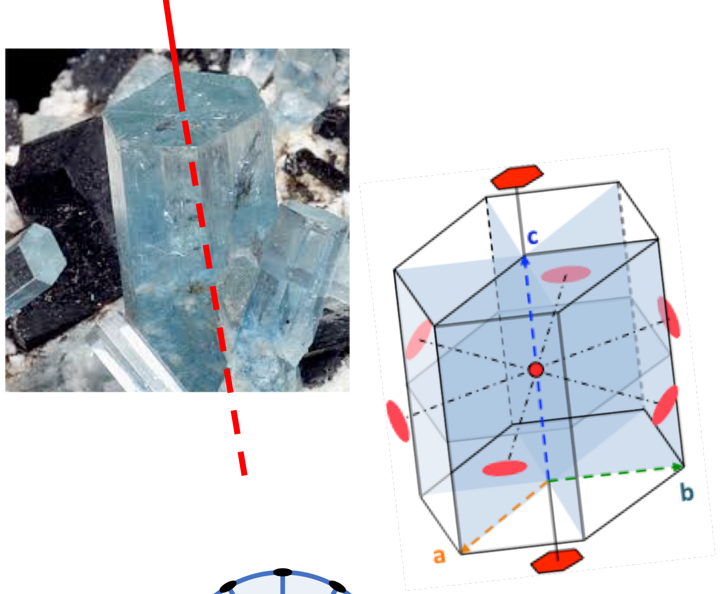
9 – Roto-inversions

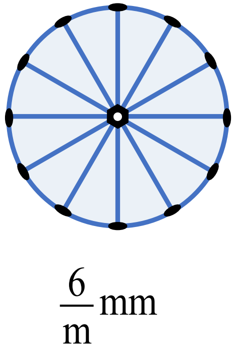
10 – The 32 crystallographic point groups

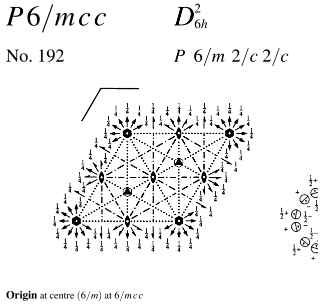
11 – The 7 crystal systems

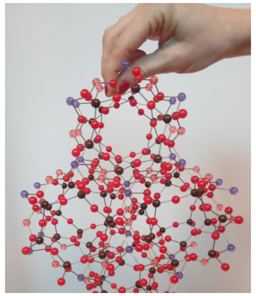
12 – The 14 Bravais lattices

13 – The 230 space-groups



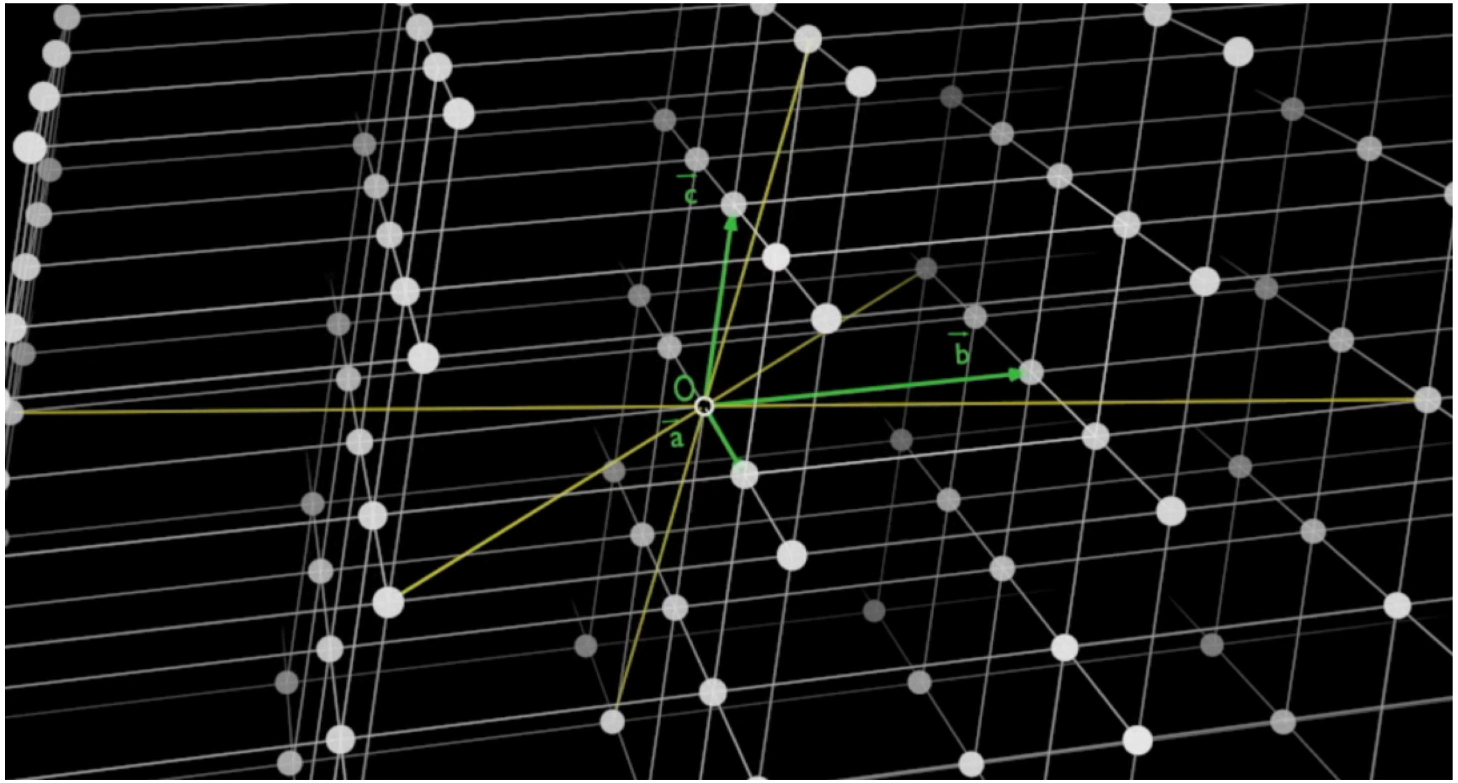






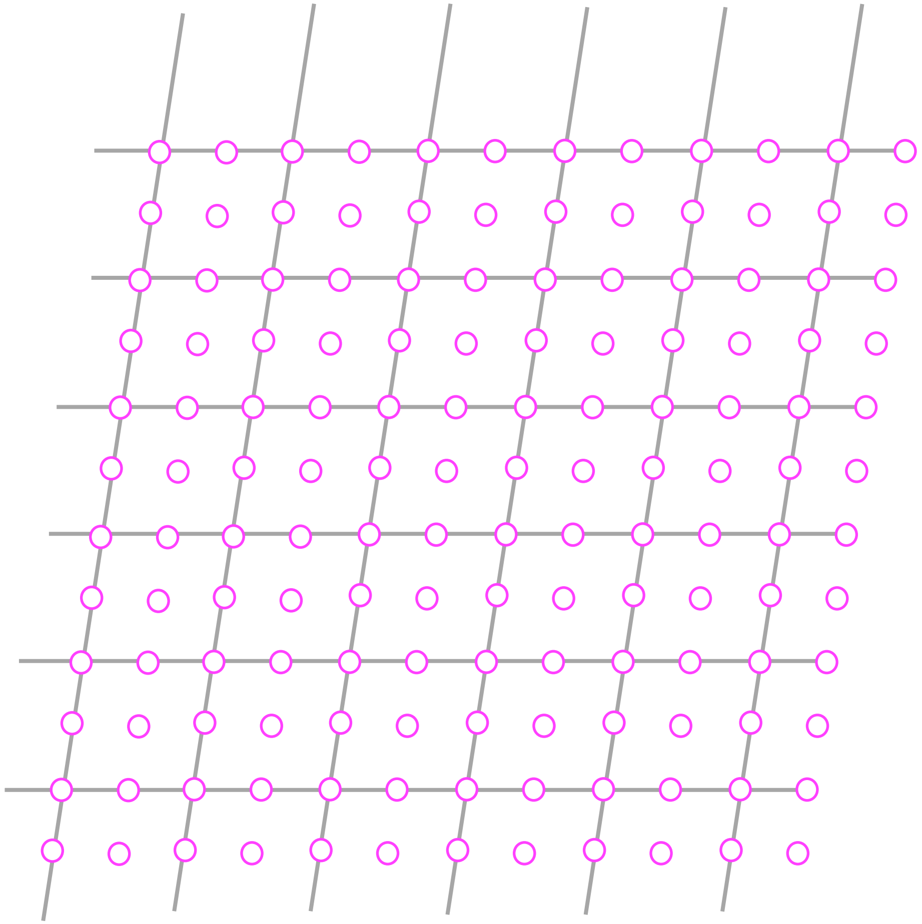
Any lattice is **centrosymmetric** with centres:

- on each lattice point
- in the middle of each cell edge
- in the middle of each cell face
- in the center of each cell



Any lattice is
centrosymmetric
with centres:

- on each lattice point
- in the middle of each cell edge
- in the middle of each cell face
- in the middle of the each cell



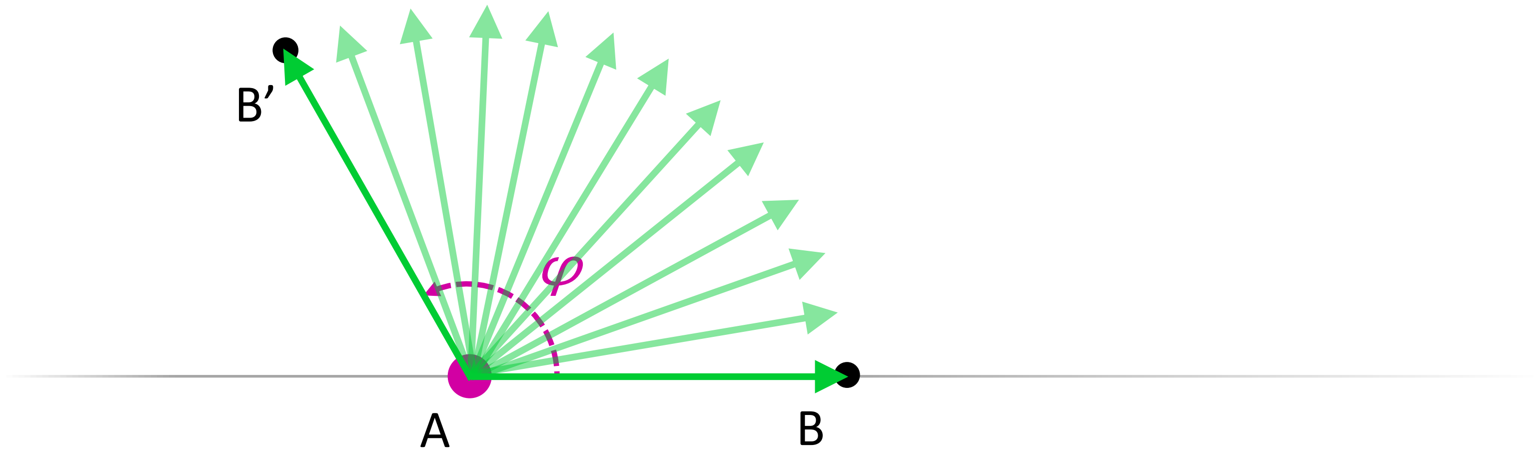
The rotation axes compatible with the crystal lattice

rotation axes $\mathbf{A_n}$ of angle $\varphi = \dfrac{2\pi}{n}$

Are other values of n possible?

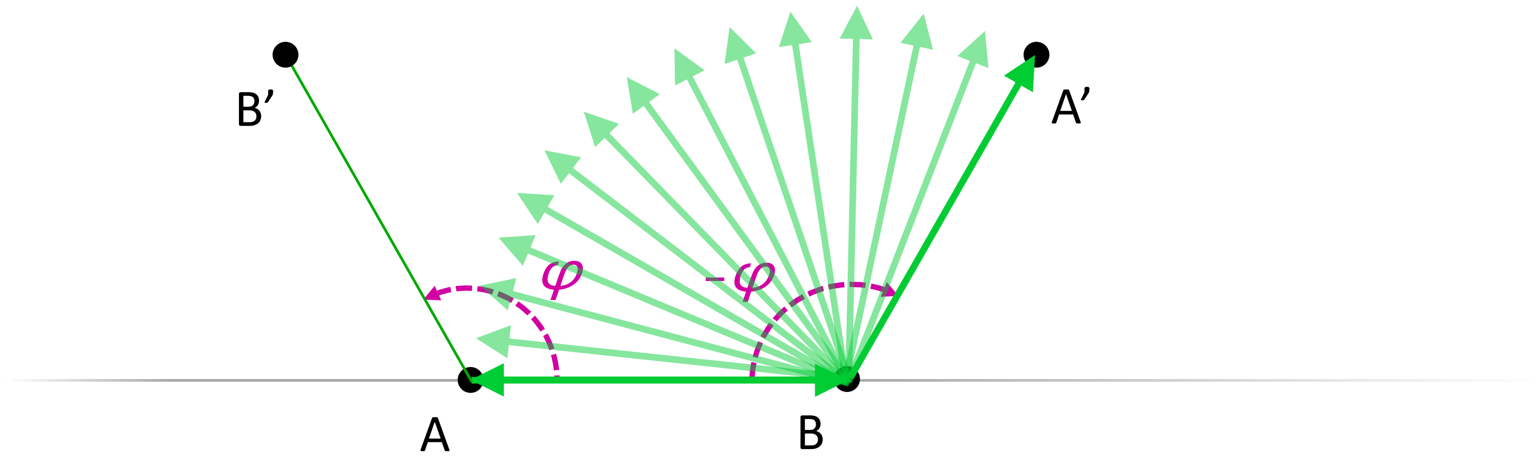
The rotation axes compatible with the crystal lattice

axis A_n of angle φ **in A**



The rotation axes compatible with the crystal lattice

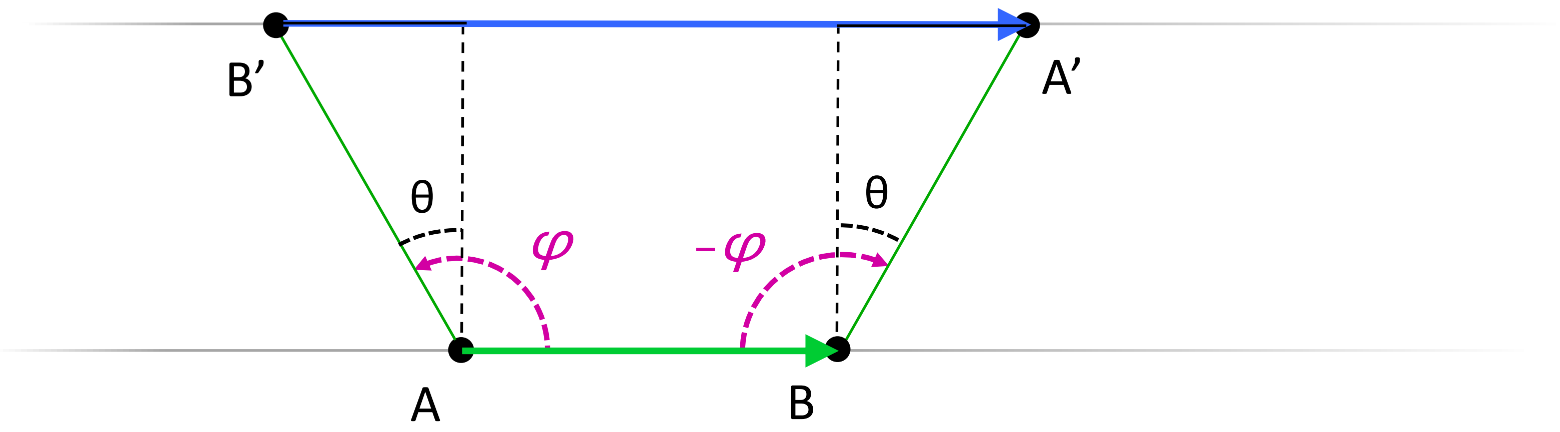
axis A_n of angle φ **in A** **in B**



The rotation axes compatible with the crystal lattice

What are the possible values of φ?

$$\varphi = \frac{2\pi}{n}$$?



B'A' = k AB with k an integer

B'A' = AB + 2 AB' sinθ where θ= φ – π/2

= AB (1 – 2 cosφ)

The rotation axes compatible with the crystal lattice

What are the possible values of φ?

$$\varphi = \frac{2\pi}{n}$$

?

B'A' = k AB

B'A' = (1 – 2 cos φ) AB

identification

$$\cos\varphi = \frac{1 - k}{2}$$

with $-1 \leq \cos\varphi \leq +1$

The rotation axes compatible with the crystal lattice

k	0	1	2	3	~~4~~	-1
$\cos\varphi = \frac{1 - k}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	-1	impossible!	1
$\varphi = \frac{2\pi}{n}$	$\frac{\pi}{3}$	$\frac{\pi}{2}$	$\frac{2\pi}{3}$	π		0
n	6	4	3	2		1
						identity

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

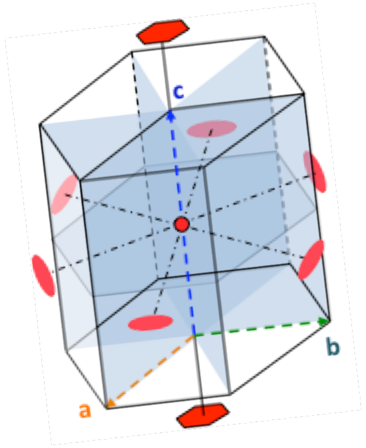
9 – Roto-inversions

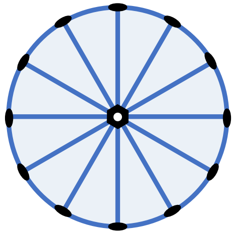
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

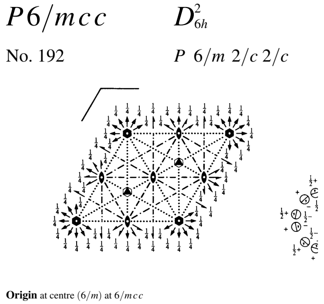
12 – The 14 Bravais lattices

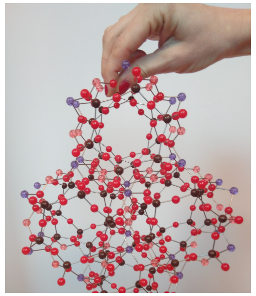
13 – The 230 space-groups



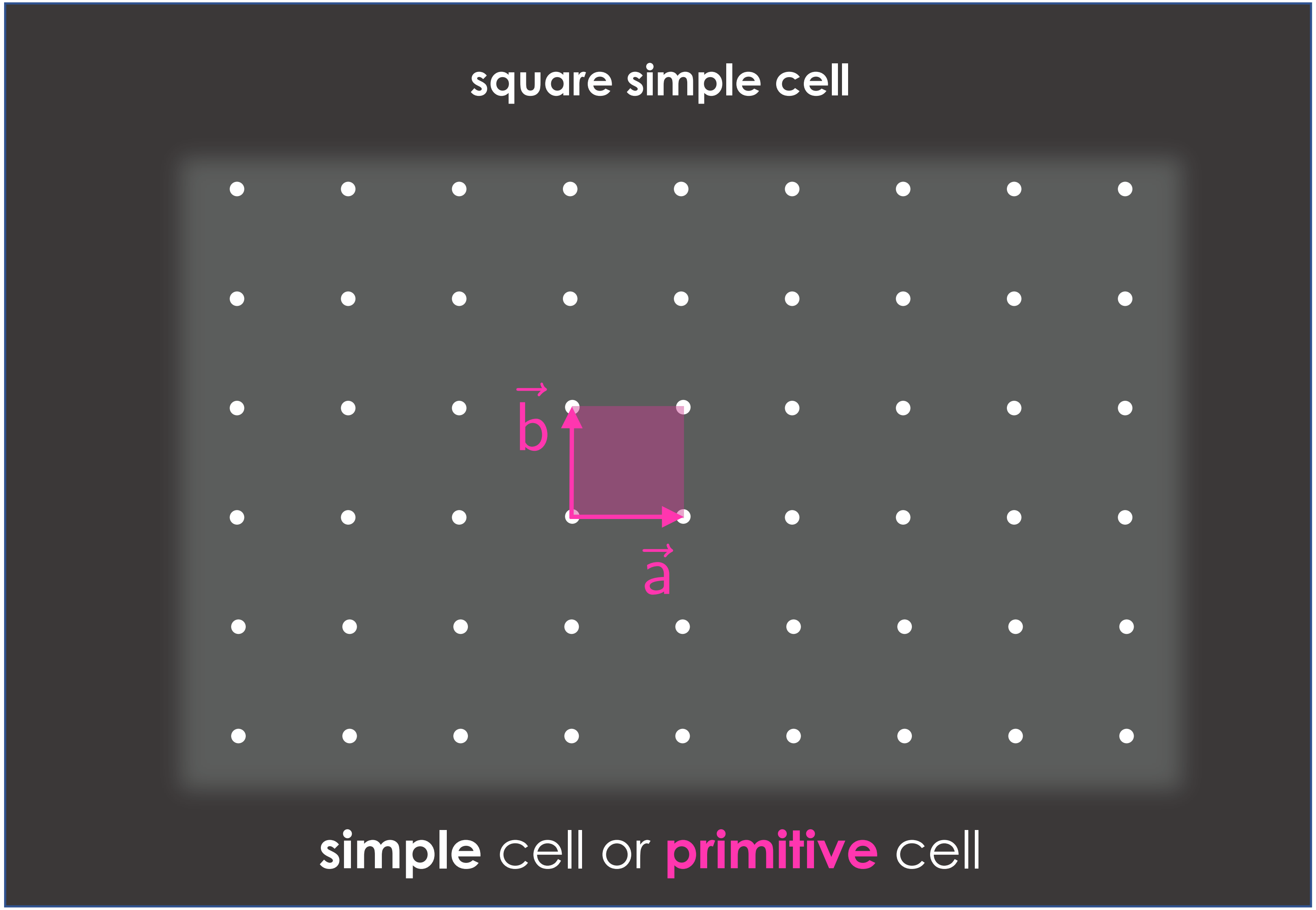


$\frac{6}{m}mm$





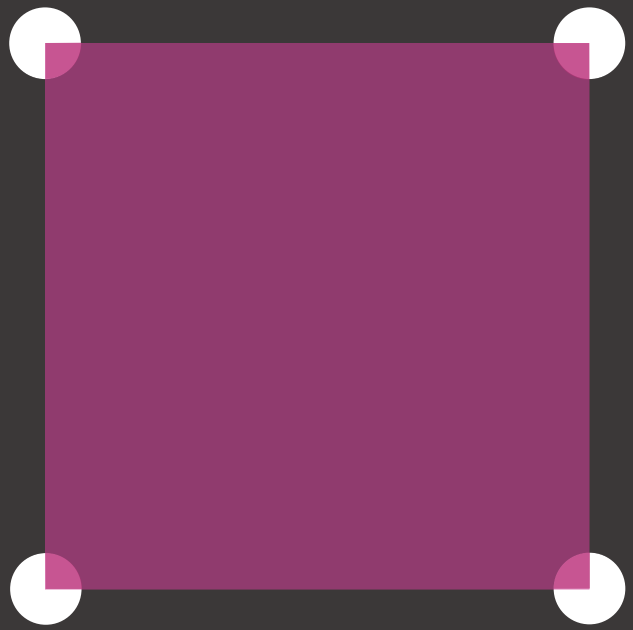
7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)

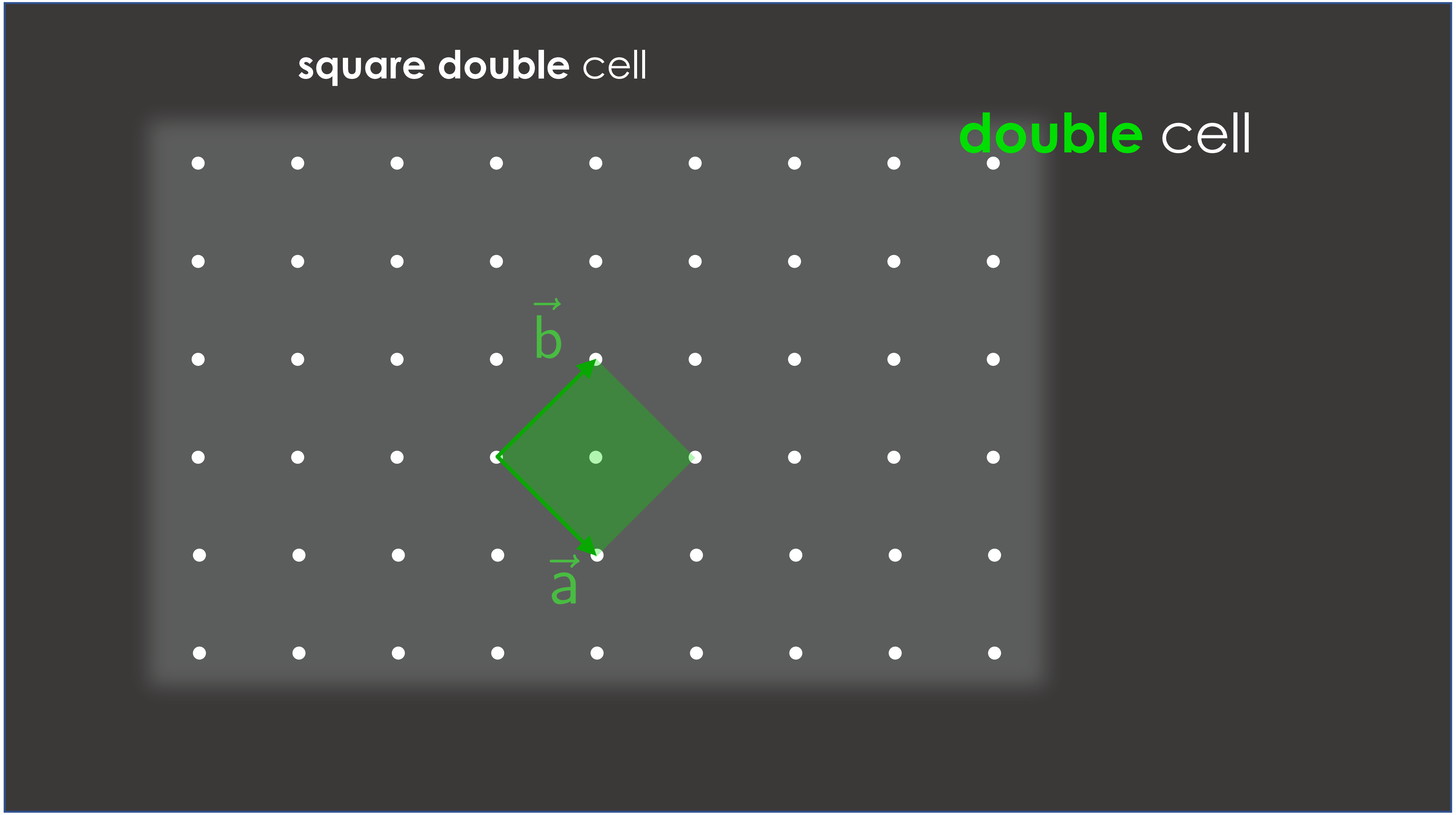
only 1 lattice point/cell

$$\frac{1}{4}+\frac{1}{4}+\frac{1}{4}+\frac{1}{4}=\mathbf{1}$$



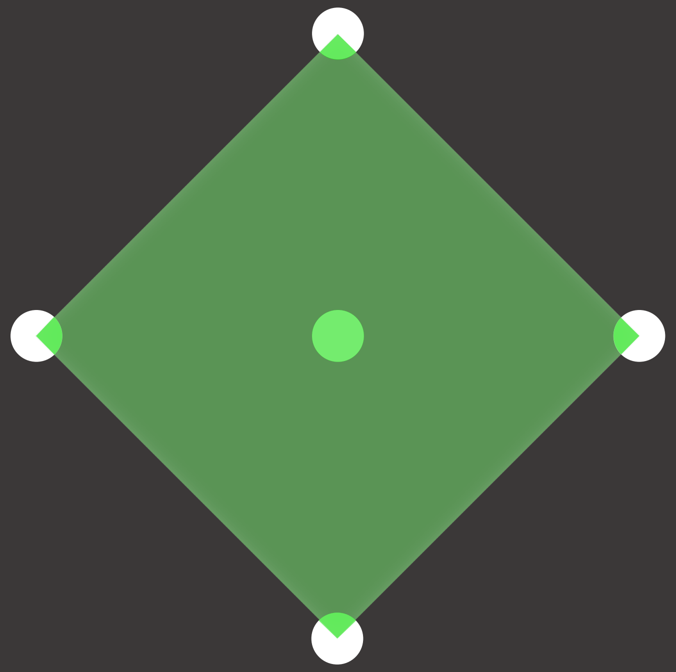
simple cell or **primitive** cell

7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)

square double cell



double cell

$$\frac{1}{4}+\frac{1}{4}+\frac{1}{4}+\frac{1}{4}+1=\mathbf{2}$$

2 lattice points /cell

7 – Conventional cell (=unit cell)

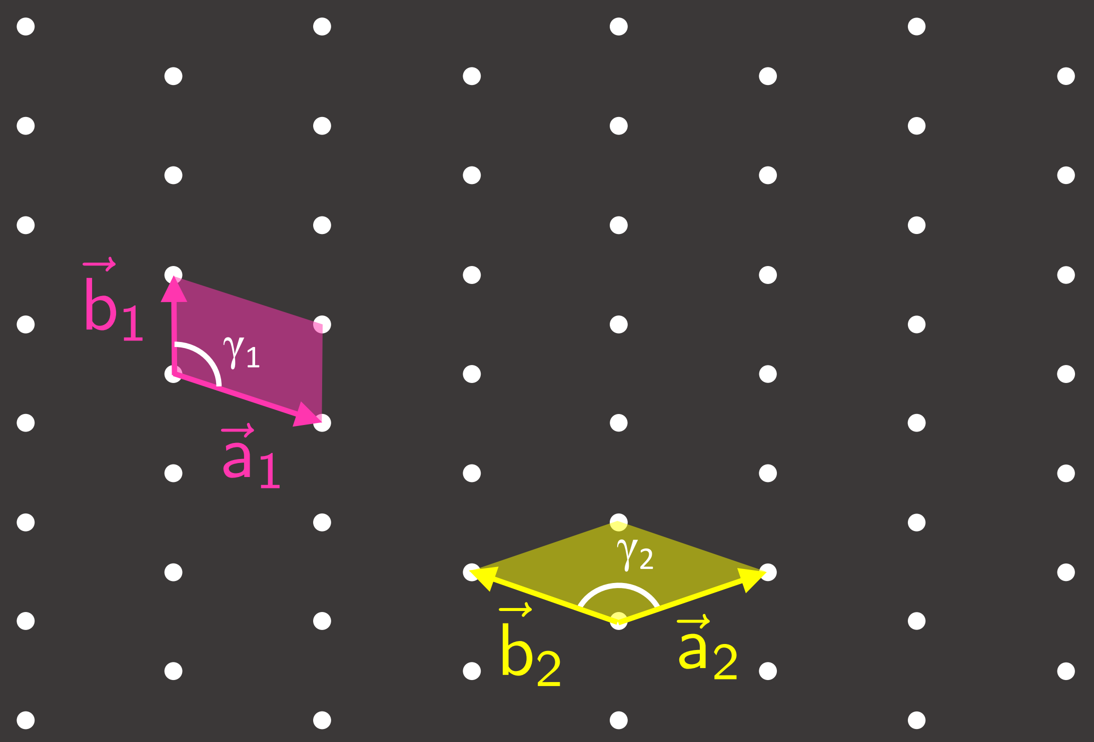
Visualize 2 simple cells with different shapes

cell 1

$a_1 \neq b_1, \gamma_1 \neq 90°$

cell 2

$a_2 = b_2, \gamma_2 \neq 90°$



7 – Conventional cell (=unit cell)

Visualize a **centred double cell**

cell 1

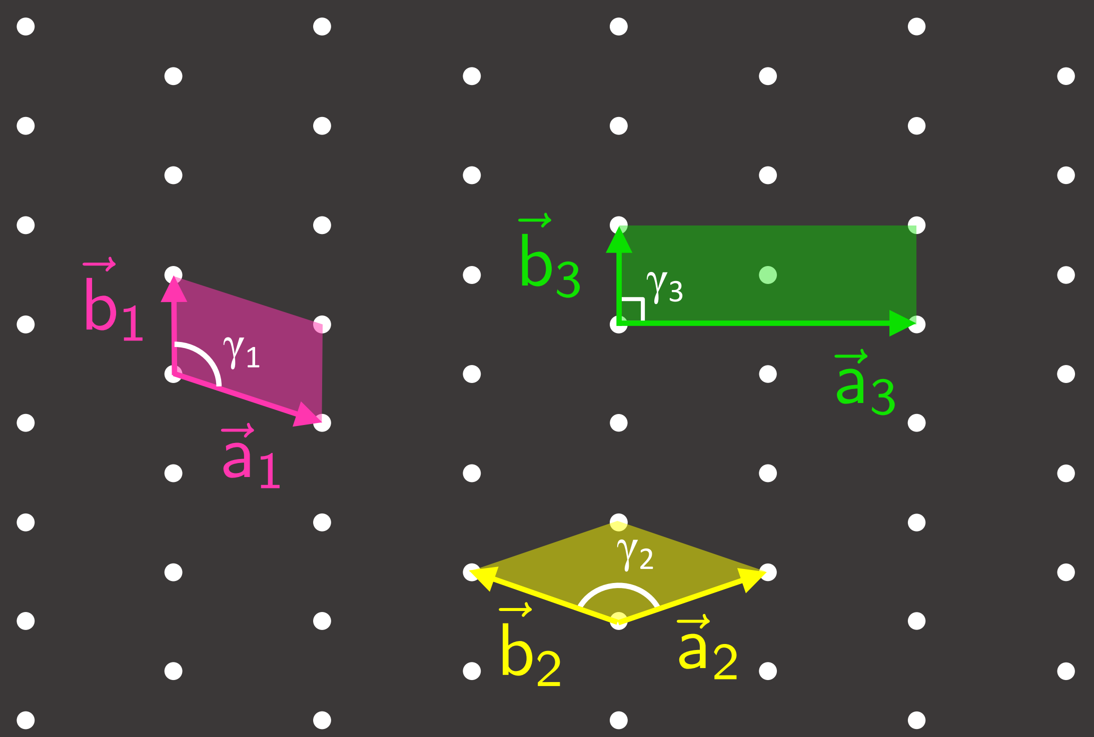
$a_1 \neq b_1, \gamma_1 \neq 90°$

cell 2

$a_2 = b_2, \gamma_2 \neq 90°$

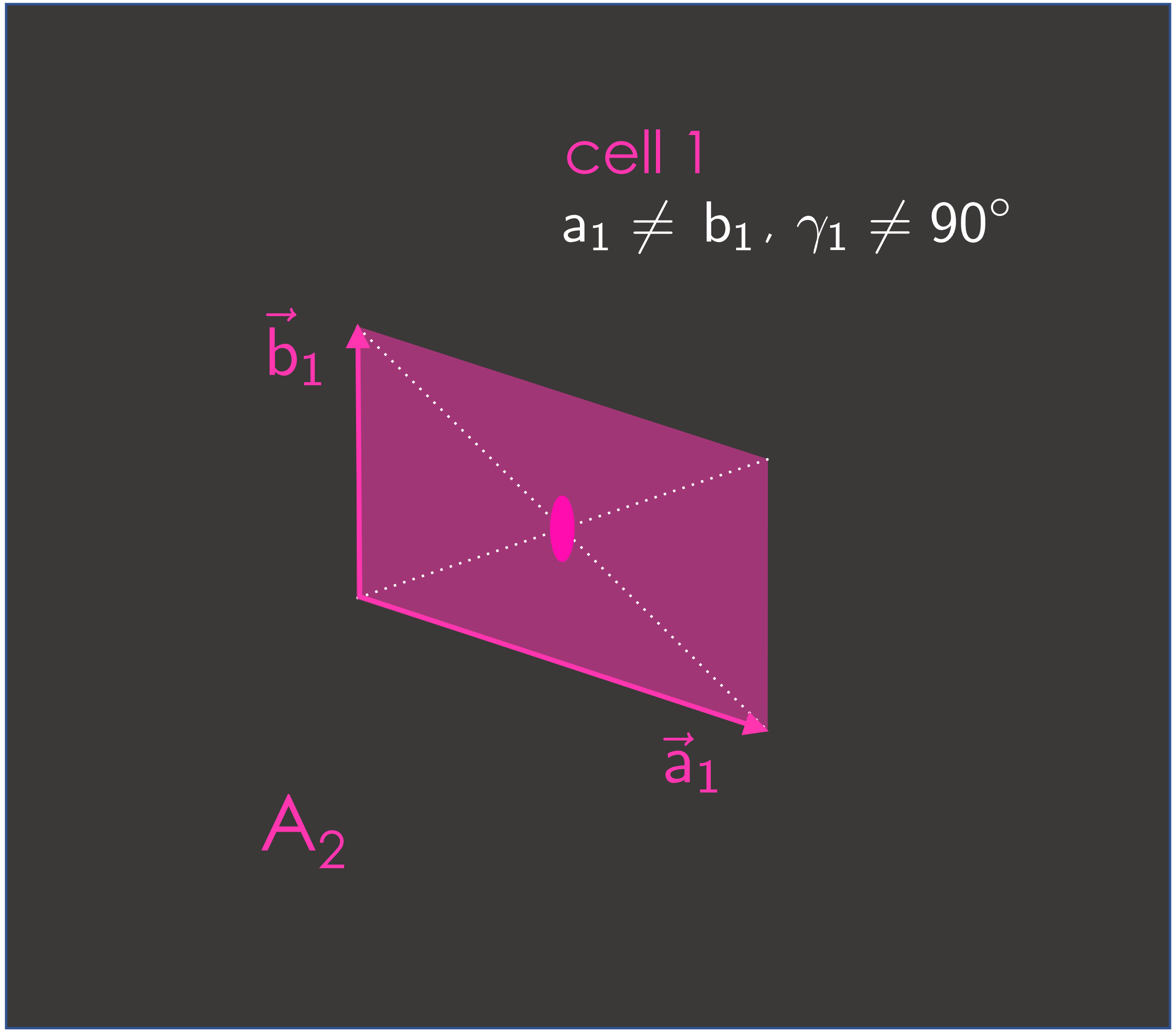
cell 3

$a_3 \neq b_3, \gamma_3 = 90°$

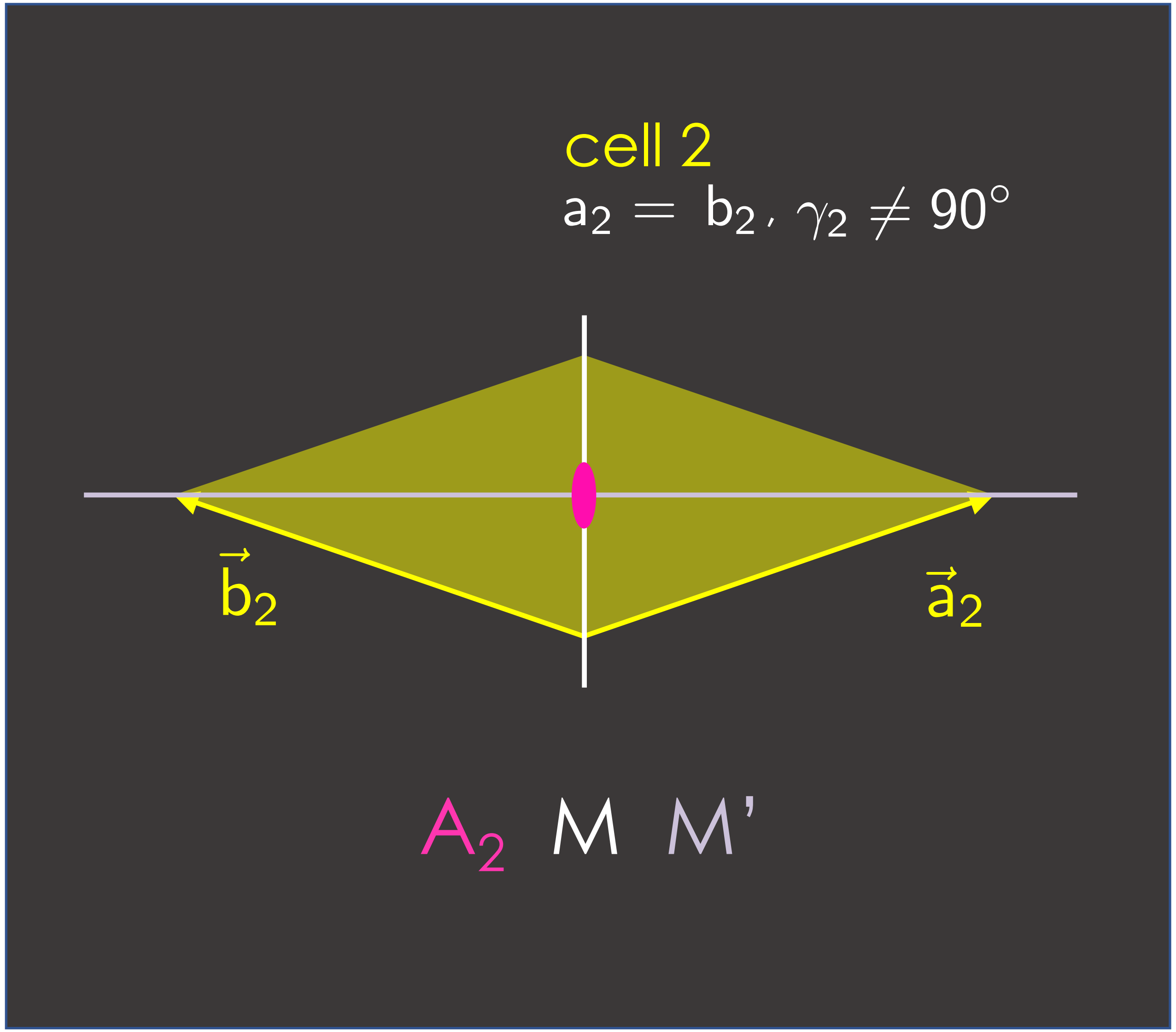


conventional cell?

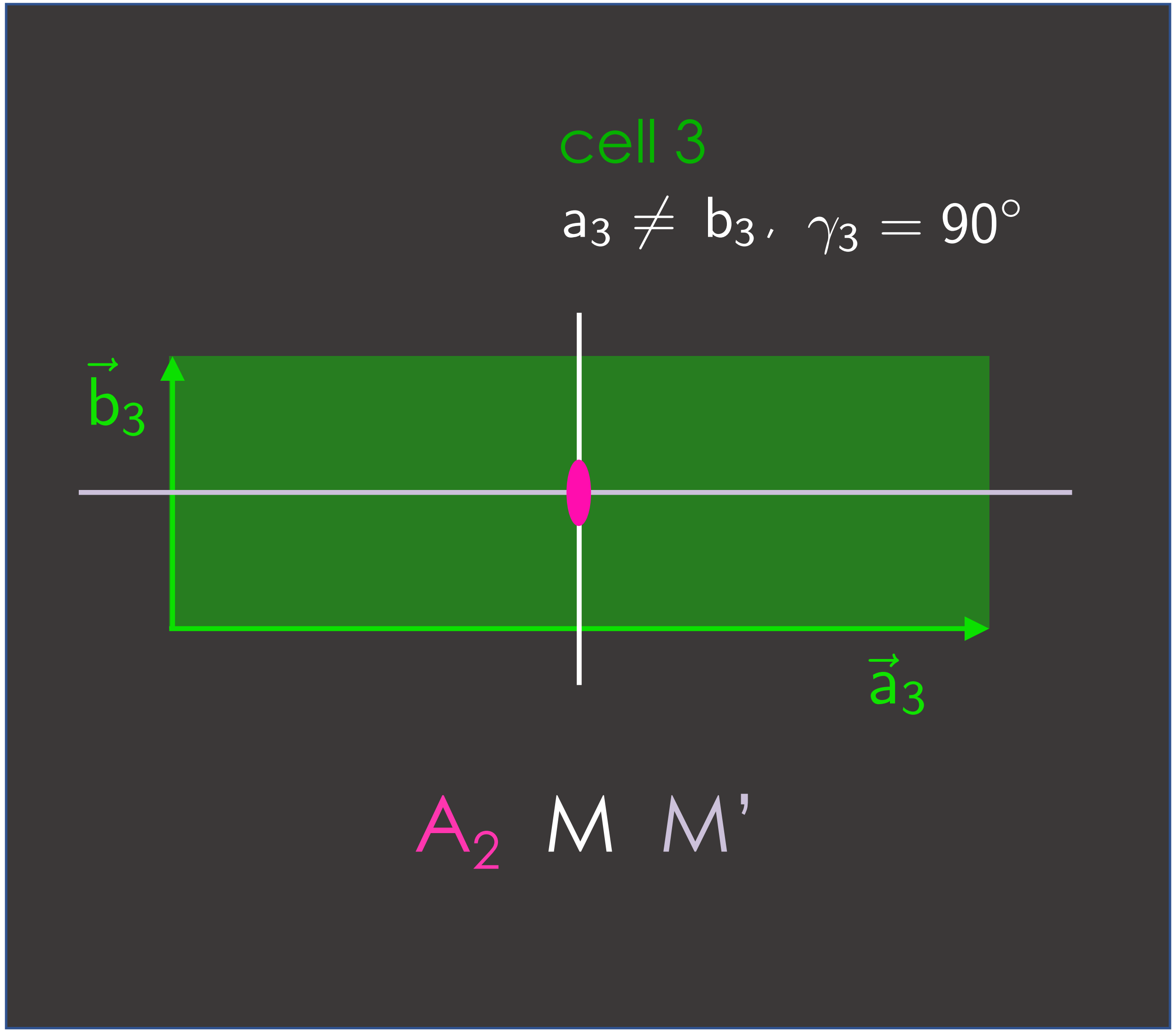
7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)



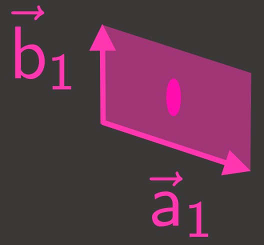
7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)

cell 1: simple

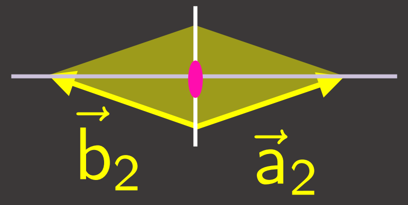
$a_1 \neq b_1, \gamma_1 \neq 90°$



A_2

cell 2: simple

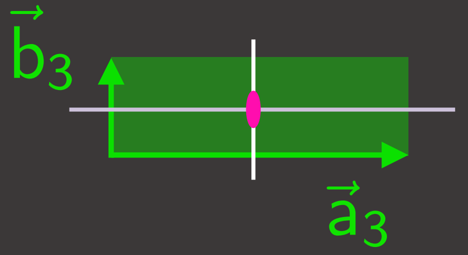
$a_2 = b_2, \gamma_2 \neq 90°$



A_2 M M'

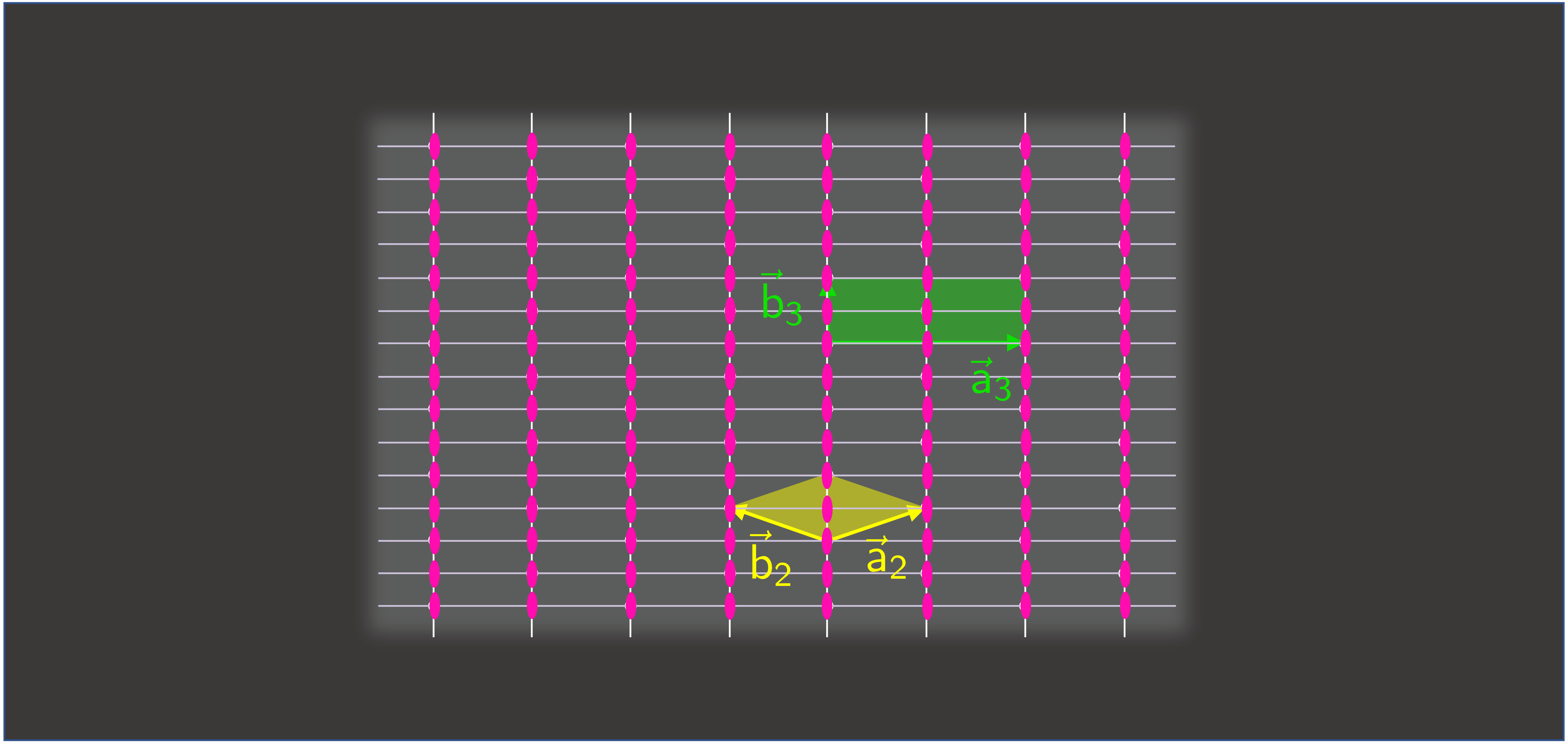
cell 3: double

$a_3 \neq b_3, \gamma_3 = 90°$



A_2 M M'

7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)

conventional cell

- it has the symmetry as the lattice
- its axes are parallel
  to symmetry directions of the lattice
- it can be a supercell (it is not always primitive)

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

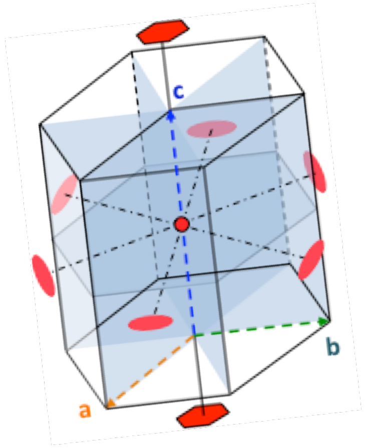
9 – Roto-inversions

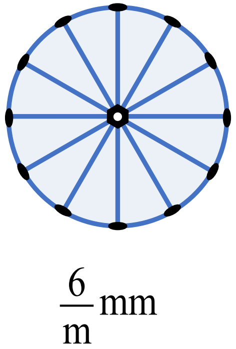
10 – The 32 crystallographic point groups

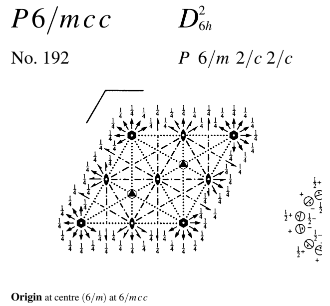
11 – The 7 crystal systems

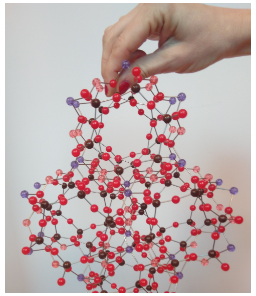
12 – The 14 Bravais lattices

13 – The 230 space-groups



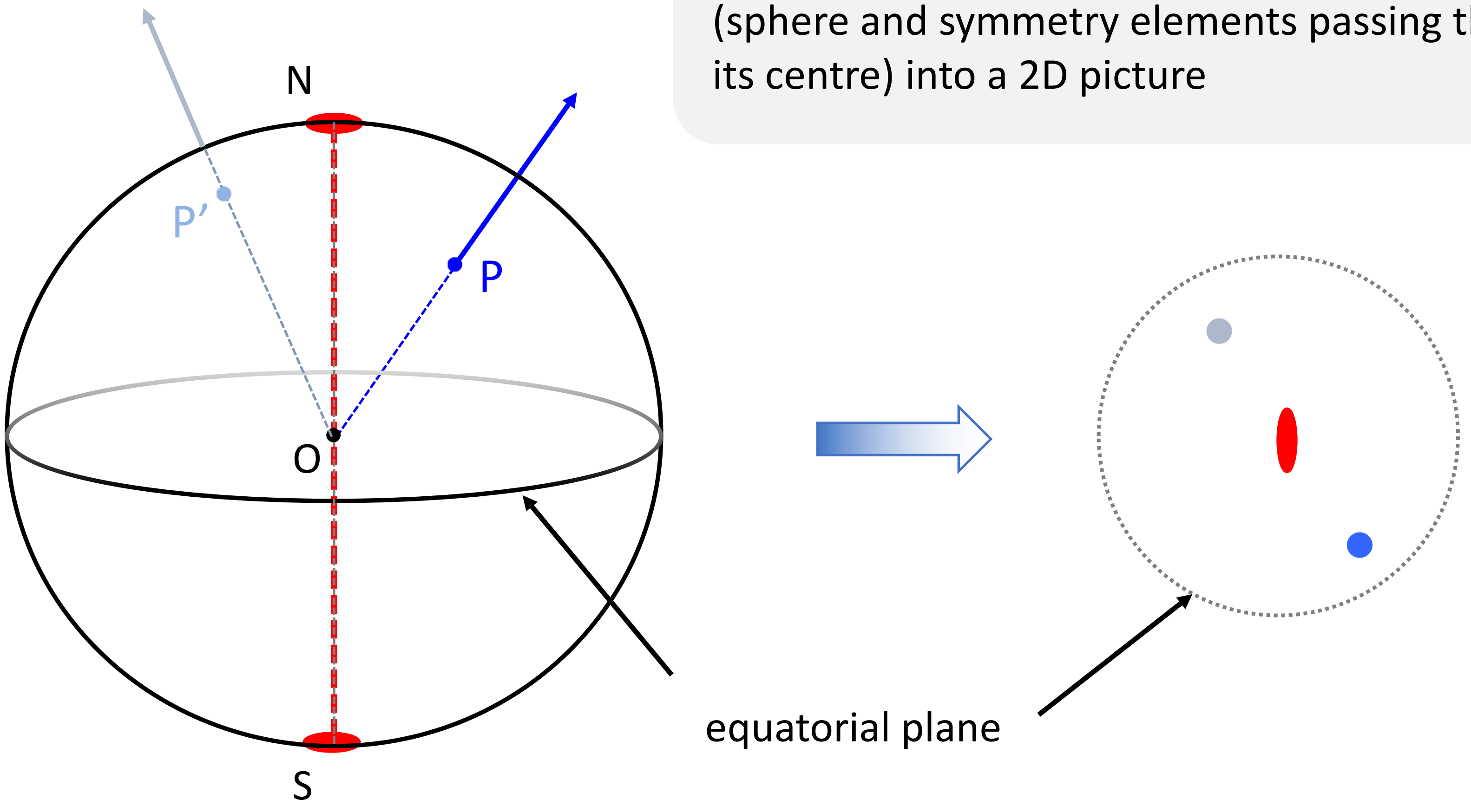






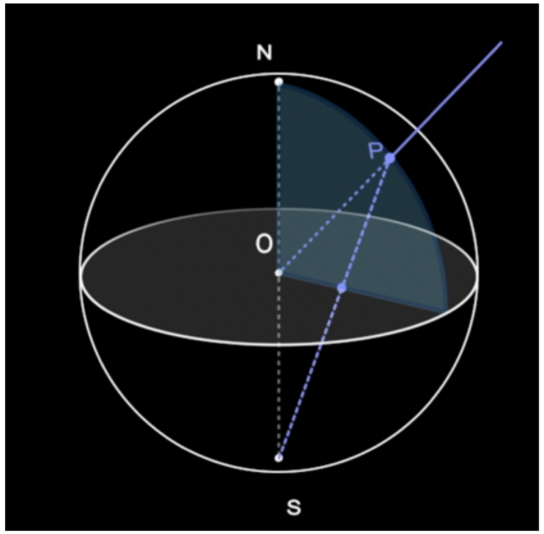
8 – Stereographic projection

Stereographic projection:
way of representing geometric objects of the 3D space (sphere and symmetry elements passing through its centre) into a 2D picture



8 – Stereographic projection

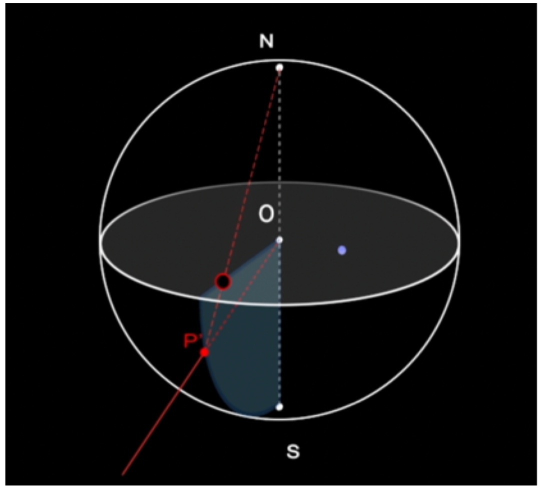
- Given a half-line OP in the North hemisphere starting from O and crossing the sphere in point P.
- The stereographic projection of OP is the intersection point of [PS] with the equatorial plane.
- It is represented (here) by a dot: ●.

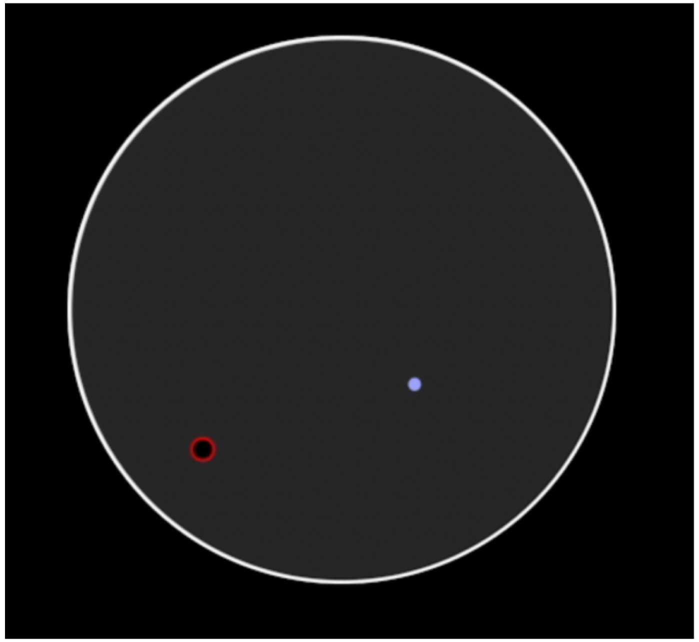


- Given a half-:ine OP’ in the South hemisphere starting from O and crossing the sphere in point P’.

•The stereographic projection of OP’ is the intersection point of [P’N] with the equatorial plane.

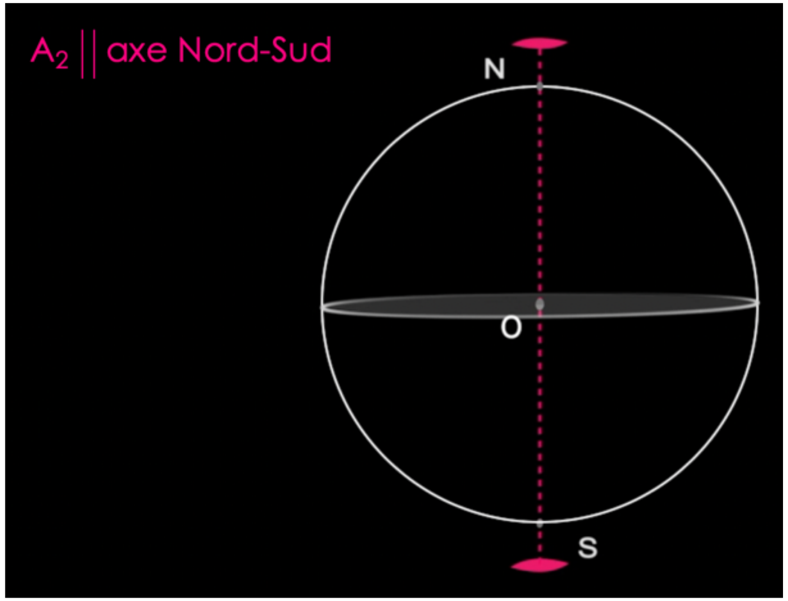
- It is represented by a small circle: **o**.

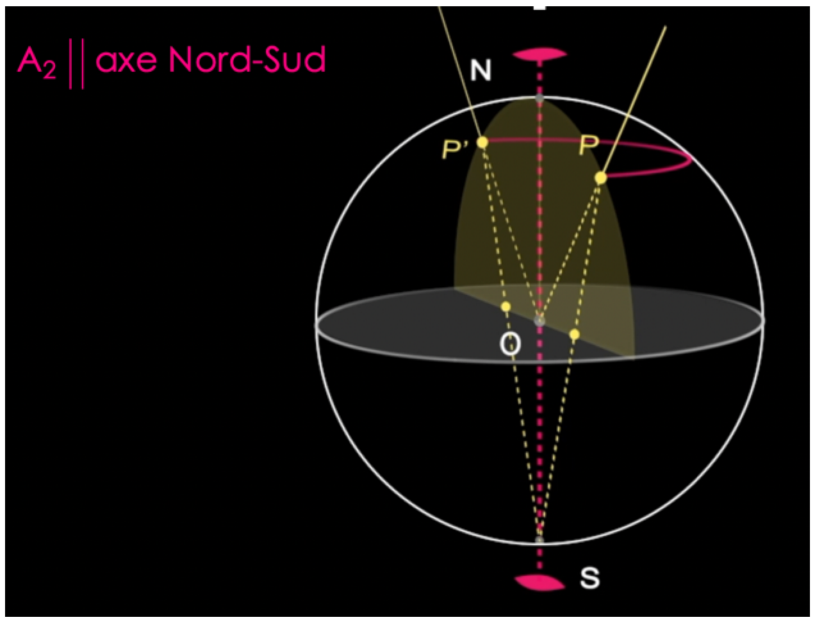


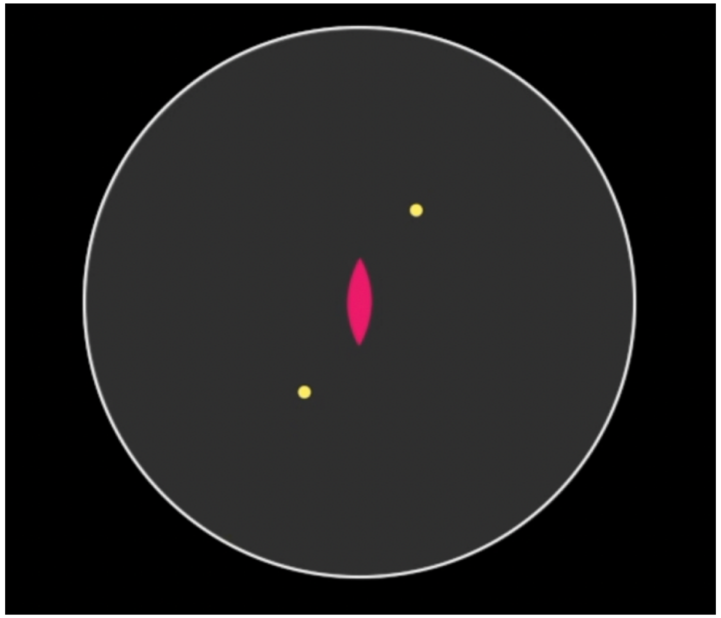


8 – Stereographic projection

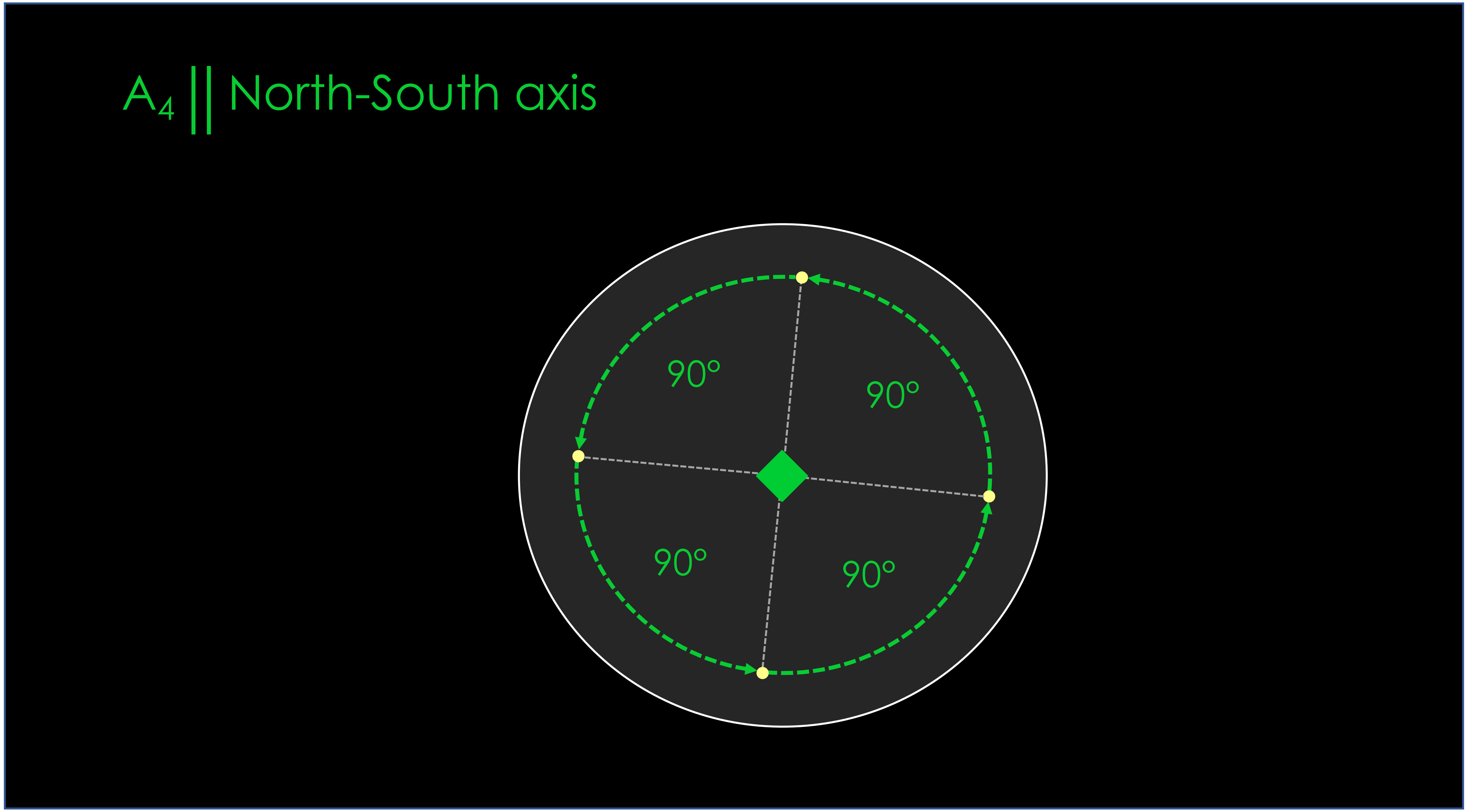
A_2 || North-South axis



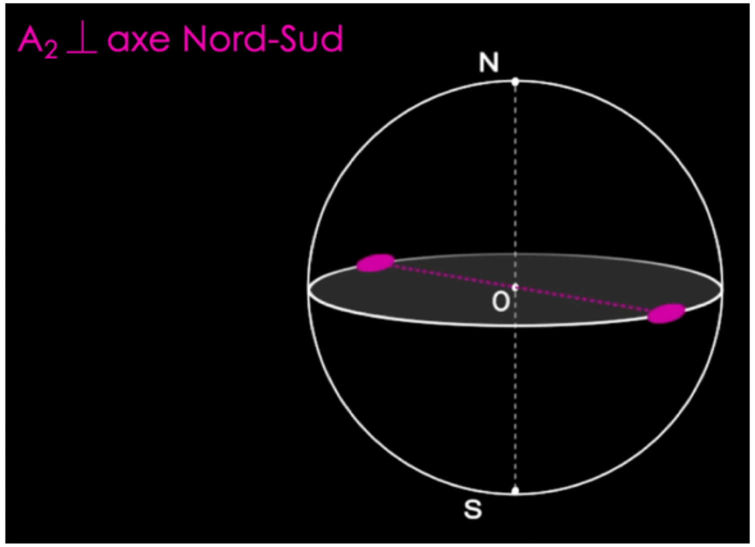




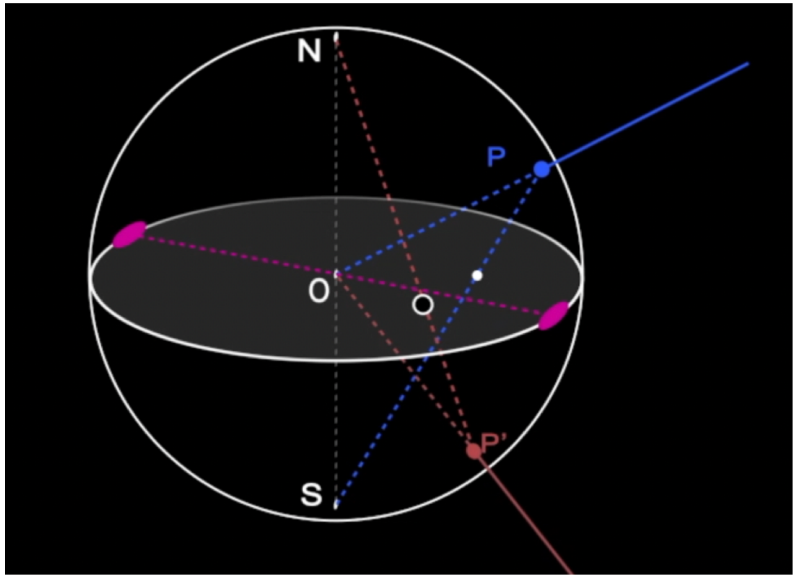
8 – Stereographic projection

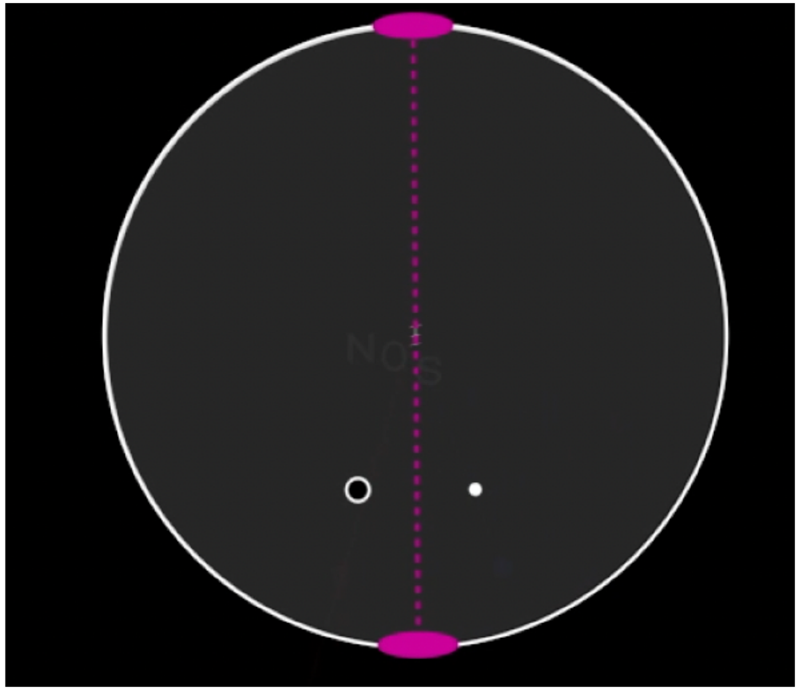


8 – Stereographic projection

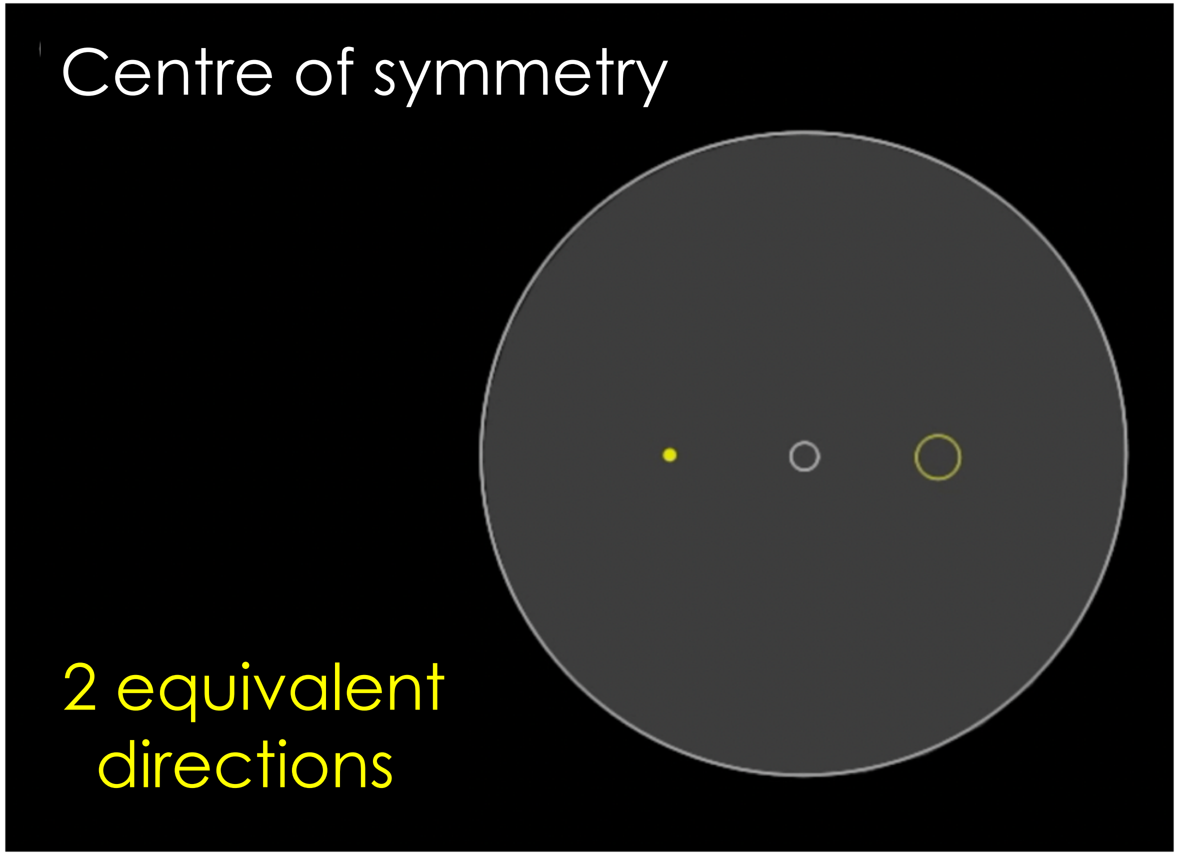


$A_2 \perp$ North-South axis

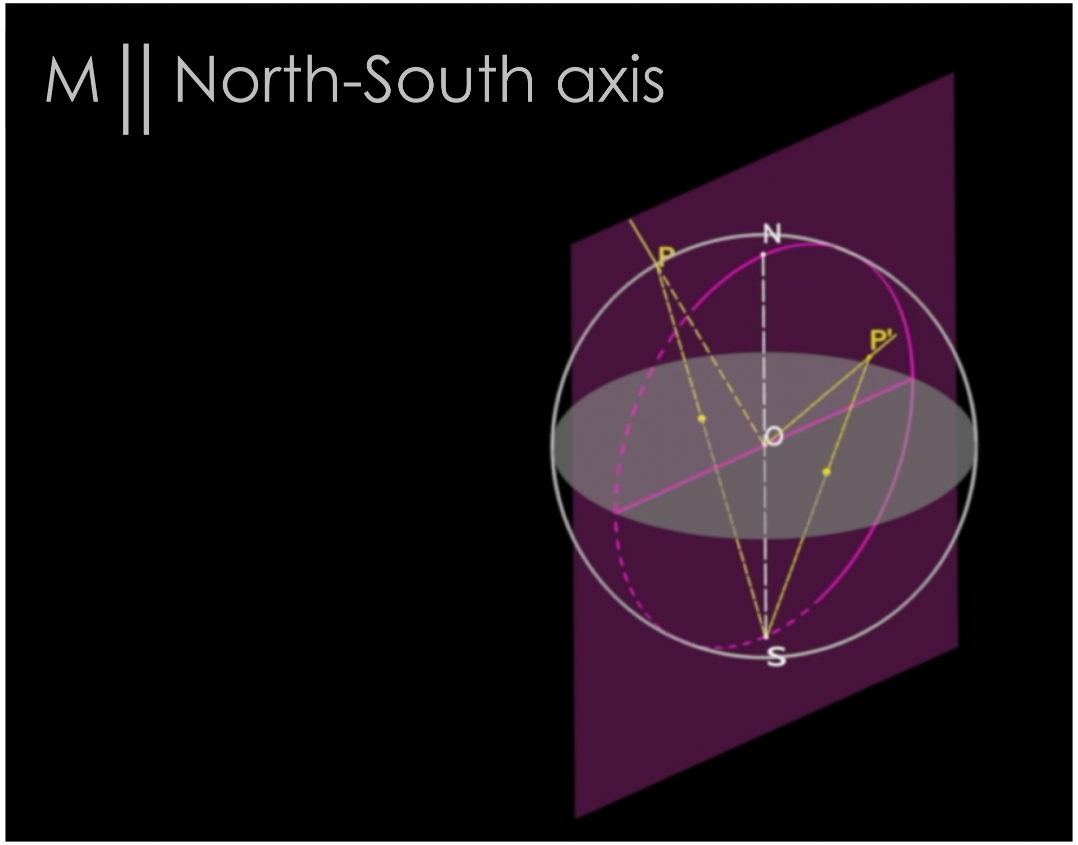


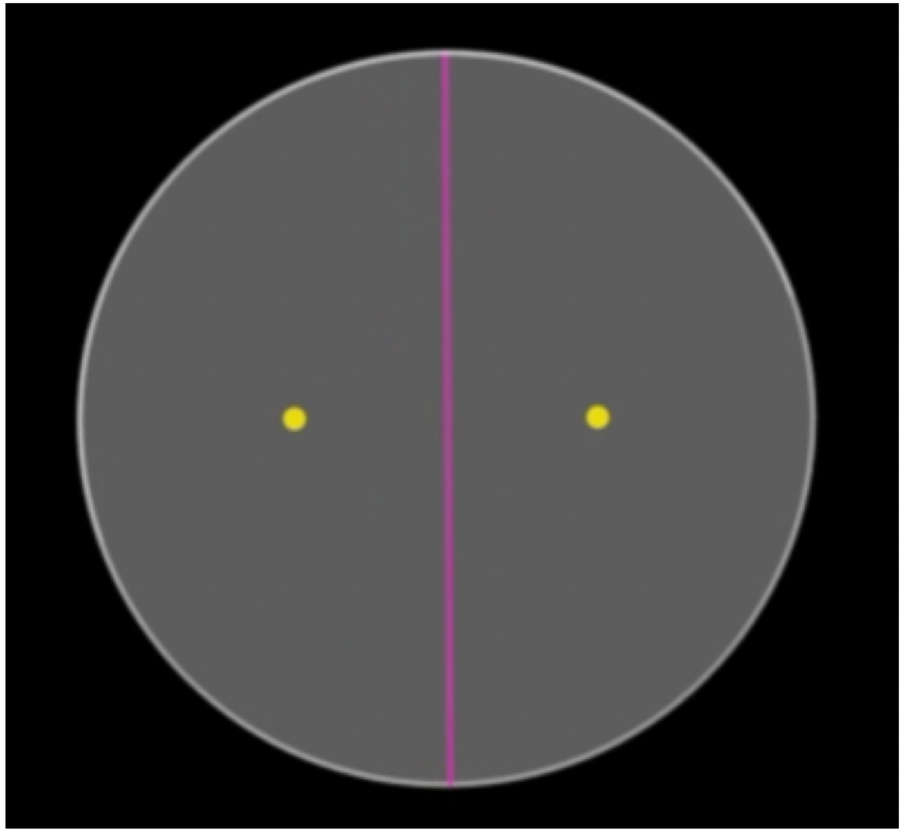


8 – Stereographic projection



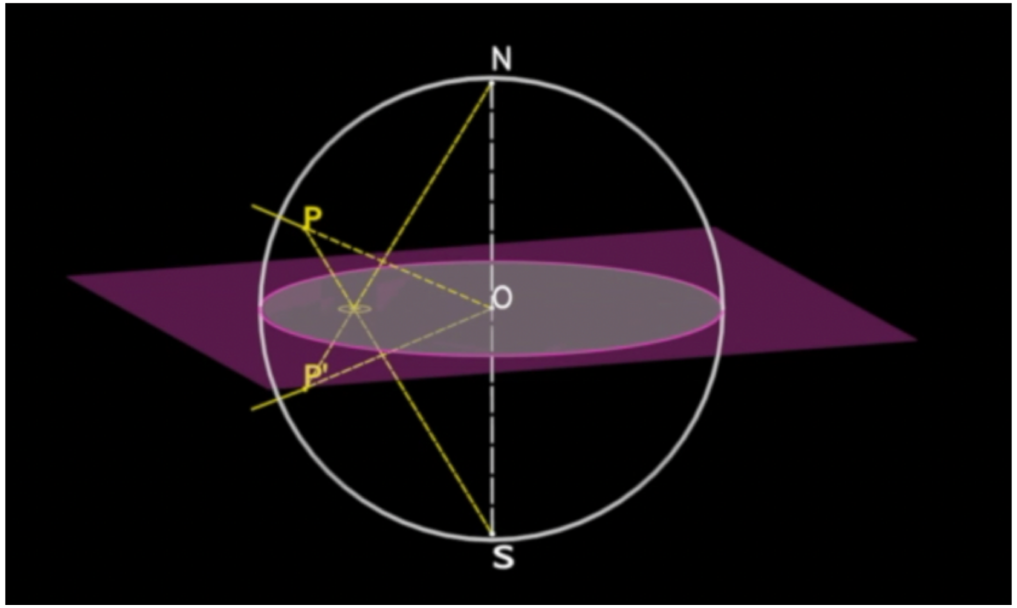
8 – Stereographic projection

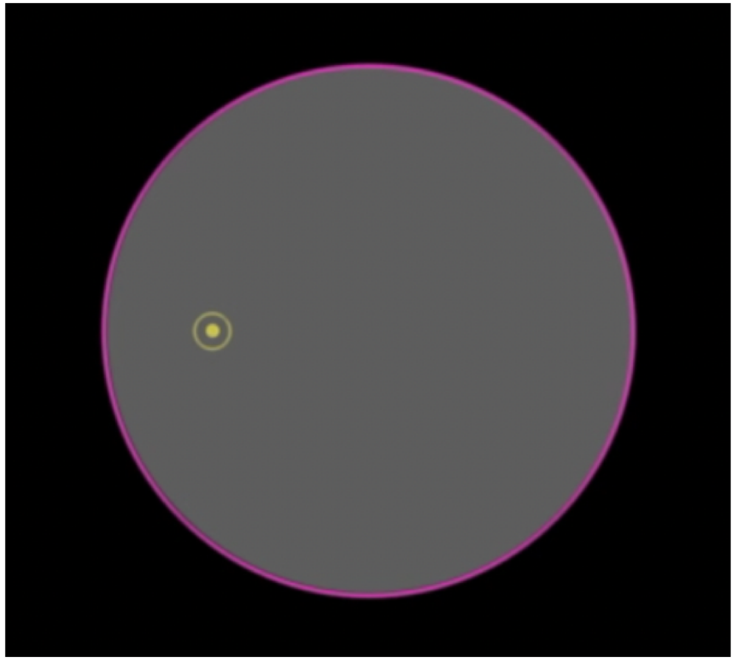




8 – Stereographic projection

M ⊥ North-South axis





Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

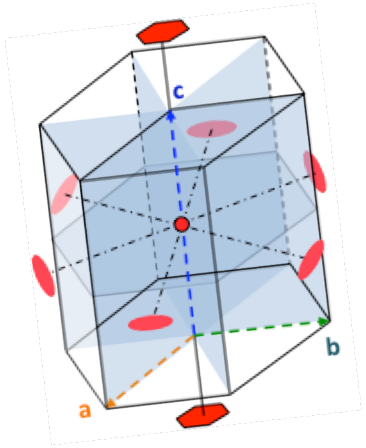
9 – Roto-inversions

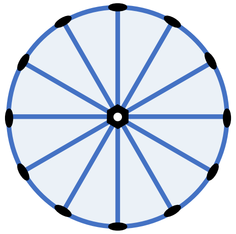
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

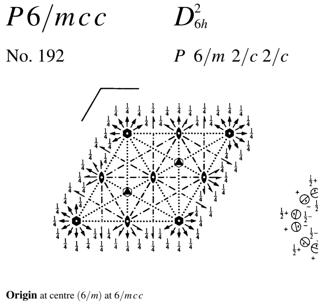
12 – The 14 Bravais lattices

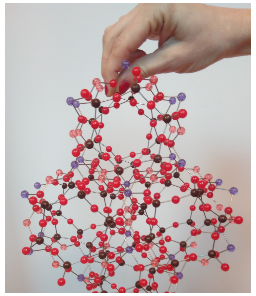
13 – The 230 space-groups





$\frac{6}{m}mm$

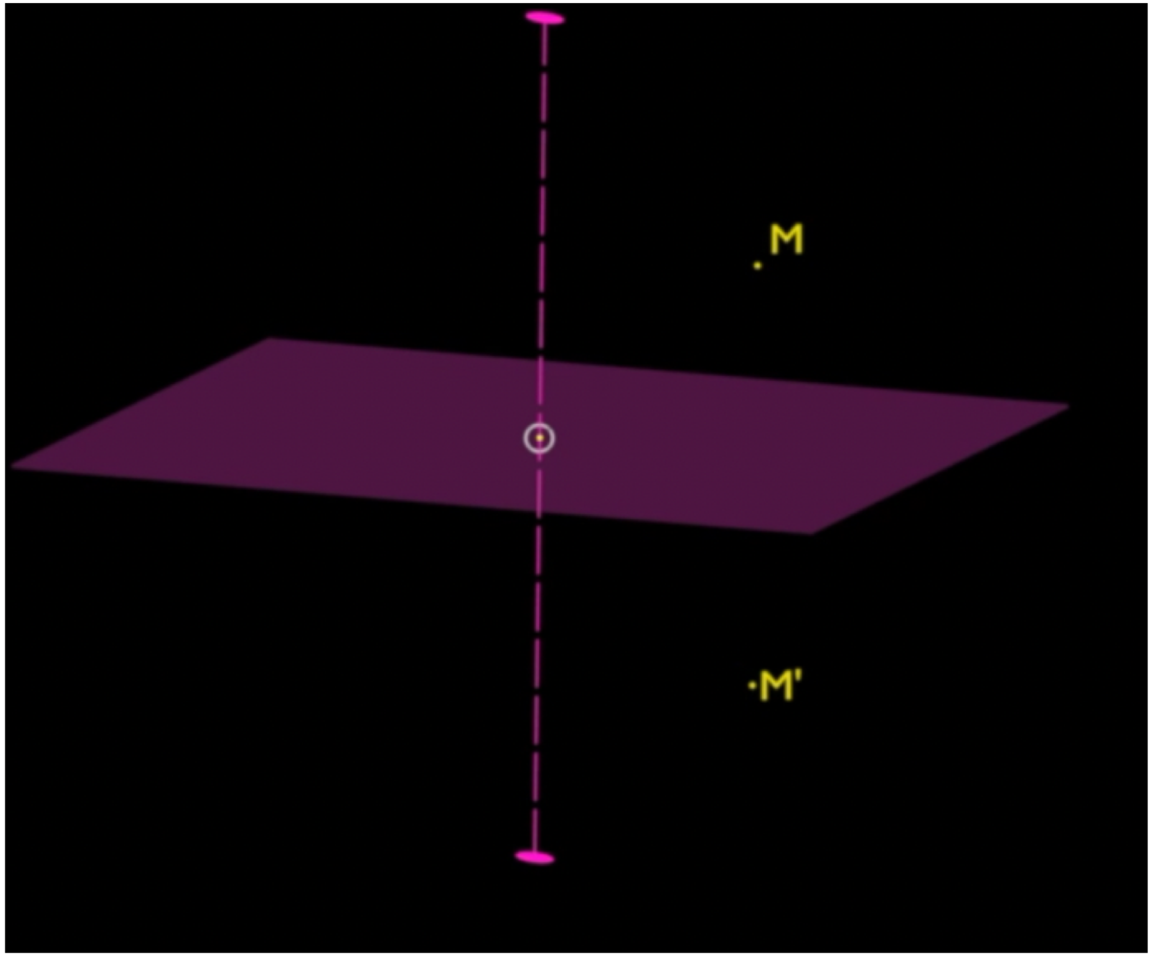




9 – Roto-inversions

$M = A_2 \times C$

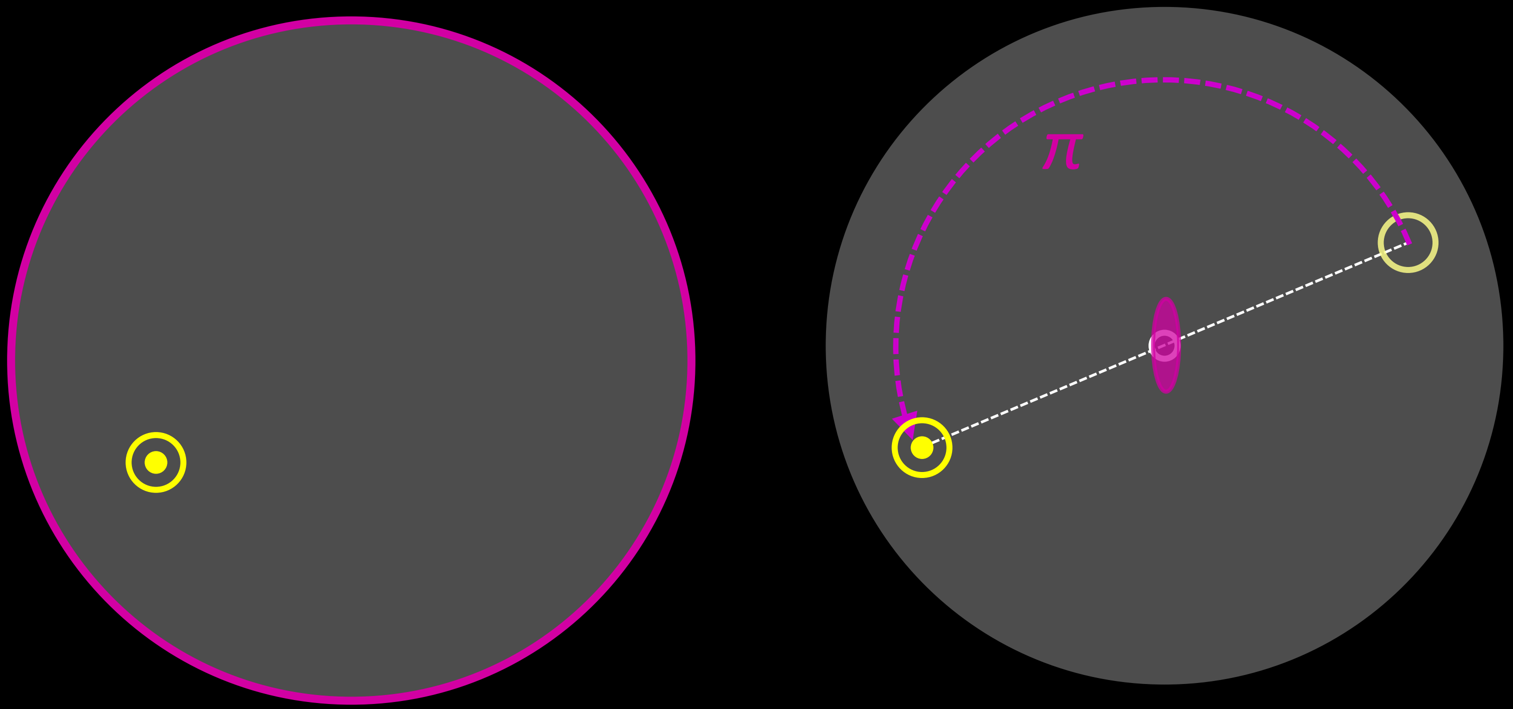
roto-inversion of order 2



$M \equiv \bar{A}_2$

9 – Roto-inversions

$M = A_2 \times C$ **roto-inversion** of order 2



$M \equiv \bar{A}_2$

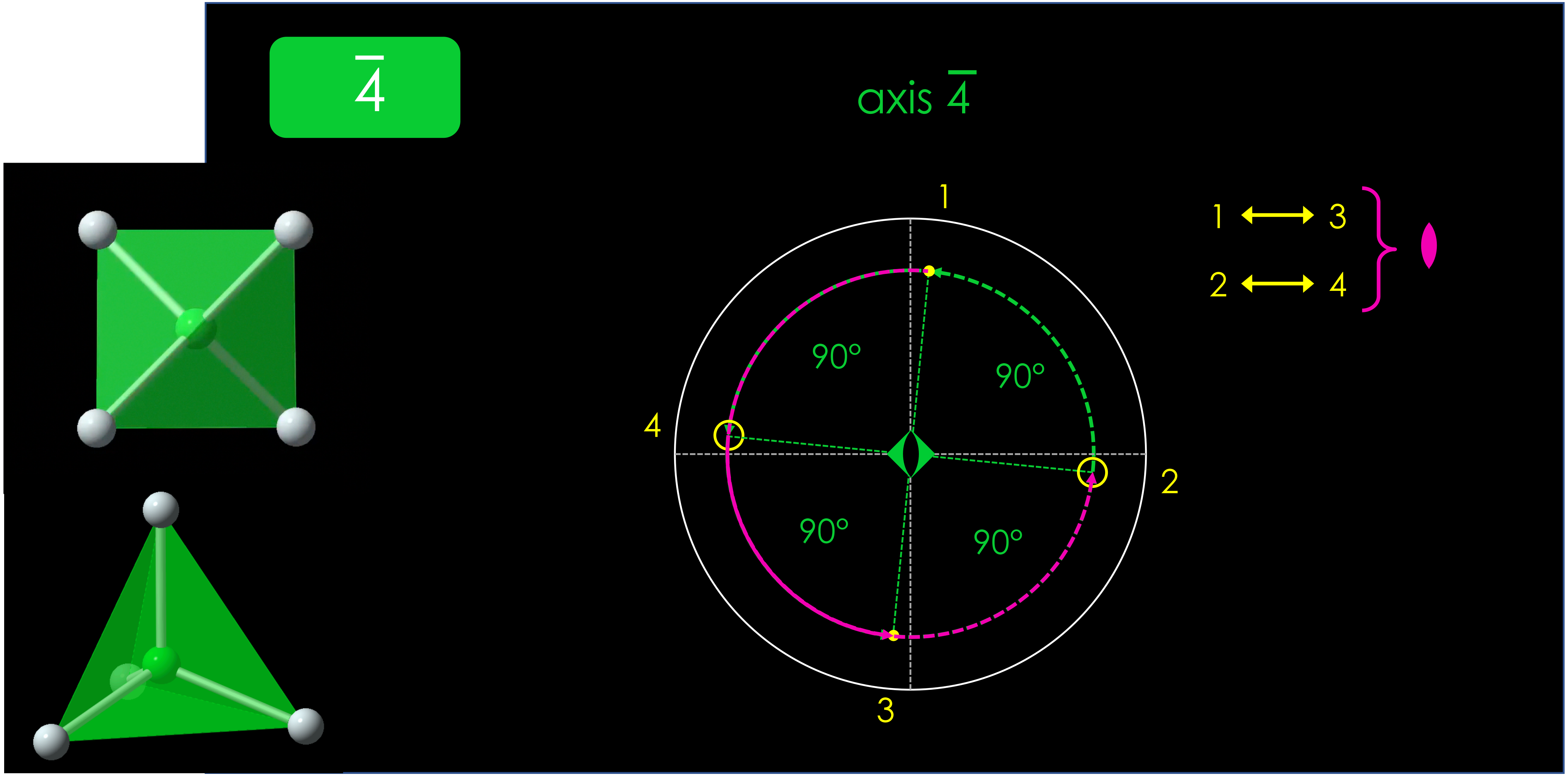
9 – Roto-inversions

A_1	A_2	A_3	A_4	A_6	
identity					
1	2	3	4	6	← Hermann-Mauguin symbols

$$\text{rotoinversion } \bar{n} = \text{rotation } \frac{2\pi}{n} \times \text{ inversion}$$

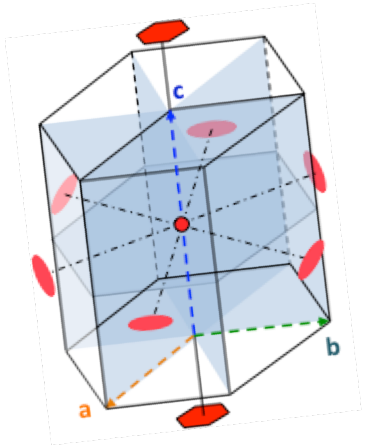
$C \equiv \bar{A}_1$	$M \equiv \bar{A}_2$	$\bar{A}_3$	$\bar{A}_4$	$\bar{A}_6$
centre				
$\bar{1}$	m	$\bar{3}$	$\bar{4}$	$\bar{6}$

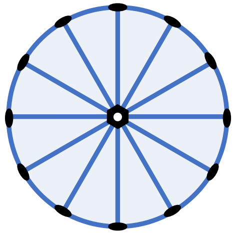
9 – Roto-inversions



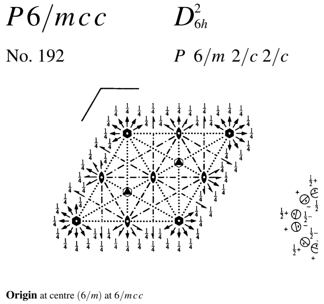
Course outline

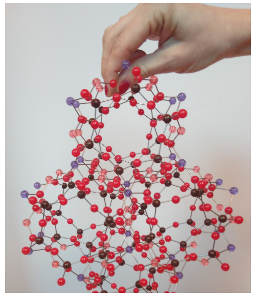
1- Symmetry observation in natural crystals
2- Internal cause of the natural crystal shape
3 – Crystal lattice, cell, motif
4 – Lattice direction and planes
5 – Reciprocal lattice
6 – Crystal lattice & symmetries
7 – Conventional cell (unit cell)
8 – Stereographic projection
9 – Roto-inversions
10 – The 32 crystallographic point groups
11 – The 7 crystal systems
12 – The 14 Bravais lattices
13 – The 230 space-groups





$\frac{6}{m}mm$





10 – The 32 crystallographic point groups

The possible ''combinations'' of the 10 rotations and rotoinversions form the **32 crystallographic point groups**, also called the **32 classes of orientation symmetry**.

crystallographic point group: set of symmetry elements that leave a central point fixed

The symmetry of the macroscopic **physical properties** of a crystal is governed by its crystallographic point group.

↳ physical properties sensitive to direction symmetries (invariant under translations)

➔ *it is important to know, for a given point group, the equivalent directions by the symmetry operations that define the group.*

10 – The 32 crystallographic point groups

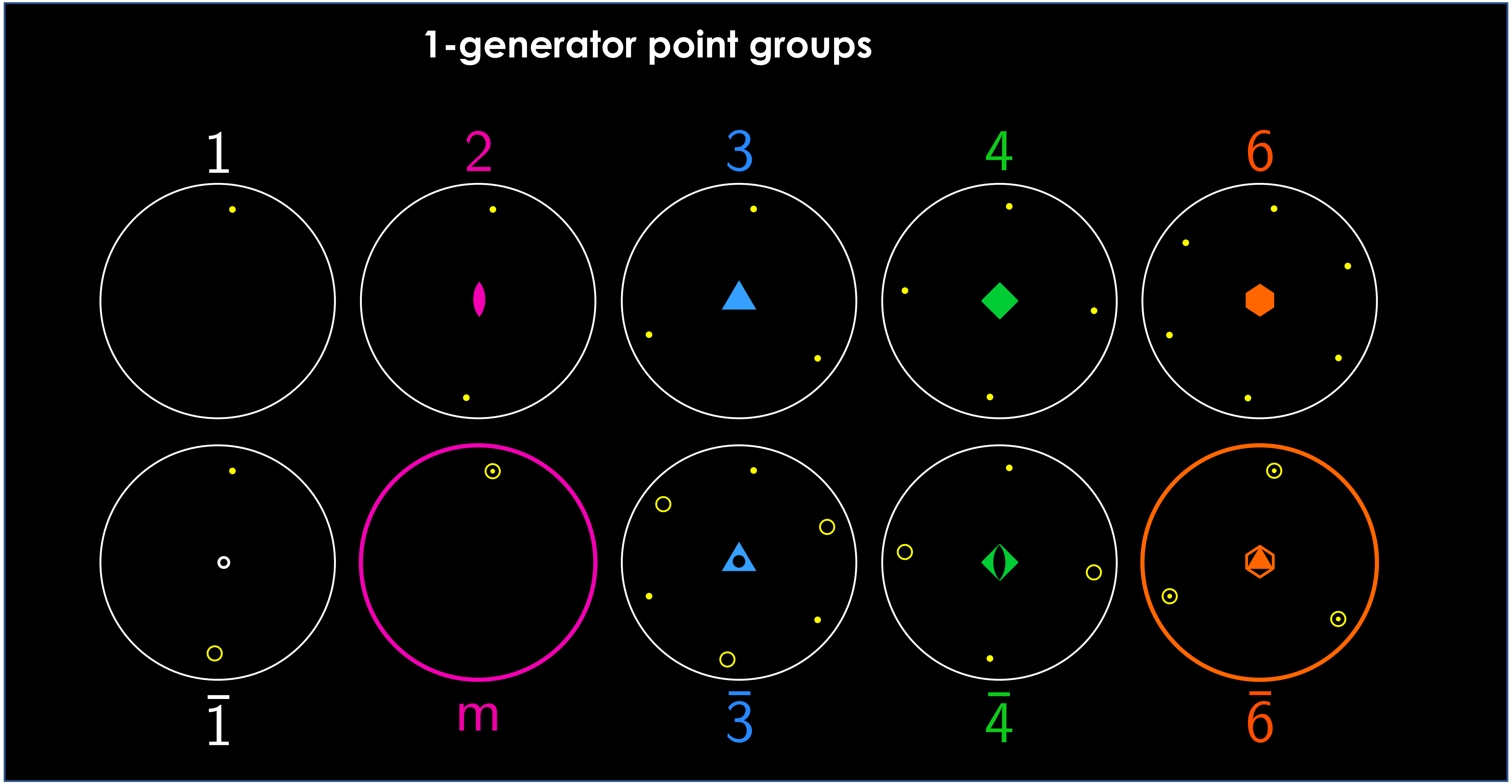
2 CATEGORIES:

- The groups containing MORE than one A_n axis with n>2
  ➔ **the 5 cubic groups**

- The other groups
  ➔ **les 27 non-cubic groups**

- We already know 10! ➔ 1-generator group
- 2- or 3-generator groups

10 – The 32 crystallographic point groups

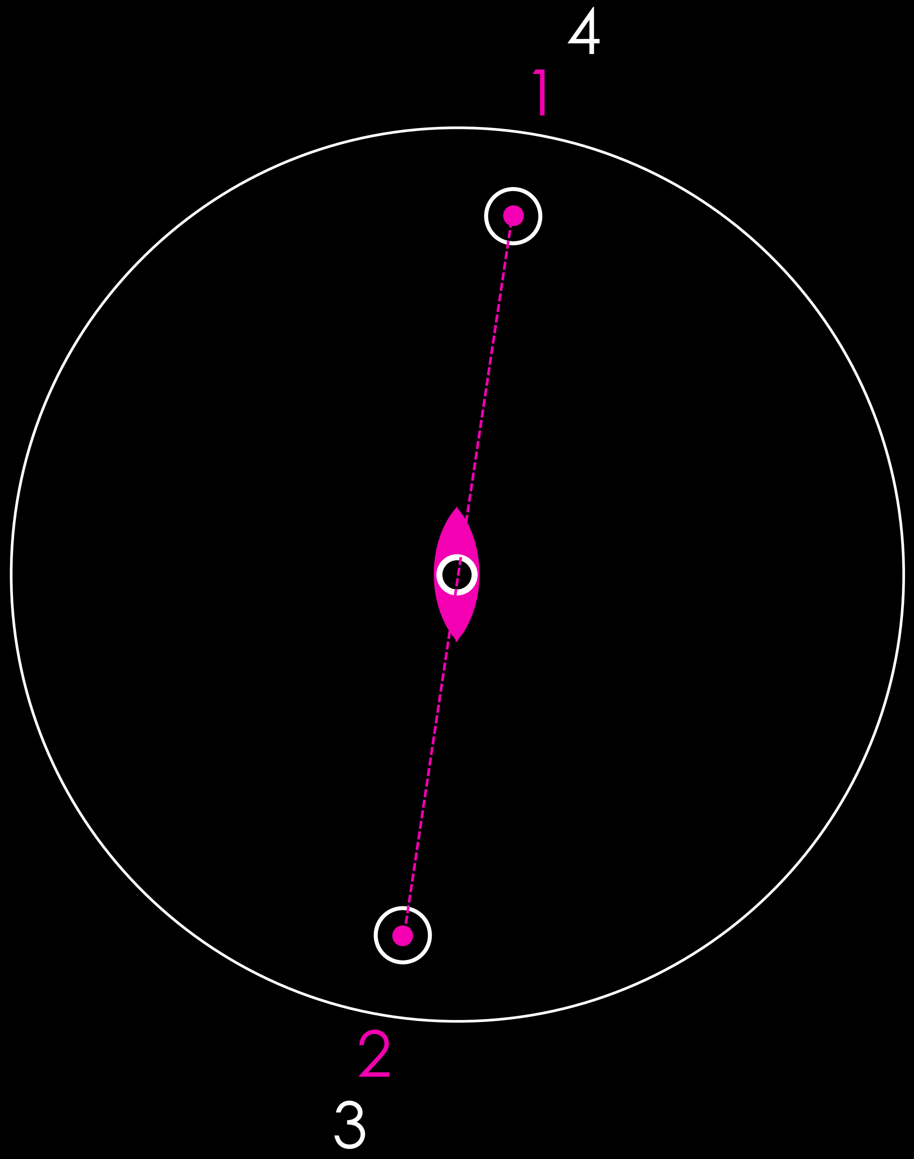


2-generator point groups

generator 1		genzrator 2
	C	C
A_2	M	M
A_3	$\bar{A}_3$	A_2
A_4	$\bar{A}_4$	$\perp$ ou $\parallel$ à A_n et $\bar{A}_n$
A_6	$\bar{A}_6$	

14 non-cubic point groups with 2 generators

A_2 & C



1 ⟶ 3

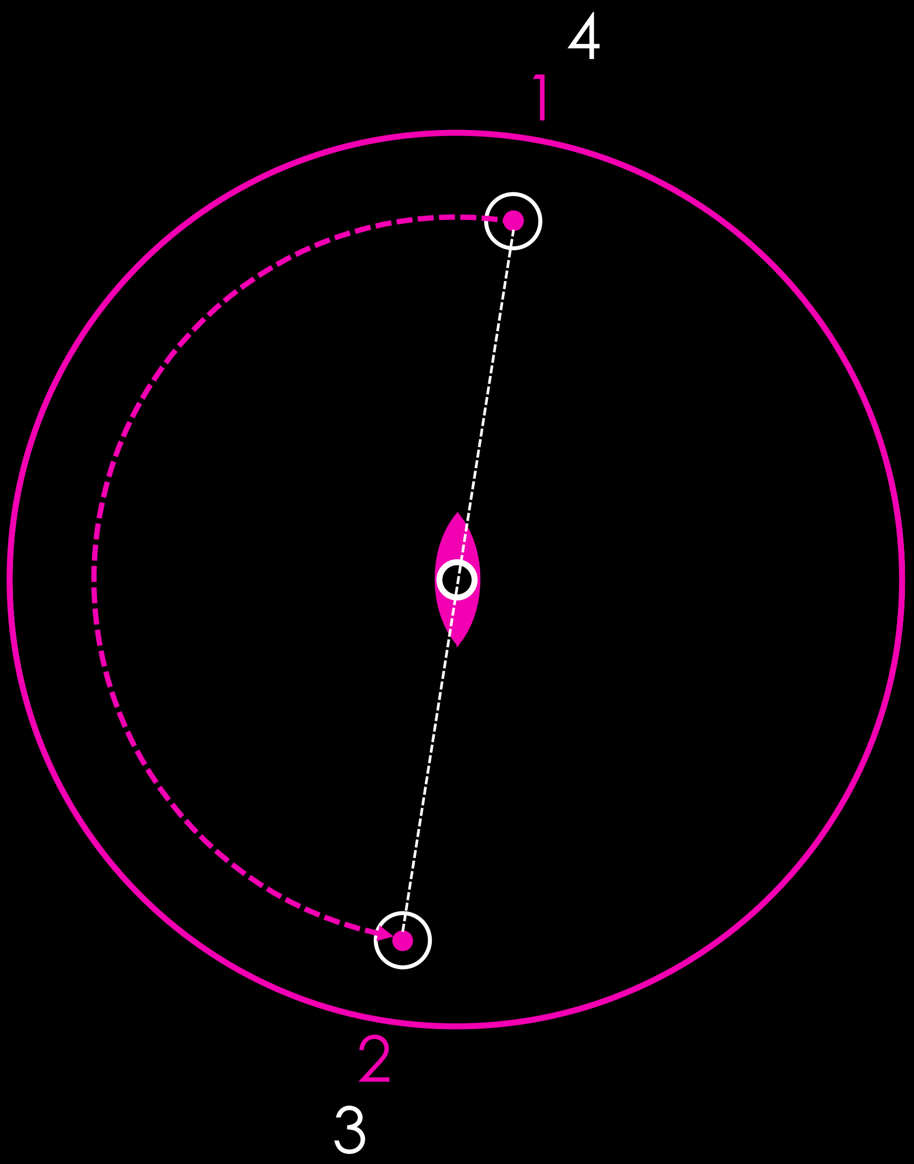
2 ⟶ 4

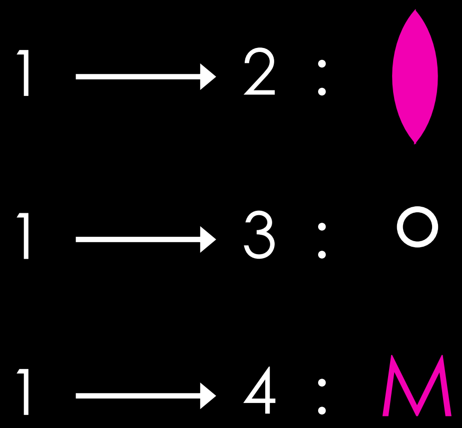
1 ⟶ 2 : ?

1 ⟶ 3 : ?

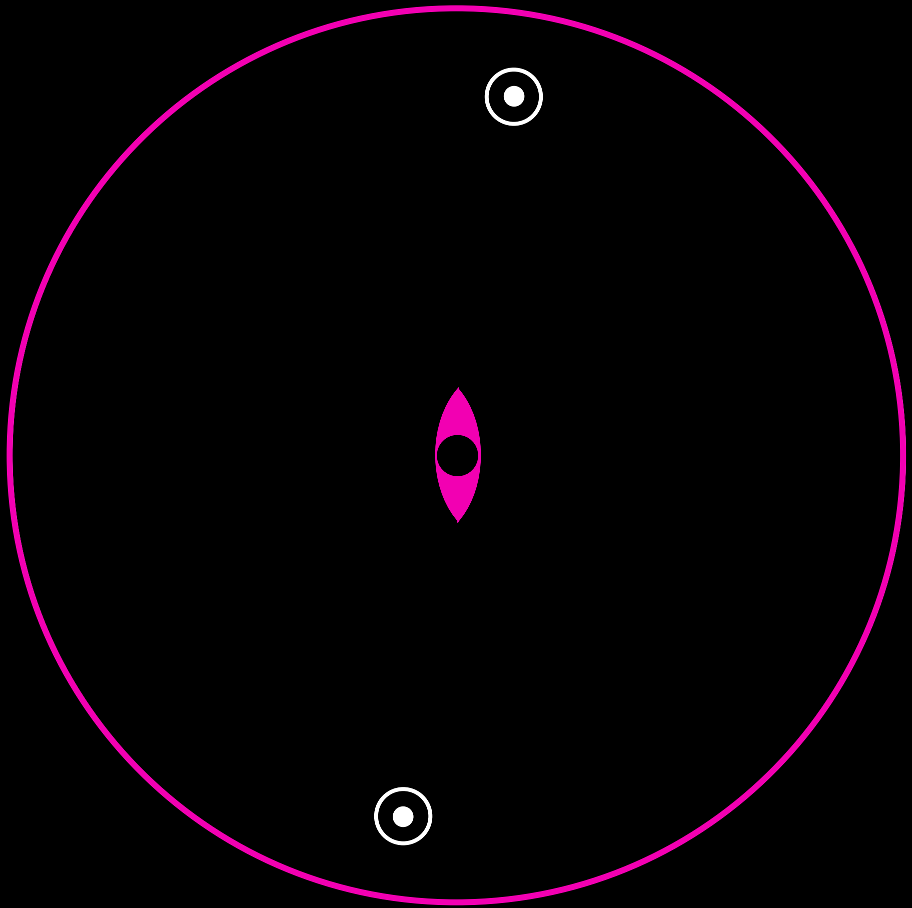
1 ⟶ 4 : ?

A_2 & C





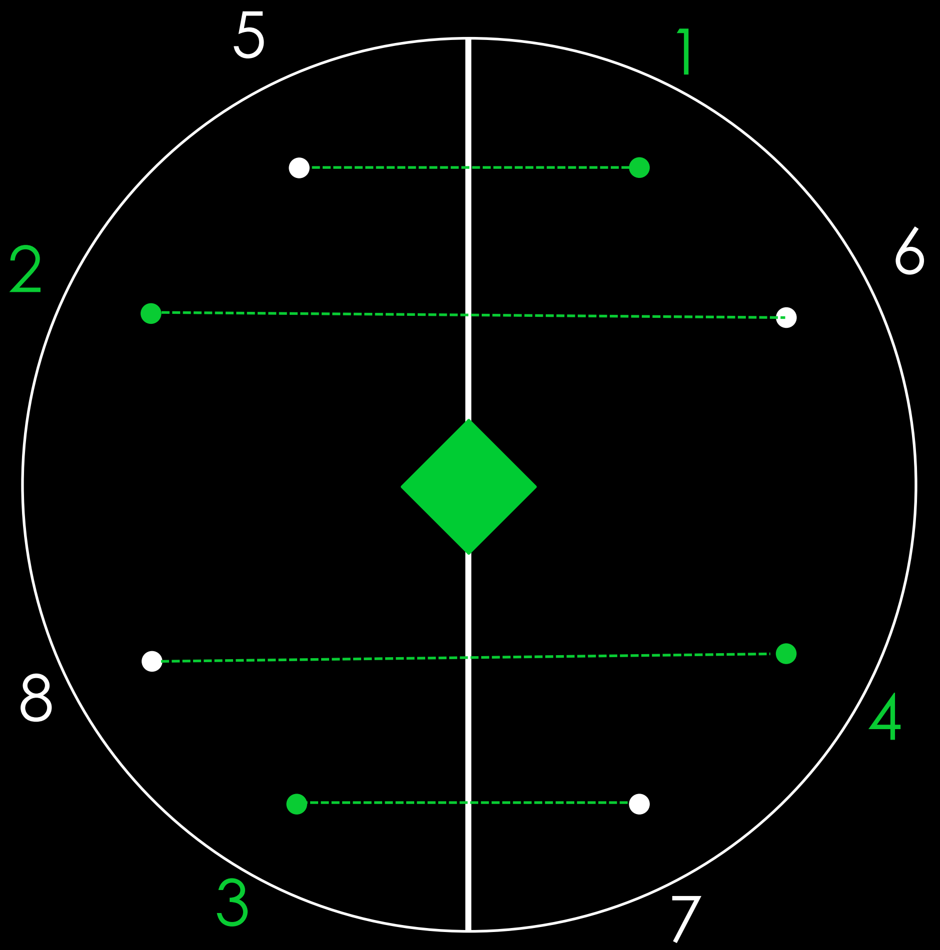
A_2 & C



$\frac{A_2}{M}C$

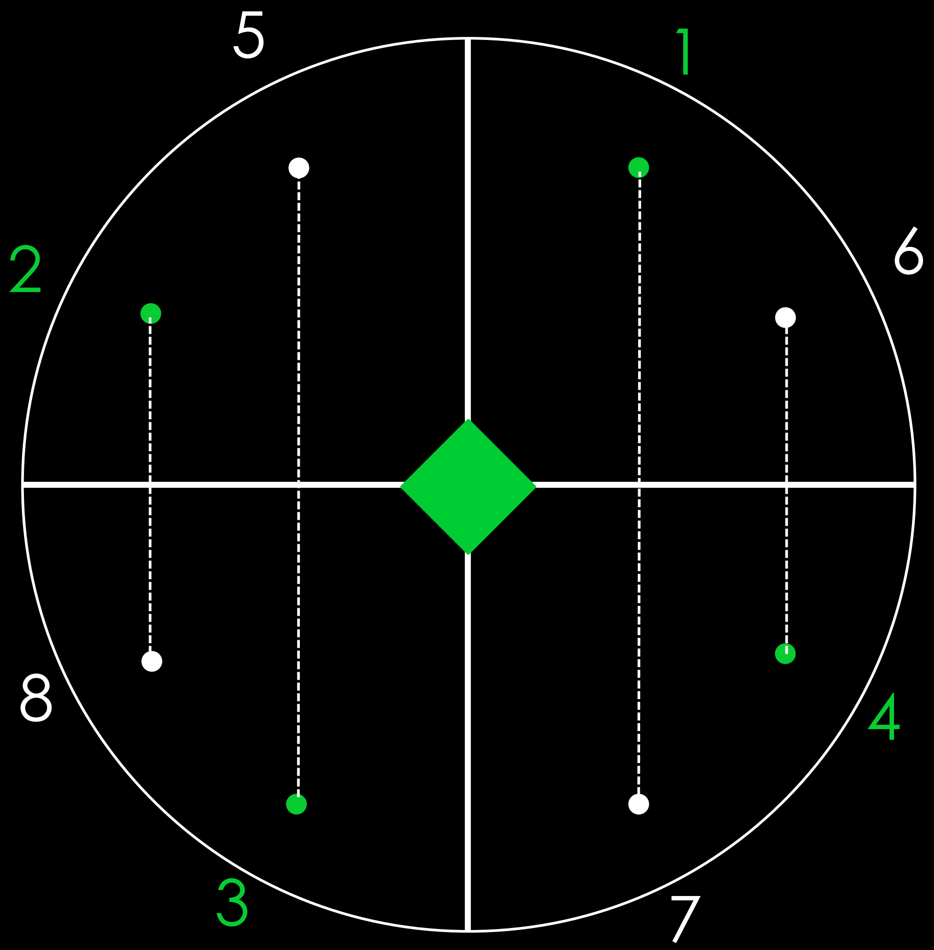
$\frac{2}{m}$

A_4 & M ||



8 equivalent directions

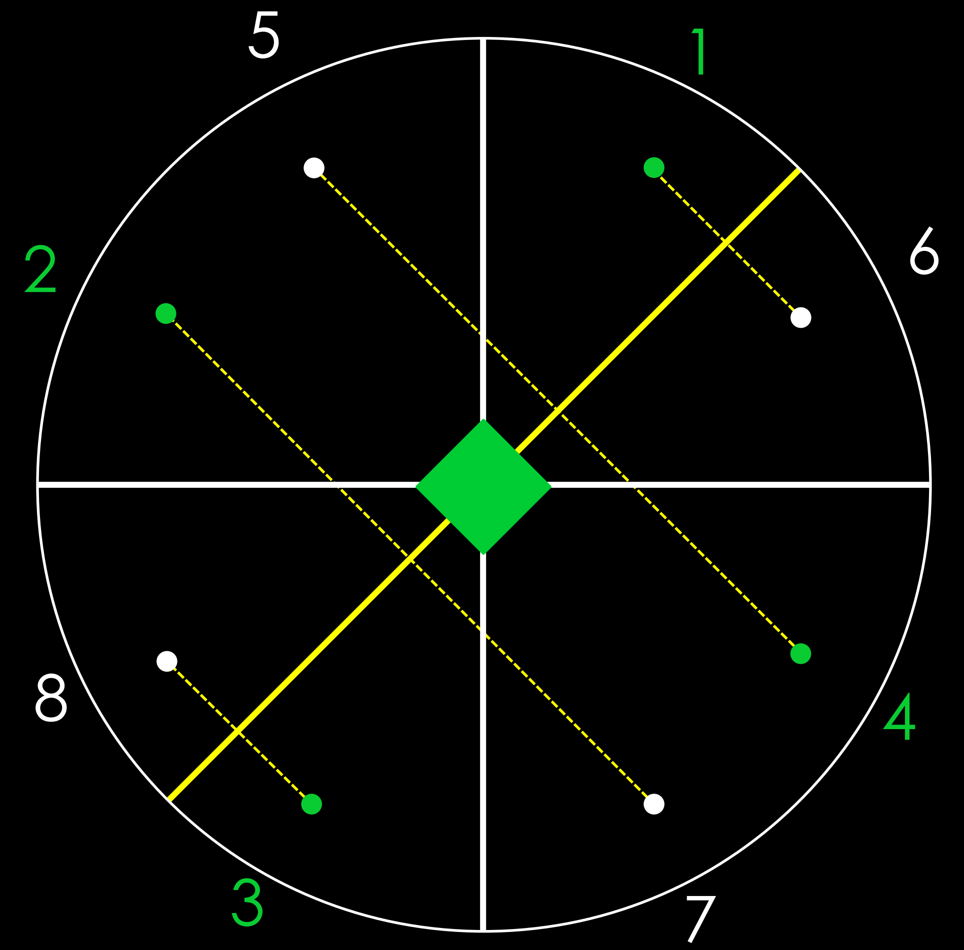
A_4 & M ||

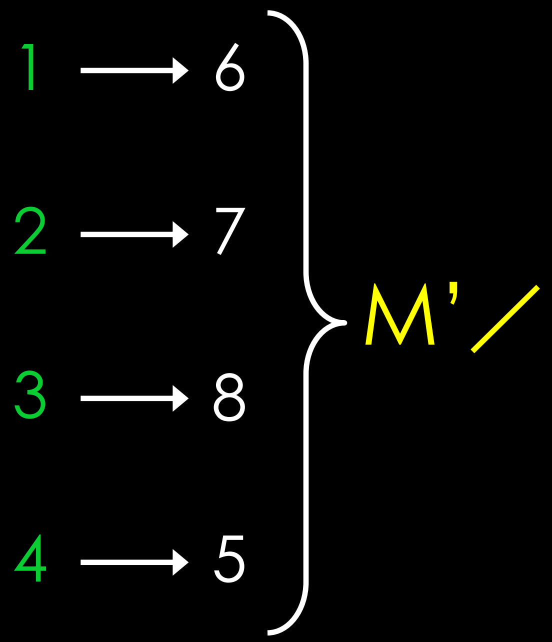


1 ⟶ 7
2 ⟶ 8
3 ⟶ 5
4 ⟶ 6

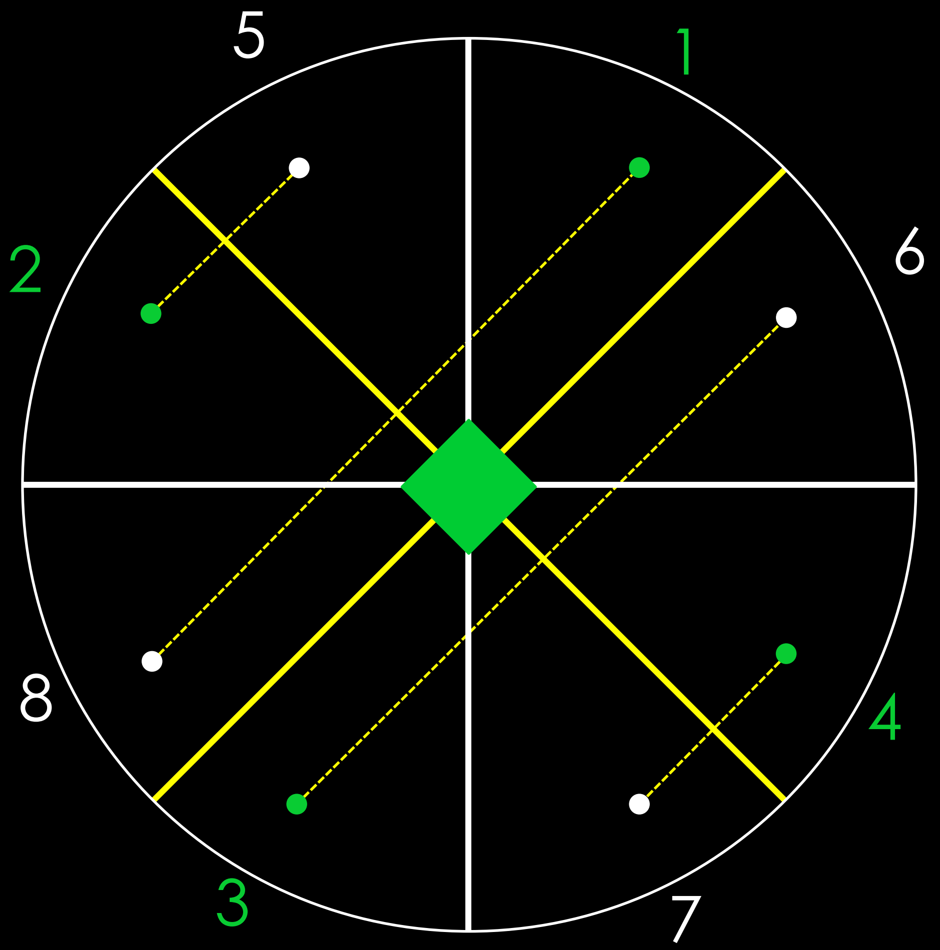
} M —

A_4 & M ||





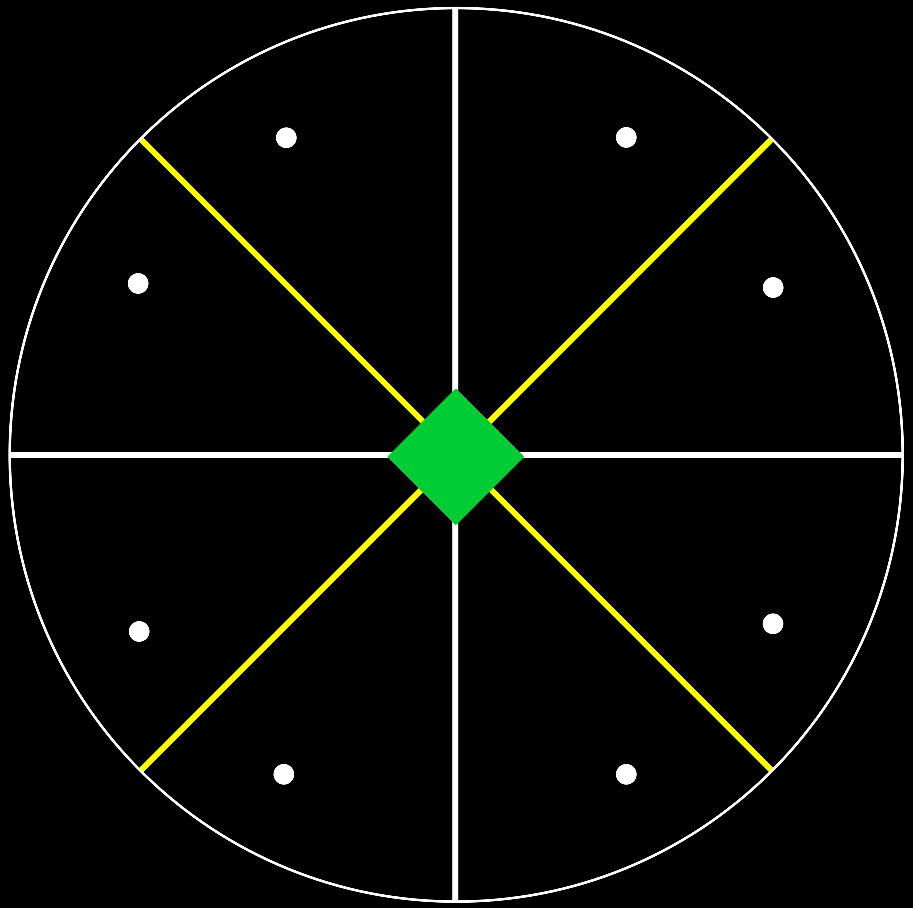
A_4 & M ∥



1 ⟶ 8
2 ⟶ 5
3 ⟶ 6
4 ⟶ 7

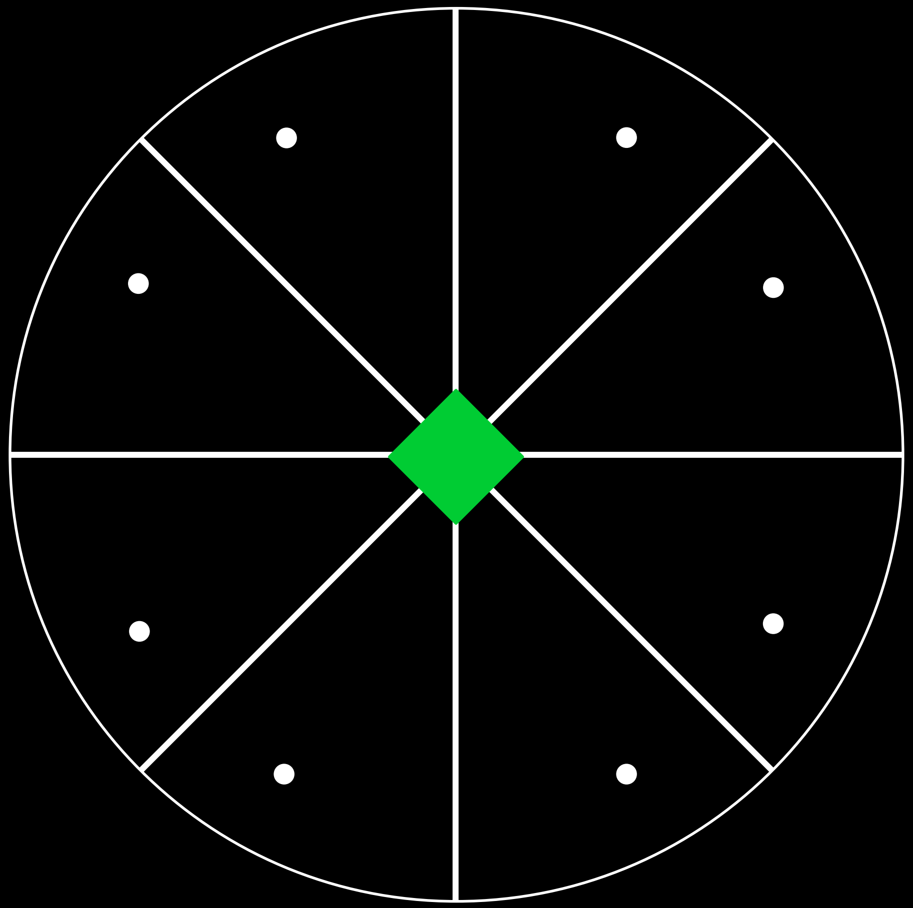
} M' ╲

A_4 & M ||



A_4 2 M 2 M'

A_4 & M ||



A_4 2 M 2 M'

4 m m

10 – The 32 crystallographic point groups

$2/m$ 222 $mm2$

$\bar{3}m$ 32 $3m$

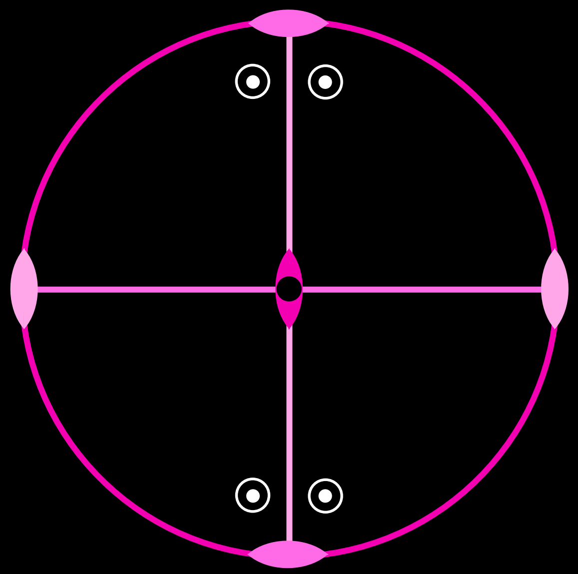
$4/m$ 422 $4mm$ $\bar{4}2m$

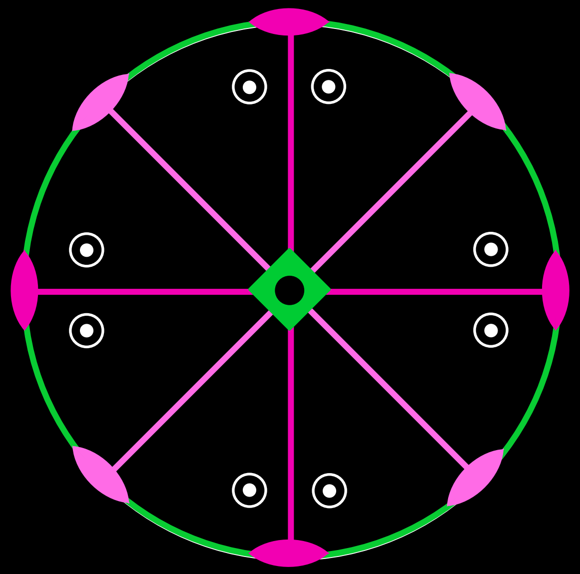
$6/m$ 622 $6mm$ $\bar{6}2m$

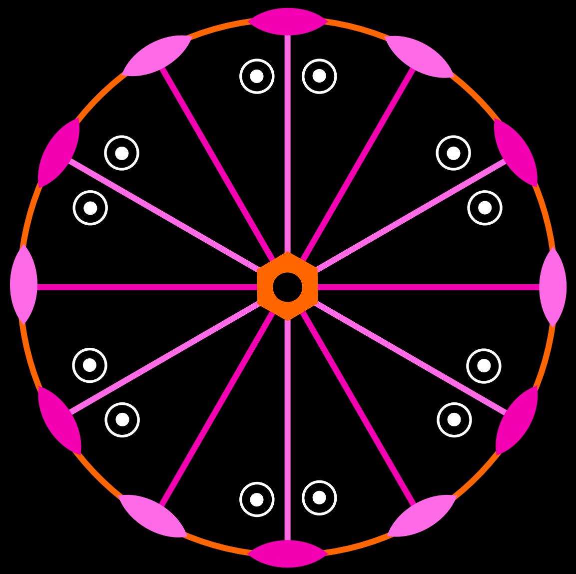
$\times\ \bar{1}$

3 non-cubic
point groups
with 3 generators

mmm $\frac{4}{m}mm$ $\frac{6}{m}mm$





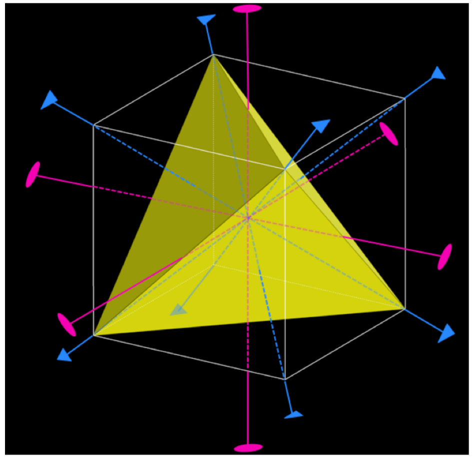


3 non-cubic point groups with 3 generators

10 – The 32 crystallographic point groups

5 cubic point groups

They contain **at least** 4 A_3 (oriented along the <111> directions) and 3 A_2 (oriented along the <100> directions)



$3A_2\ \ 4A_3$	2 3	T	**rotation group of the regular tetrahedron**
$\frac{3A_2}{3M}\ \ 4\bar{A}_3\ \ C$	m $\bar{3}$	T_h	obtained by adding a centre to 2 3
$3\bar{A}_4\ \ 4A_3\ \ 6M'$	$\bar{4}$ 3 m	T_d	obtained from 2 3 by replacing A_2 par $\bar{A}_4$ **symmetry group of the regular tetrahedron**
$3A_4\ \ 4A_3\ \ 6A'_2$	4 3 2	O	obtained from 2 3 by replacing A_2 by A_4 **rotation group of the regular octahedron**
$\frac{3A_4}{3M}\ \ 4\bar{A}_3\ \ \frac{6A'_2}{6M'}\ \ C$	m $\bar{3}$ m	O_h	obtained by adding a centre to 4 3 2 **symmetry group of the regular octahedron**

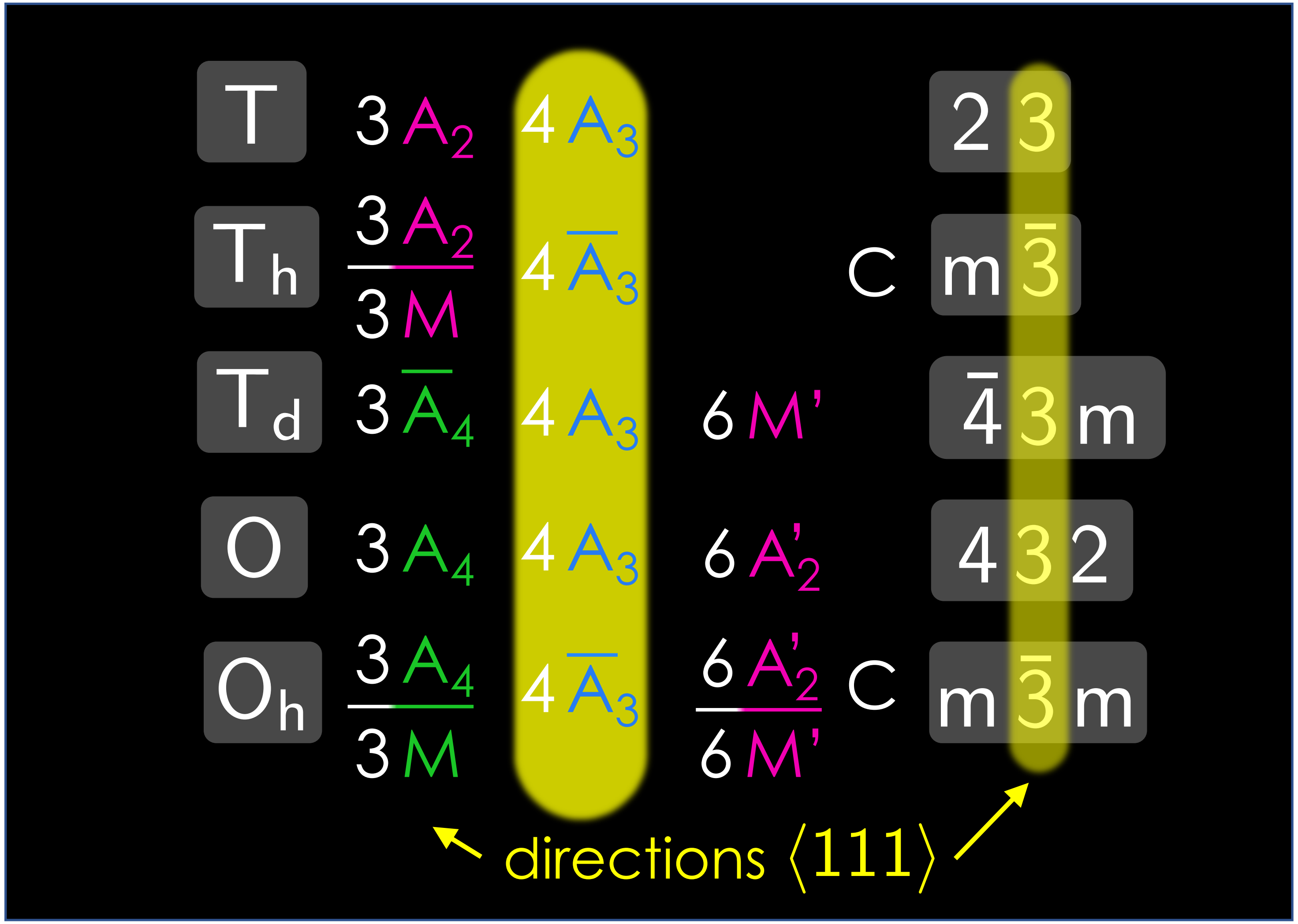
5 cubic point groups

T	$3A_2$	$4A_3$			$2\,3$
T_h	$\frac{3A_2}{3M}$	$4\bar{A}_3$		C	$m\,\bar{3}$
T_d	$3\bar{A}_4$	$4A_3$	$6M'$		$\bar{4}\,3\,m$
O	$3A_4$	$4A_3$	$6A'_2$		$4\,3\,2$
O_h	$\frac{3A_4}{3M}$	$4\bar{A}_3$	$\frac{6A'_2}{6M'}$	C	$m\,\bar{3}\,m$

directions $\langle 001 \rangle$

10 – The 32 crystallographic point groups

5 cubic point groups



5 cubic point groups

T	$3A_2$	$4A_3$			2 3
T_h	$\frac{3A_2}{3M}$	$4\bar{A}_3$		C	$m\bar{3}$
T_d	$3\bar{A}_4$	$4A_3$	$6M'$		$\bar{4}3m$
O	$3A_4$	$4A_3$	$6A'_2$		4 3 2
O_h	$\frac{3A_4}{3M}$	$4\bar{A}_3$	$\frac{6A'_2}{6M'}$	C	$m\bar{3}m$

directions $\langle 011 \rangle$

5 cubic point groups

T	$3A_2$	$4A_3$			2 3
T_h	$\frac{3A_2}{3M}$	$4\bar{A}_3$		C	m $\bar{3}$
T_d	$3\bar{A}_4$	$4A_3$	$6M'$		$\bar{4}$ 3 m
O	$3A_4$	$4A_3$	$6A'_2$		4 3 2
O_h	$\frac{3A_4}{3M}$	$4\bar{A}_3$	$\frac{6A'_2}{6M'}$	C	m $\bar{3}$ m

5 cubic point groups

T	$3A_2$	$4A_3$			$2\,3$
T_h	$\frac{3A_2}{3M}$	$4\overline{A}_3$		C	$m\,\bar{3}$
T_d	$3\overline{A}_4$	$4A_3$	$6M'$		$\bar{4}\,3\,m$
O	$3A_4$	$4A_3$	$6A'_2$		$4\,3\,2$
O_h	$\frac{3A_4}{3M}$	$4\overline{A}_3$	$\frac{6A'_2}{6M'}$	C	$m\,\bar{3}\,m$

holoédrie

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

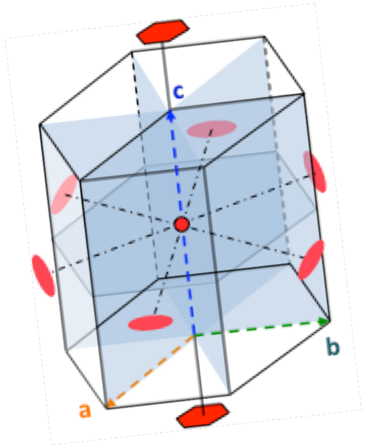
9 – Roto-inversions

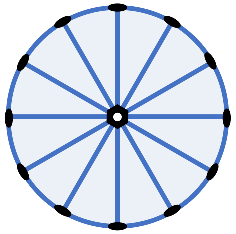
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

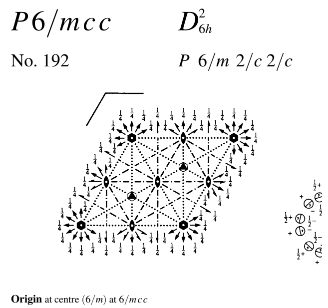
12 – The 14 Bravais lattices

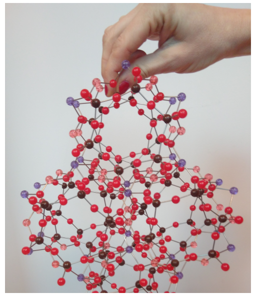
13 – The 230 space-groups





$\frac{6}{m}mm$

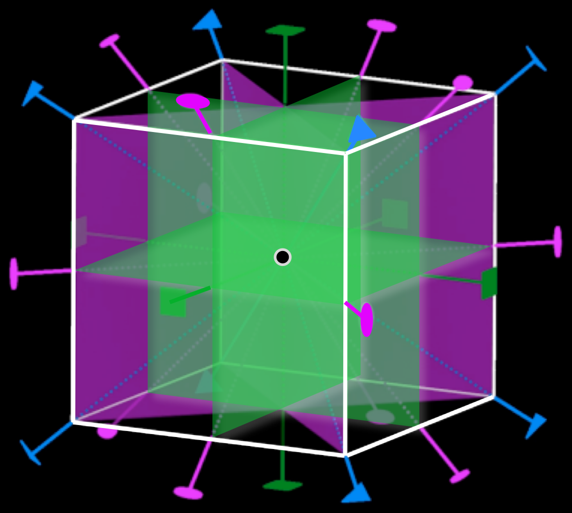




11 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

cubic system



- $2\,3$
- $m\,\bar{3}$
- $\bar{4}\,3\,m$
- $4\,3\,2$
- $m\,\bar{3}\,m$ ← holohedry

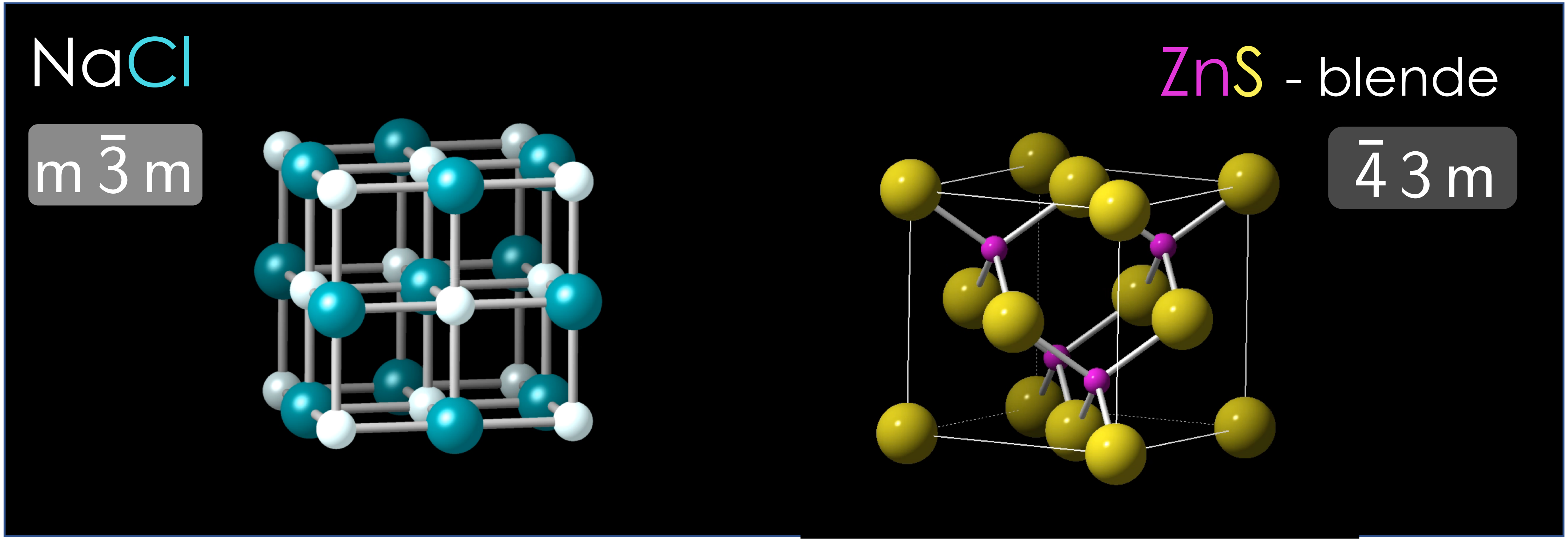
$a = b = c$

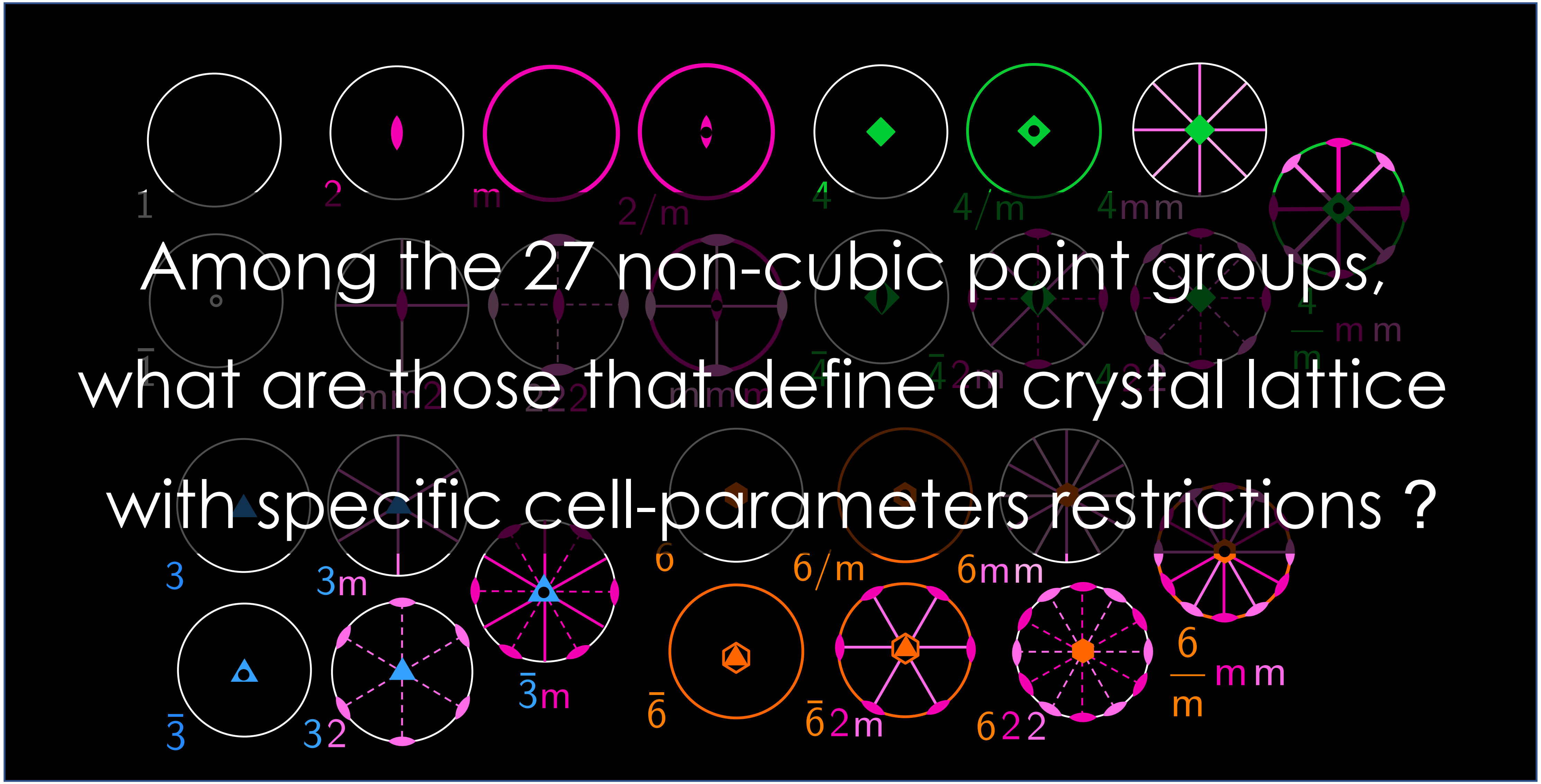
$\alpha = \beta = \gamma = 90°$

11 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

crystal symmetry ≤ lattice symmetry



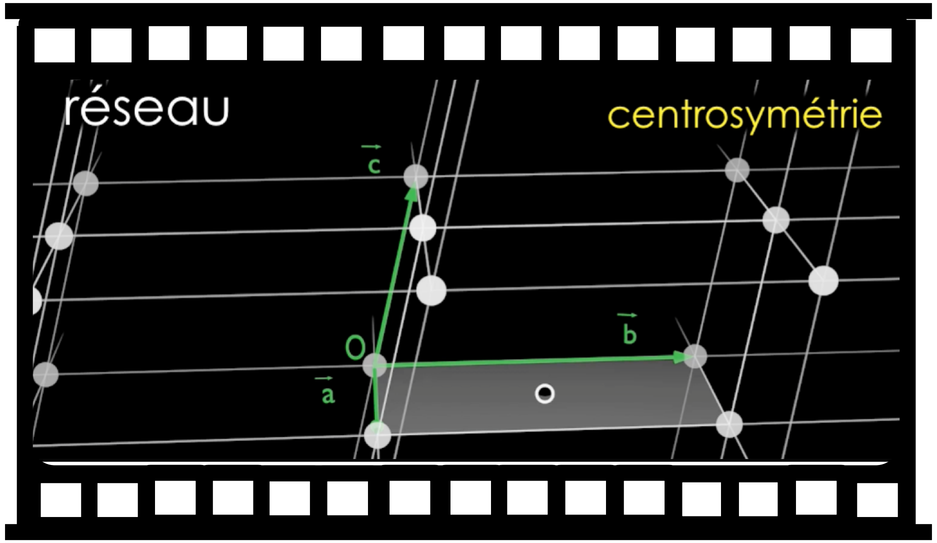

1
2
m
2/m
4
4/m
4mm
Among the 27 non-cubic point groups,
what are those that define a crystal lattice
with specific cell-parameters restrictions ?
3
3m
6
6/m
6mm
$\bar{3}$
32
$\bar{3}$m
$\bar{6}$
$\bar{6}$2m
622
$\frac{6}{m}$mm

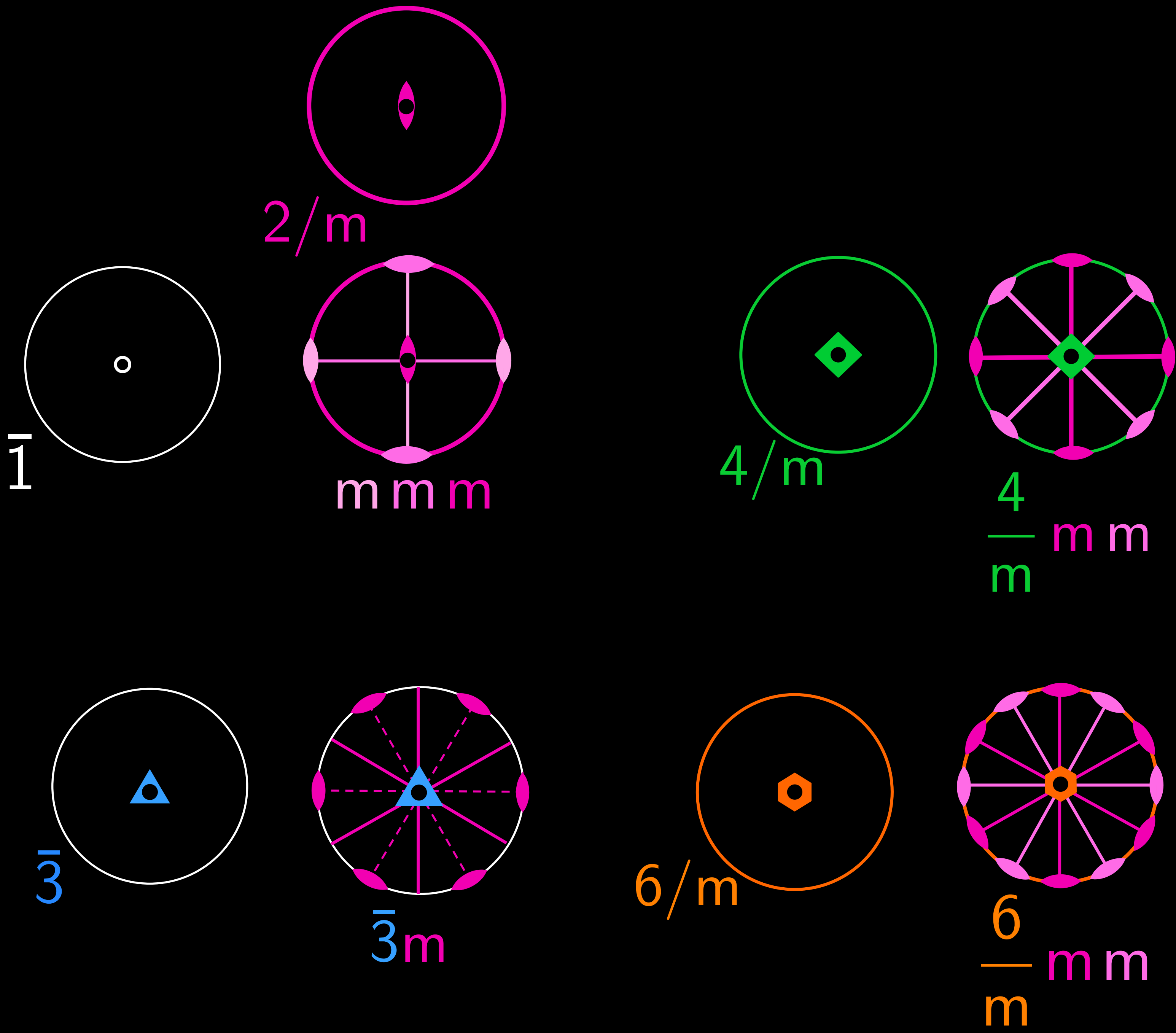
11 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

crystal symmetry ≤ lattice symmetry

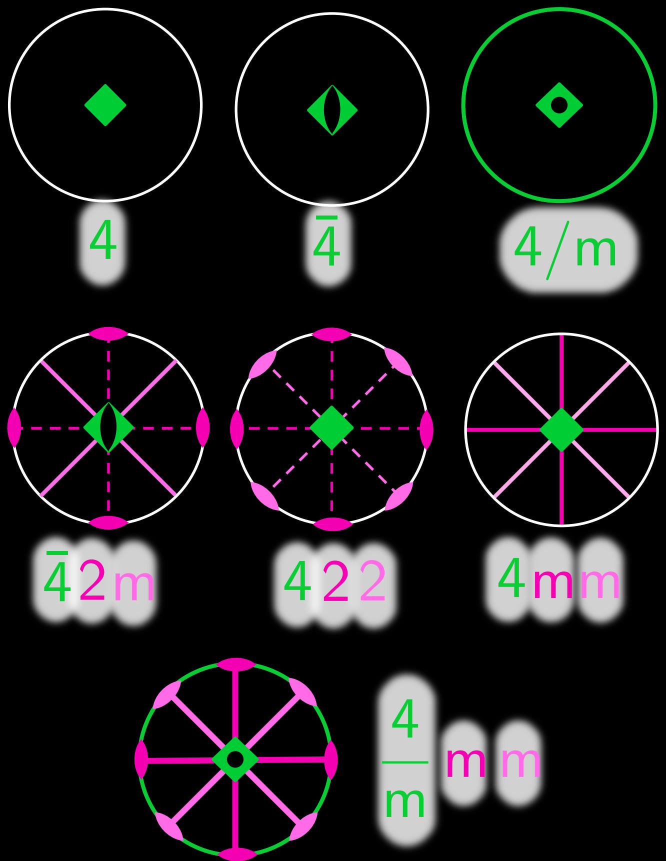
any lattice is centrosymmetric

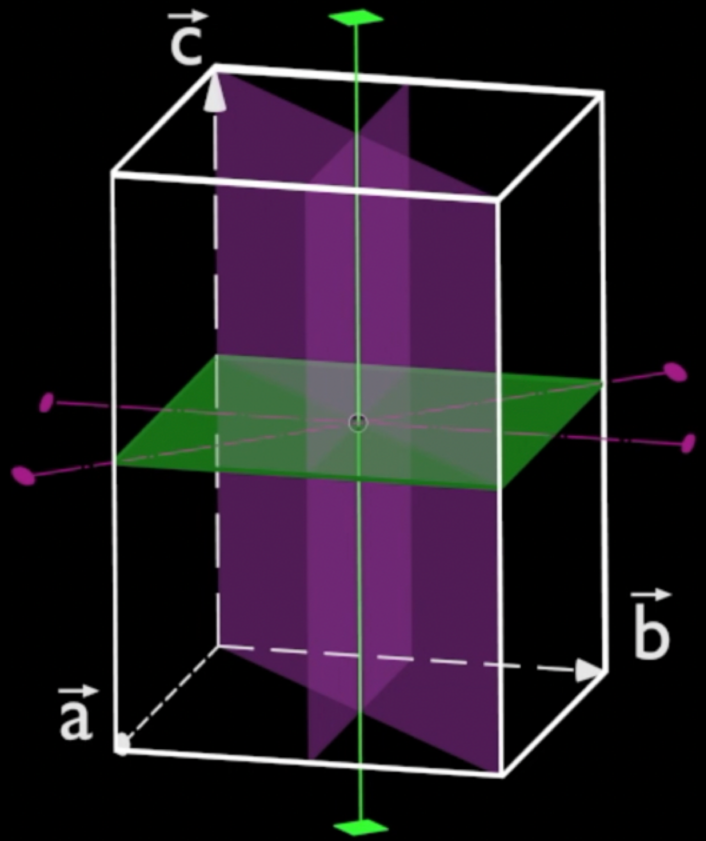




Laue classes

tetragonal system





$a = b$

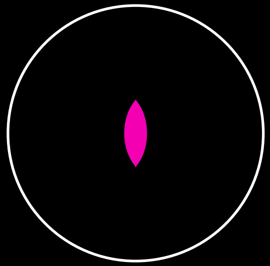
$\alpha = \beta = \gamma = 90°$

direction [001]

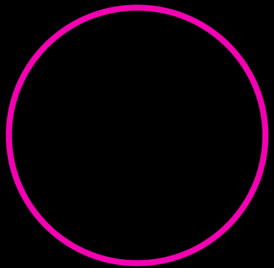
directions [100] & [010]

directions [110] & [$\bar{1}$10]

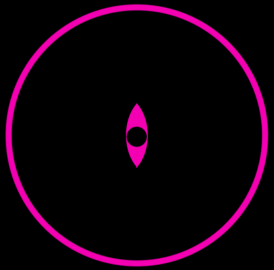
monoclinic system



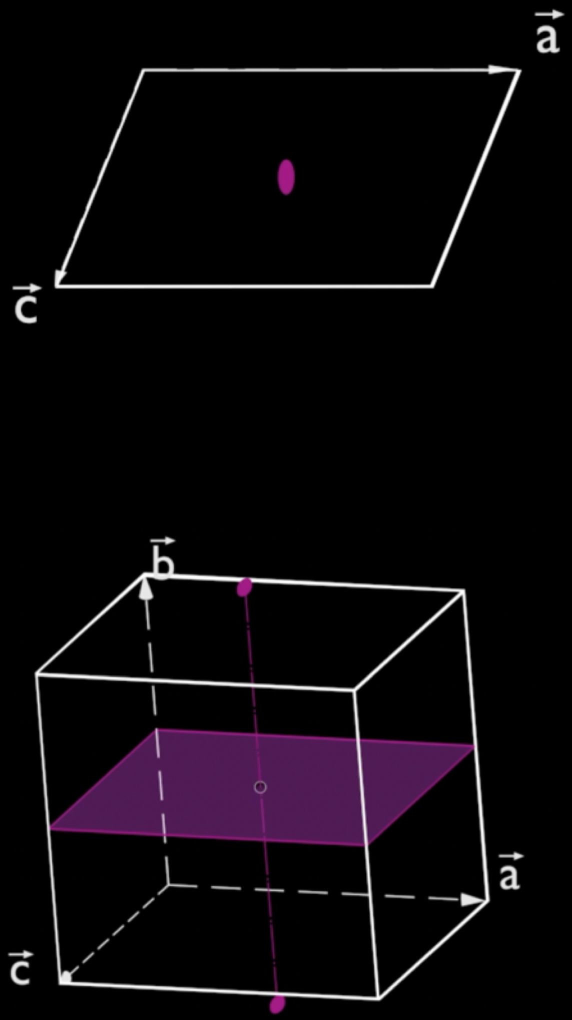
2



m

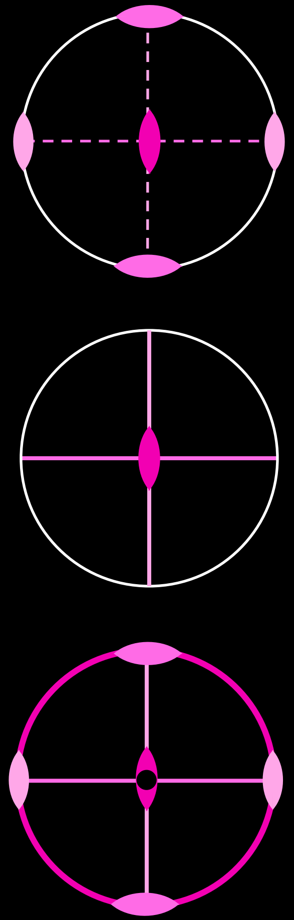


2/m



$$\alpha = \gamma = 90°$$

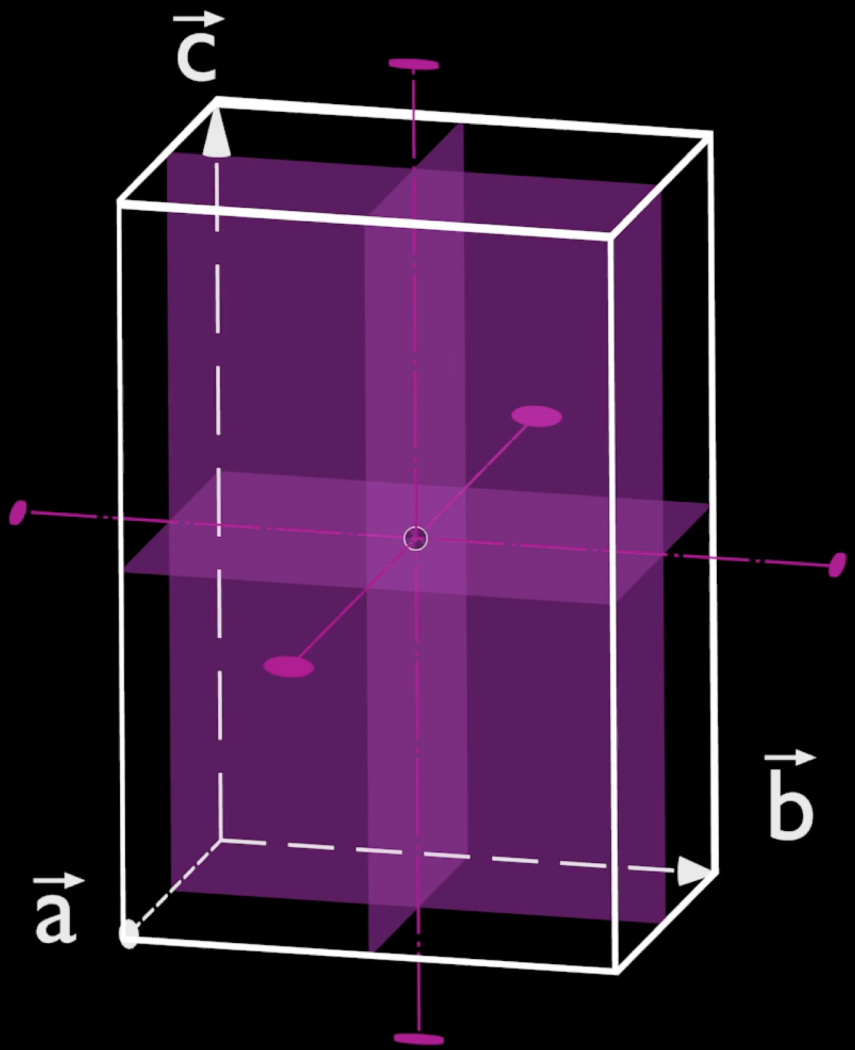
orthorhombic system



2 2 2

m m 2

m m m



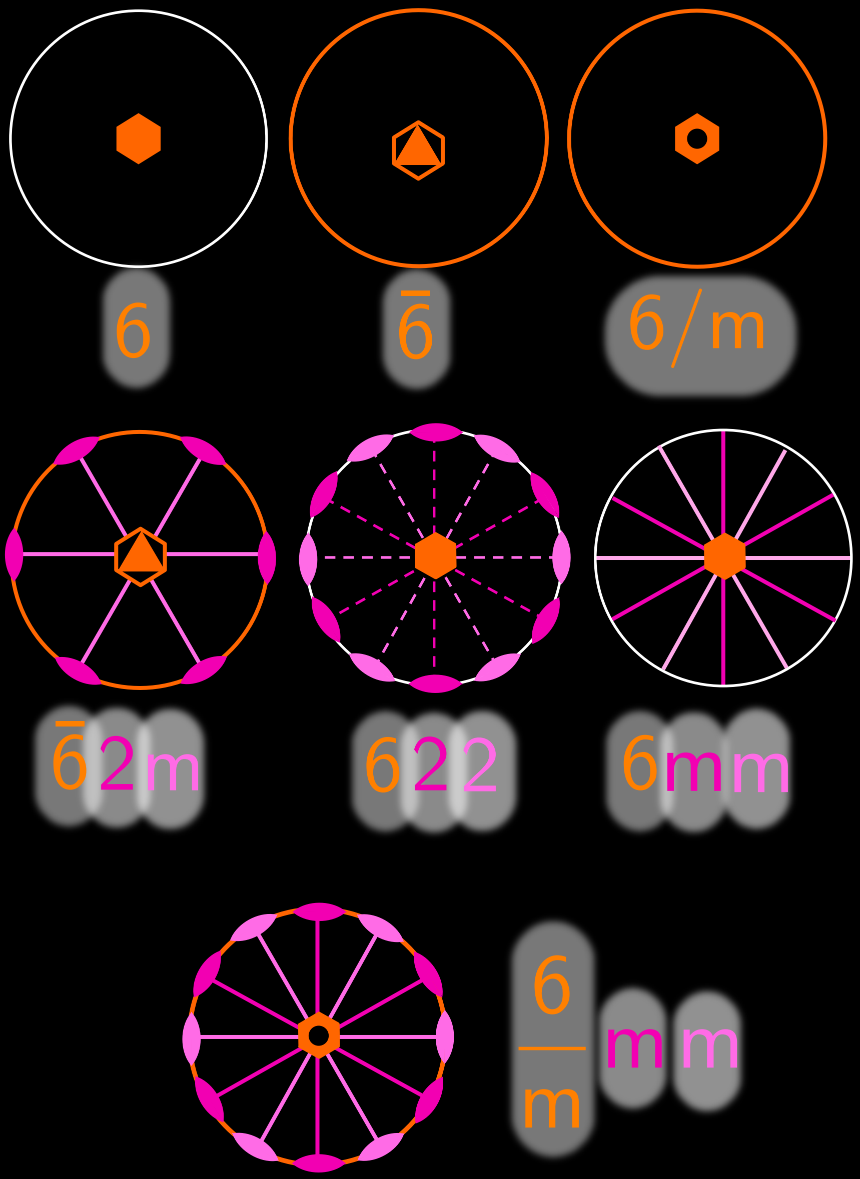
$$\alpha = \beta = \gamma = 90°$$

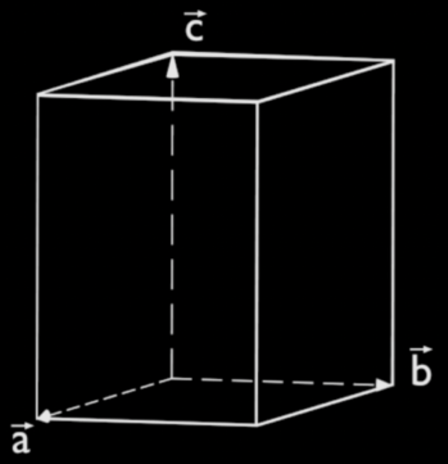
direction [100]

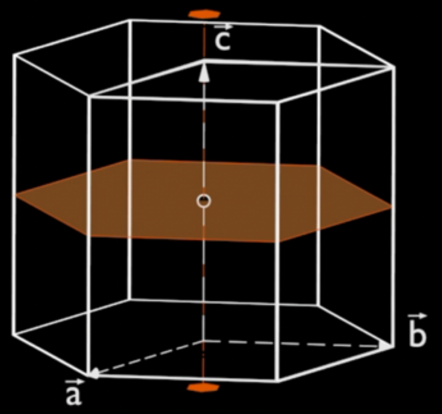
direction [010]

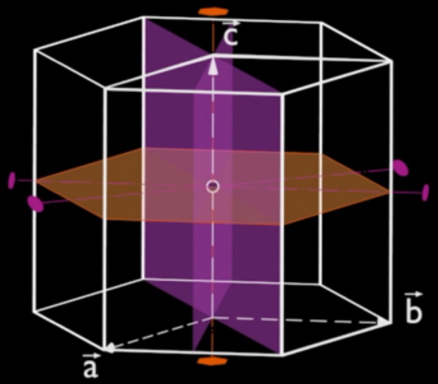
direction [001]

hexagonal system









$a = b$

$\gamma = 120°$

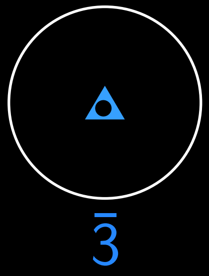
$\alpha = \beta = 90°$

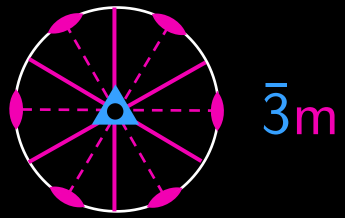
direction [001]

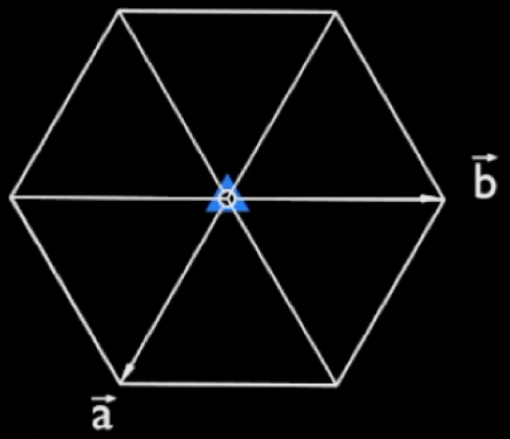
directions
[100], [010], [$\bar{1}\bar{1}0$]

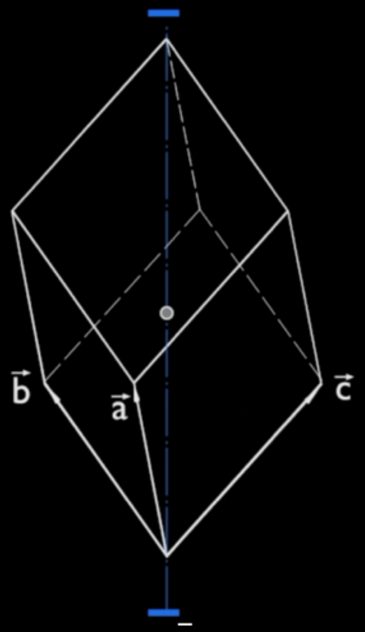
directions
[$1\bar{1}0$], [120], [$\bar{2}\bar{1}0$]

trigonal system







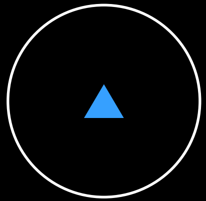


rhombohedral cell

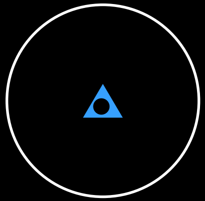
$$a = b = c$$

$$\alpha = \beta = \gamma$$

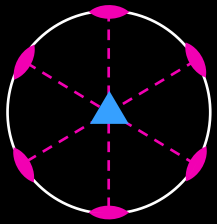
trigonal system



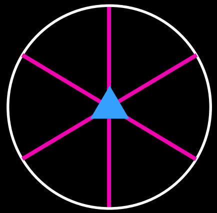
3



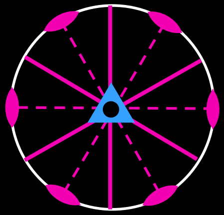
$\bar{3}$



32

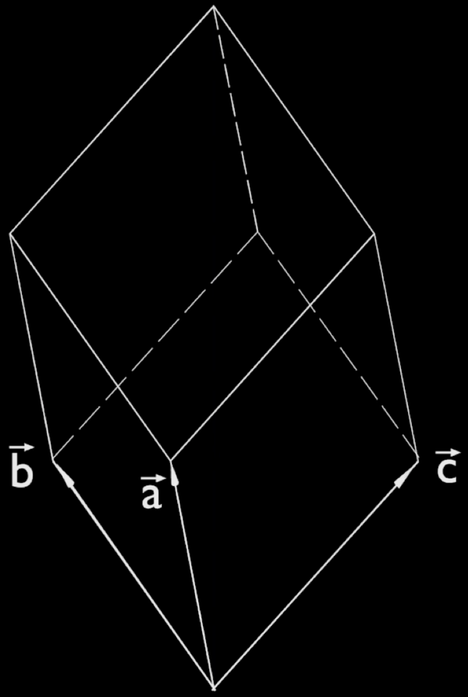


3m

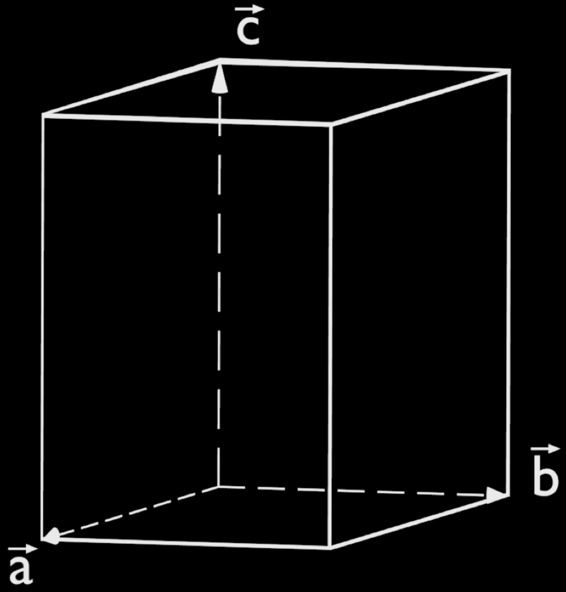


$\bar{3}$m

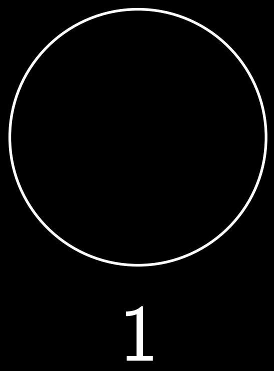
rhombohedral axes

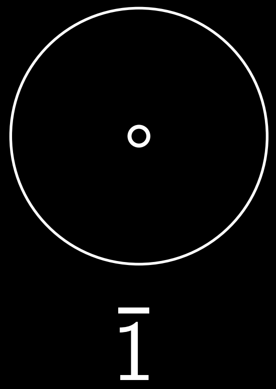


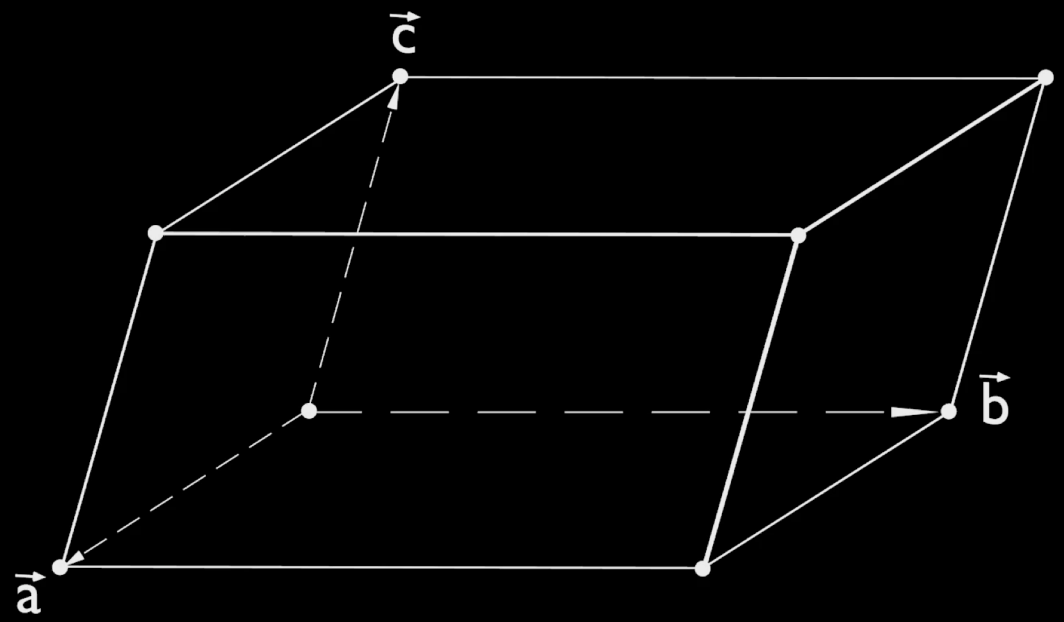
hexagonal axes



triclinic system







Classification of the 32 point groups

crystal symmetry ≤ lattice symmetry

We have classified **the 32 point groups** according to the **3-dimensional lattice symmetry**, that defines 2 criteria:

1. Any lattice is centrosymmetric.
2. Any lattice that has a symmetry axis of order n>2 also presents n mirrors plane parallel to this axis.

➔ The 11 Laue classes (criterion 1) lead to 7 holohedries (criterion 2), which are each associated with one crystal system (with spectific restrictions on the cell parameters).

➔ The other 25 groups have lower symmetry. In order to find the symmetry of their lattice, just add to the symmetry elements of the group those which are necessary to satisfy criteria 1 and 2.

11 – The 7 crystal systems

The 11 laue classes do not define 11 distinct lattices (with 11 different cells), but only 7.

Using criterion 2, we define **7 holohedries**, leading to the **7 crystal systems**.

$\bar{A}_1$ → any parallele-piped

$\frac{A_2}{M}C$ → paralle-logram-based straight prism

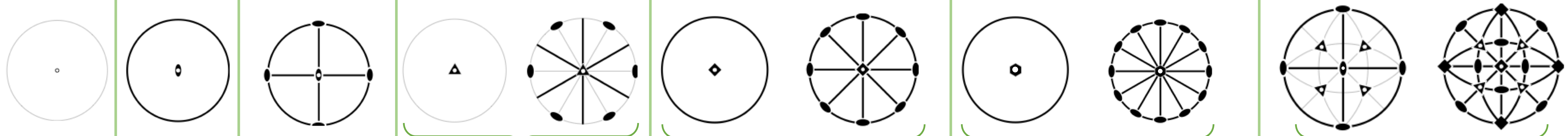
$\frac{A_2}{M}\frac{A_2'}{M'}\frac{A_2''}{M''}C$ → *rectangle-based straight prism "shoe box"*

$\bar{A}_3$, $\bar{A}_3\frac{3A_2'}{3M'}C$ → rhombohedron

$\frac{A_4}{M}C$, $\frac{A_4}{M}\frac{2A_2'}{2M'}\frac{2A_2''}{2M''}C$ → squared-based straight prism

$\frac{A_6}{M}C$, $\frac{A_6}{M}\frac{3A_2'}{3M'}\frac{3A_2''}{3M''}C$ → 1/3 of a hexagonal-based straight prism

$\frac{3A_2}{3M}4\bar{A}_3C$, $\frac{3A_4}{3M}4\bar{A}_3\frac{6A_2'}{6M'}C$ → cube



11 – The 7 crystal systems

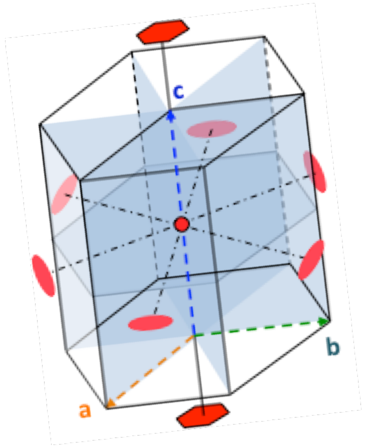
Crystal system	*This course*	Hermann-Mauguin	Schoenflies	Group order
triclinic	$\mathrm{A_1}$	1	C_1	1
	C	$\bar{1}$	$C_i \equiv S_2$	2
monoclinic	$\mathrm{A_2}$	2	C_2	2
	$\mathrm{M} \equiv \bar{\mathrm{A}}_2$	m	$C_{1h} \equiv C_s$	2
	$\frac{\mathrm{A_2}}{\mathrm{M}}\ \mathrm{C}$	$2/m$	C_{2h}	4
orthorhombic	$\mathrm{A_2\ M'\ M''}$	$m\ m\ 2$	C_{2v}	4
	$\mathrm{A_2\ A'_2\ A''_2}$	$2\ 2\ 2$	D_2	4
	$\frac{\mathrm{A_2}}{\mathrm{M}}\ \frac{\mathrm{A'_2}}{\mathrm{M'}}\ \frac{\mathrm{A''_2}}{\mathrm{M''}}\ \mathrm{C}$	$m\ m\ m$	D_{2h}	8
tetragonal	$\mathrm{A_4}$	4	C_4	4
	$\bar{\mathrm{A}}_4$	$\bar{4}$	S_4	4
	$\mathrm{A_4\ 2M'\ 2M''}$	$4\ m\ m$	C_{4v}	8
	$\frac{\mathrm{A_4}}{\mathrm{M}}\ \mathrm{C}$	$4/m$	C_{4h}	8
	$\bar{\mathrm{A}}_4\ \mathrm{2A'_2\ 2M''}$	$\bar{4}\ 2\ m$ (ou $\bar{4}\ m\ 2$)	D_{2d}	8
	$\mathrm{A_4\ 2A'_2\ 2A''_2}$	$4\ 2\ 2$	D_4	8
	$\frac{\mathrm{A_4}}{\mathrm{M}}\ \frac{\mathrm{2A'_2}}{\mathrm{2M'}}\ \frac{\mathrm{2A''_2}}{\mathrm{2M''}}\ \mathrm{C}$	$4/m\ m\ m$	D_{4h}	16

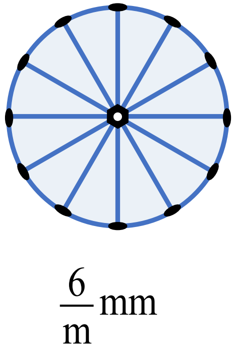
11 – The 7 crystal systems

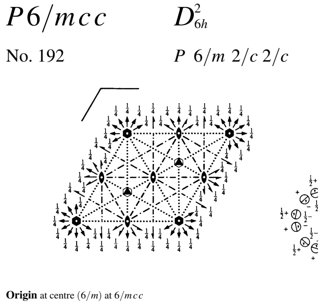
trigonal	A_3	3	C_3	3
	$\bar{A}_3$	$\bar{3}$	$C_{3i} \equiv S_6$	6
	$A_3\ 3M'$	$3\ m$	C_{3v}	6
	$A_3\ 3A'_2$	$3\ 2$	D_3	6
	$\bar{A}_3\ \frac{3A'_2}{3M'}\ C$	$\bar{3}\ m$	D_{3d}	12
hexagonal	A_6	6	C_6	6
	$\bar{A}_6$	$\bar{6}$	$C_{3h} \equiv S_3$	6
	$A_6\ 3M'\ 3M''$	$6\ m\ m$	C_{6v}	12
	$\frac{A_6}{M}\ C$	$6/m$	C_{6h}	12
	$\bar{A}_6\ 3A'_2\ 3M''$	$\bar{6}\ 2\ m$	D_{3h}	12
	$A_6\ 3A'_2\ 3A''_2$	$6\ 2\ 2$	D_6	12
	$\frac{A_6}{M}\ \frac{3A'_2}{3M'}\ \frac{3A''_2}{3M''}\ C$	$6/m\ m\ m$	D_{6h}	24
cubic	$3A_2\ 4A_3$	$2\ 3$	T	12
	$\frac{3A_2}{3M}\ 4\bar{A}_3\ C$	$m\ \bar{3}$	T_h	24
	$3\bar{A}_4\ 4A_3\ 6M'$	$\bar{4}\ 3\ m$	T_d	24
	$3A_4\ 4A_3\ 6A'_2$	$4\ 3\ 2$	O	24
	$\frac{3A_4}{3M}\ 4\bar{A}_3\ \frac{6A'_2}{6M'}\ C$	$m\ \bar{3}\ m$	O_h	48

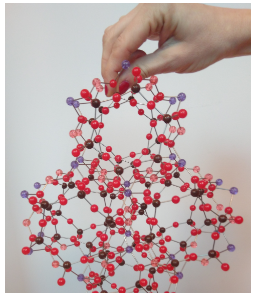
Course outline

1- Symmetry observation in natural crystals
2- Internal cause of the natural crystal shape
3 – Crystal lattice, cell, motif
4 – Lattice direction and planes
5 – Reciprocal lattice
6 – Crystal lattice & symmetries
7 – Conventional cell (unit cell)
8 – Stereographic projection
9 – Roto-inversions
10 – The 32 crystallographic point groups
11 – The 7 crystal systems
12 – The 14 Bravais lattices
13 – The 230 space-groups







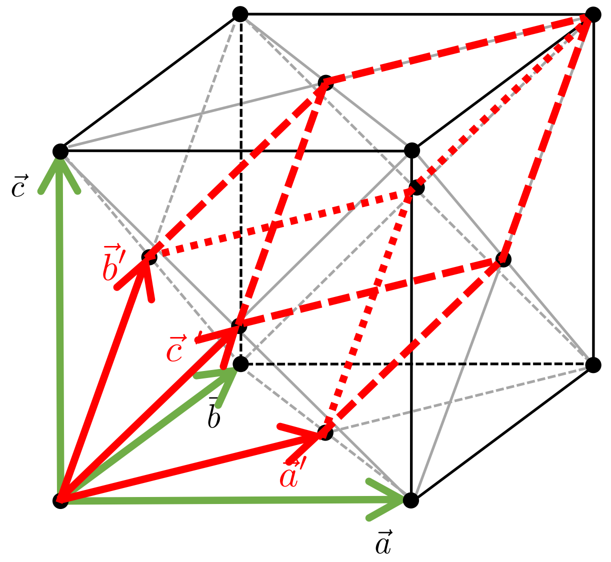


<u>Conventional cell=unit cell (the cell chosen to define a crystal lattice)</u>:
smallest volume with the same symmetry as the lattice
and defined by 3 basis-vectors **a**, **b** and **c**.

1 Bravais lattice ➔ 1 **conventional** cell **= unit** cell = **holohedral** cell

➔ When the most symmetric cell is the smallest, the conventional cell is **primitive**.

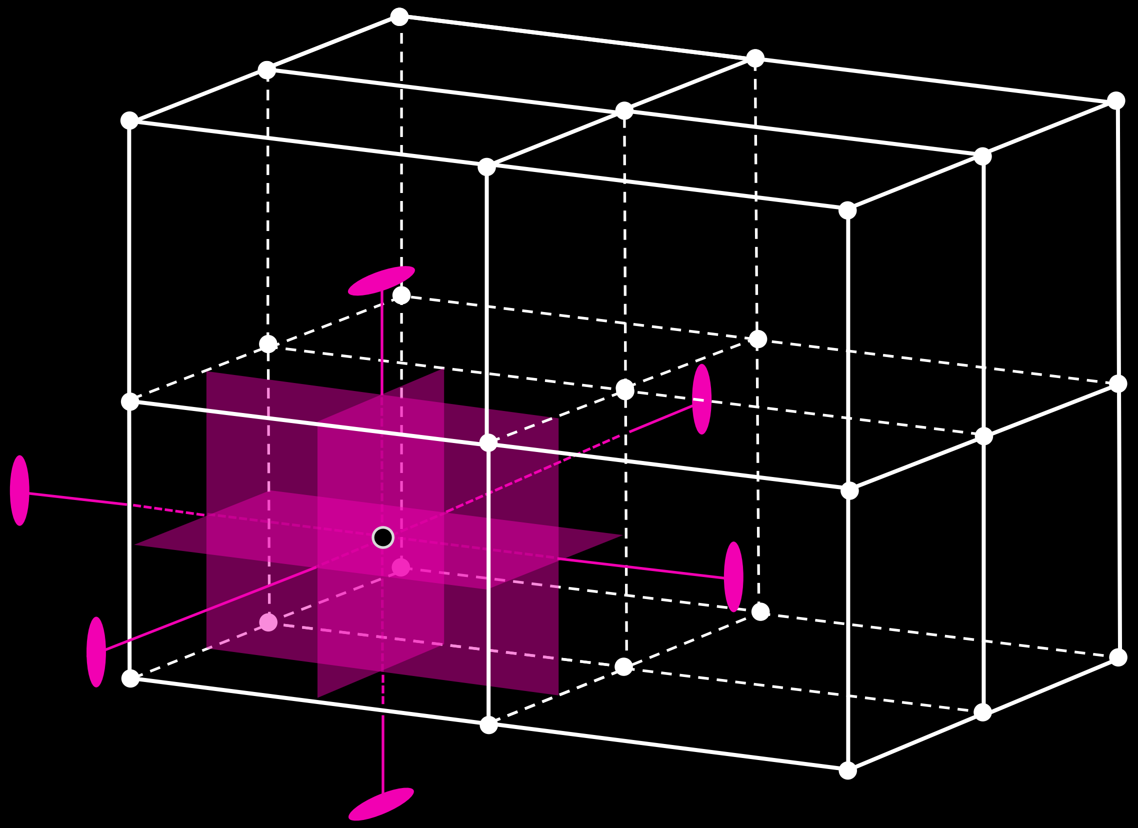
➔ When the most symmetric is not the smallest, the conventional cell is a **supercell** (multiple cell).



ex: fcc cell

Is it possible to **add extra lattice points** while **conserving the lattice symmetry**?

If yes, at which **positions** in the lattice?



- at the centre of the cell
- at the centre of the faces
- at the middle of the edges

12 – The 14 Bravais lattices

3D supercells

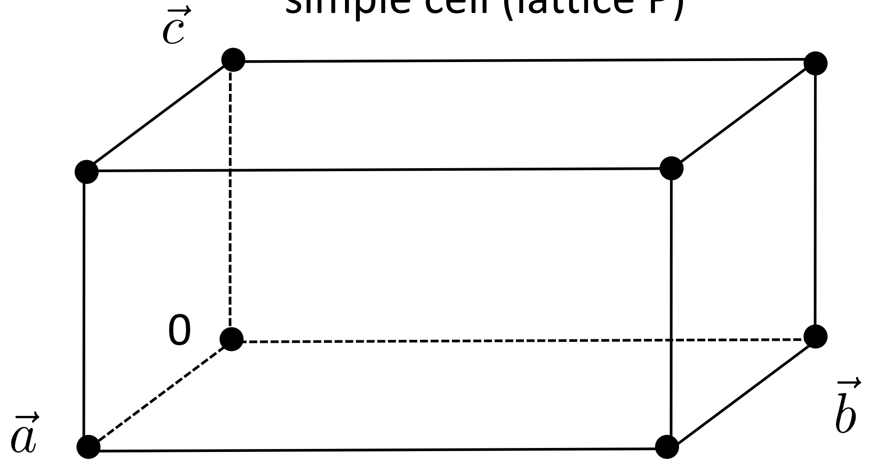
Translations	Cell	Lattice type	Cell Multiplicity
$\vec{a},\ \vec{b},\ \vec{c}$	simple or primitive	P	1
$\vec{a},\ \vec{b},\ \vec{c},\ \dfrac{\vec{b}+\vec{c}}{2}$	centred on face $(\vec{b},\ \vec{c})$	A	2
$\vec{a},\ \vec{b},\ \vec{c},\ \dfrac{\vec{a}+\vec{c}}{2}$	centred on face $(\vec{a},\ \vec{c})$	B	2
$\vec{a},\ \vec{b},\ \vec{c},\ \dfrac{\vec{a}+\vec{b}}{2}$	centred on face $(\vec{a},\ \vec{b})$	C	2
$\vec{a},\ \vec{b},\ \vec{c},\ \dfrac{\vec{a}+\vec{b}}{2},\ \dfrac{\vec{b}+\vec{c}}{2},\ \dfrac{\vec{a}+\vec{c}}{2}$	all-faces centred	F	4
$\vec{a},\ \vec{b},\ \vec{c},\ \dfrac{\vec{a}+\vec{b}+\vec{c}}{2}$	body centred	I	2

➔ **4 modes de réseau** (i.e. 4 groupes de translations)

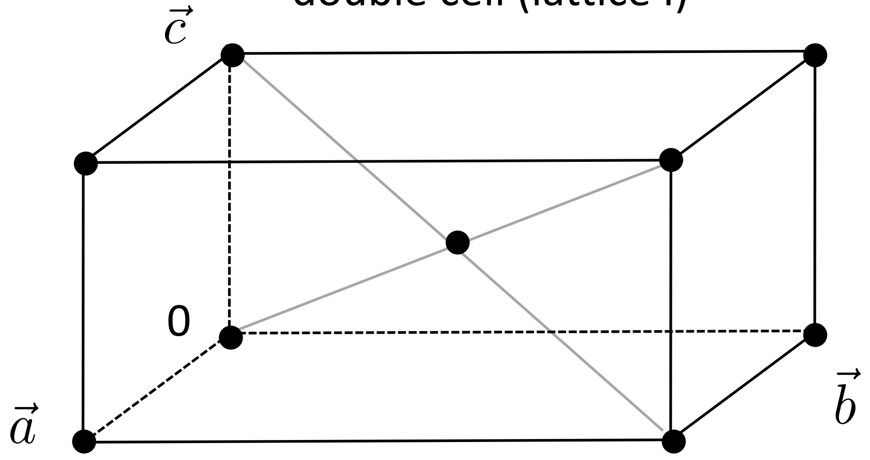
12 – The 14 Bravais lattices

3D supercells

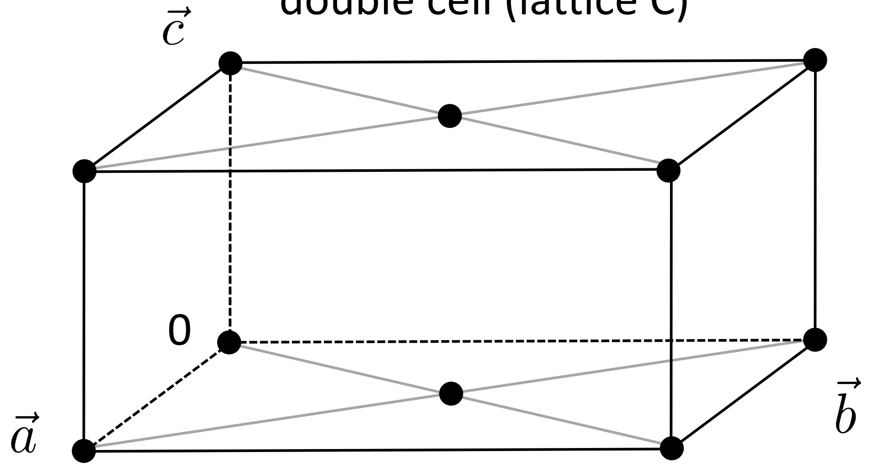
simple cell (lattice P)



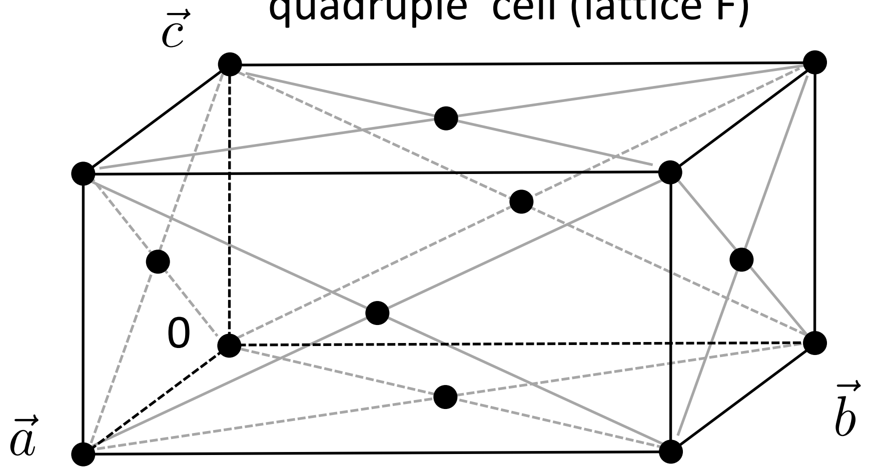
double cell (lattice I)



double cell (lattice C)



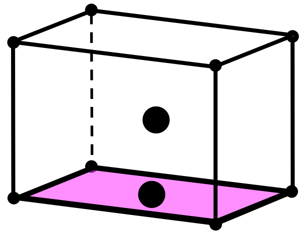
quadruple cell (lattice F)



Bravais lattice: associates a crystal system with a lattice type

7 crystal systems
4 lattice types
} 28 possibilities?

➔ only 14 Bravais lattices



Is the starting holohedry conserved in the new primitive cell?

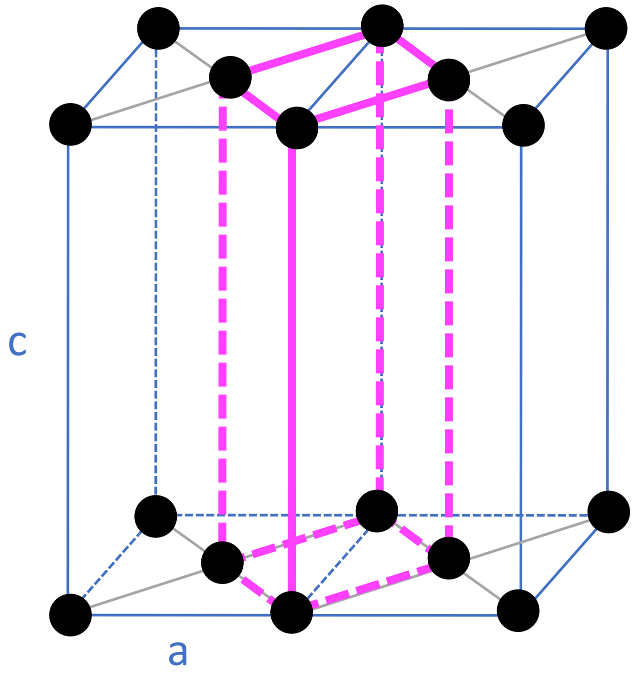
yes → Bravais lattice with **primitive cell**

no → Bravais lattice with **supercell**

12 – The 14 Bravais lattices

- tetragonal P (*tP*)
- tetragonal I (*tI*)

Why does not the tetragonal C lattice exist?



It is possible to define a smaller tetragonal cell with parameters

a' = a / √2

c' = c

➔ ➔ It is equivalent to **tetragonal P** Bravais lattice

12 – The 14 Bravais lattices

- cubic P (*cP*)
- cubic I (*cI*)
- cubic F (*cF*)

- orthorhombic P (*oP*)
- orthorhombic I (*oI*)
- orthorhombic with centred base (*oS*)

  oA *oB* *oC*

- orthorhombic F (*oF*)

12 – The 14 Bravais lattices

➡ triclinic P (*aP*)

« *anortic* »

➡ monoclinic P (*mP*)

➡ monoclinic
with double cell (*mS*)

unique axis $\vec{b}$

mC *mA* *mI*

Il en reste 2…

12 – The 14 Bravais lattices

hexagonal system ➔ one unique Bravais lattice *hP*

trigonal system

$\bar{3}$ m

→ hexagonal cell ➔ Bravais lattice *hP*

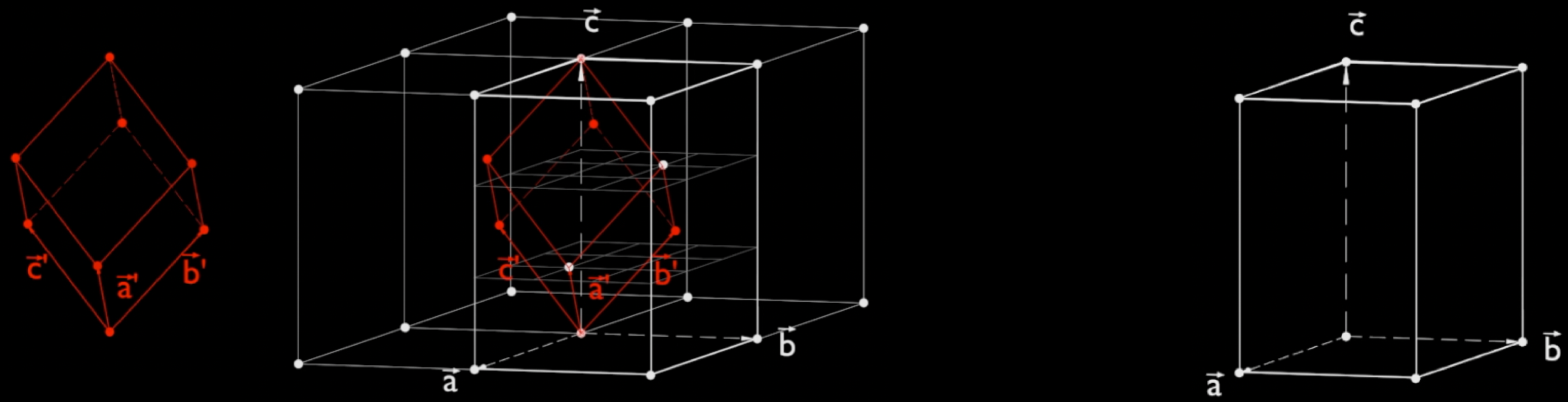
→ rhombohedral cell ➔ Bravais lattice *hR, which is also primitive*

↳ *but in pratice, hR lattice are commonly described using a triple hexagonal cell*

12 – The 14 Bravais lattices

h R Bravais lattice

h P Bravais lattice



$$+\left(\frac{1}{3},\frac{2}{3},\frac{2}{3}\right)+\left(\frac{2}{3},\frac{1}{3},\frac{1}{3}\right)$$

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

8 – Stereographic projection

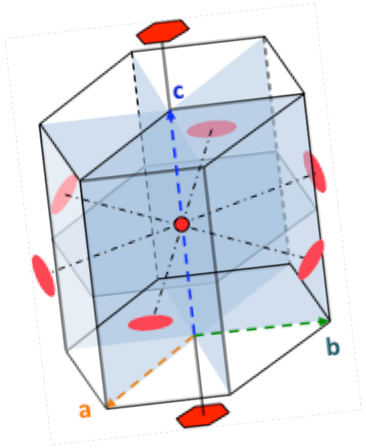
9 – Roto-inversions

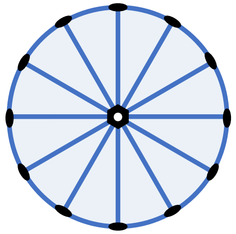
10 – The 32 crystallographic point groups

11 – The 7 crystal systems

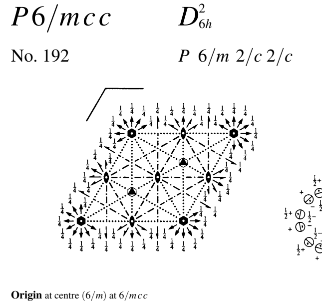
12 – The 14 Bravais lattices

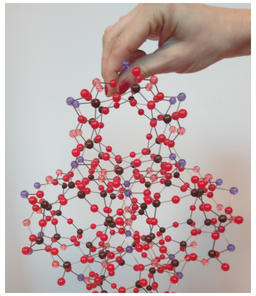
13 – The 230 space-groups





$\frac{6}{m}mm$





13 – Space groups

Orientation symmetry ➔ 32 crystallographic point groups

set of the symmetry operations that let invariant crystal morphology and its physical properties

7 crystal systems (6 crystal families)

+ 4 lattice types (translation groups)

14 Bravais lattices

Position symmetry ➔ the 230 space groups

set of the symmetry operations that let invariant the atomic structure

International Tables of Crystallography volume A

The symmorphic groups (73)

*Association of the symmetry elements of the crystallographic point groups with the Bravais lattice translation groups: the generators **are neither** screw axes **nor** glide planes)*

Hermann-Mauguin symbols: Lattice-type letter (P, A, B, C, I, F, R) followed by the Hermann-Mauguin symbol of the crystallographic point group

ex : *P m m m*, *F m m m*, *P 4 m m*, *I 4 m m*

The non-symmorphic groups(157)

Space groups whose generators are screw axes and/or glide planes.

ex : *I b a* 2, *P* 4_1, *P* 4_2 *c m*

Elements de position symmetry

- The symmetry elements of the crystallographic point groups
- New symmetry elements resulting from products:
  - $m \times \vec{t}$ → **glide planes**
  - $\mathrm{A}_n \times \vec{t}$ → **screw axes**

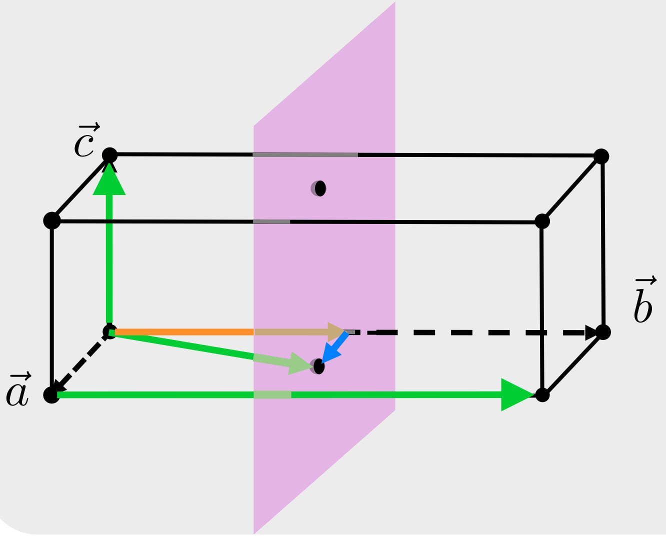
Position symmetry: mirror × lattice translation

mirror plane m × $\vec{t}$

case 1: $\vec{t} \parallel$ mirror $\qquad \vec{t} = \vec{c}$

case 2: $\vec{t} \perp$ mirror $\qquad \vec{t} = \vec{b}$

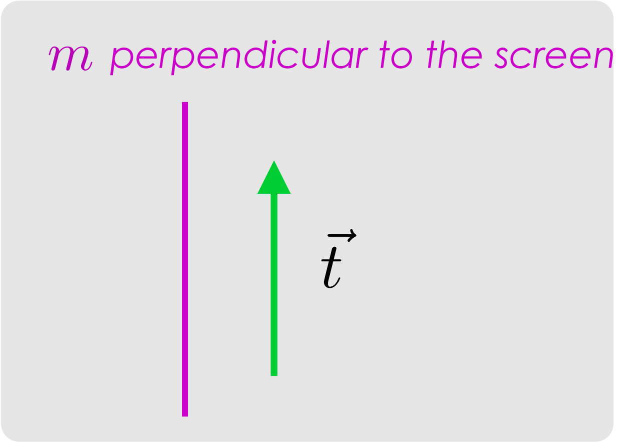
case 3: $\vec{t}$ oblique / mirror $\qquad \vec{t} = \frac{\vec{a}+\vec{b}}{2} \qquad \vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$



$\vec{t}_{\perp}$ & $\vec{t}_{\parallel}$ *are not lattice translation*

Position symmetry: mirror × lattice translation

case 1: $m \times \vec{t}$ with $\vec{t} \parallel m$

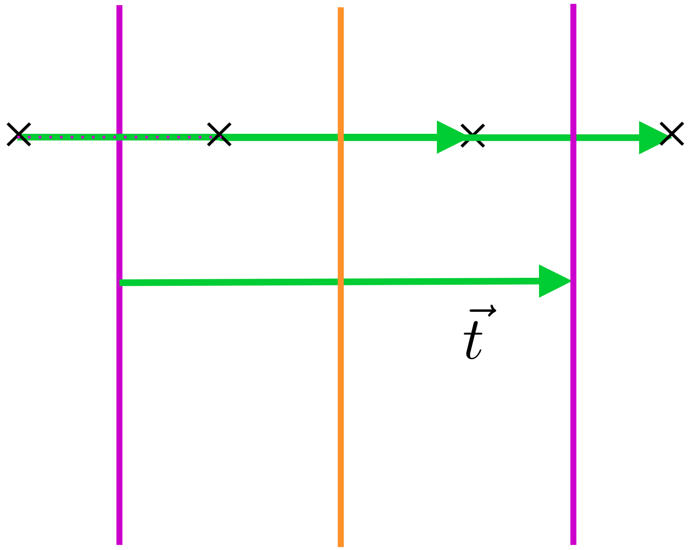


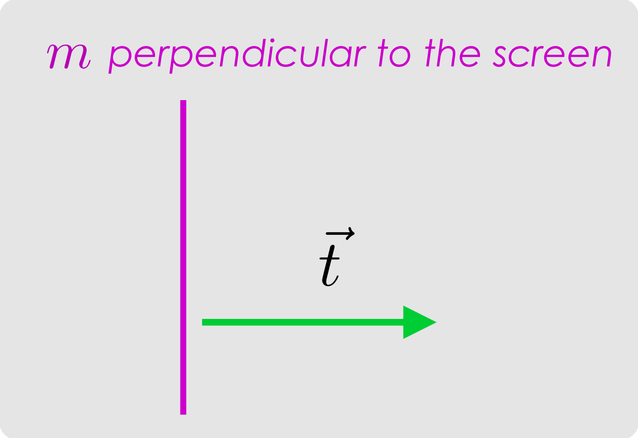
any mirror plane m is infinite

Any translation $\vec{t} \parallel m$
has no effect on it

Position symmetry: mirror × lattice translation

case 2: $m \times \vec{t}$ with $\vec{t} \perp m$





new mirror plane m at $\dfrac{\vec{t}}{2}$ from the first one

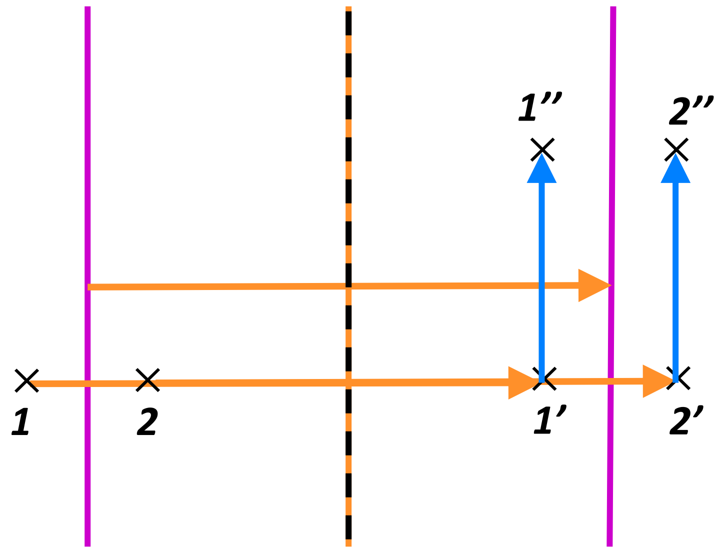
Position symmetry: mirror × lattice translation

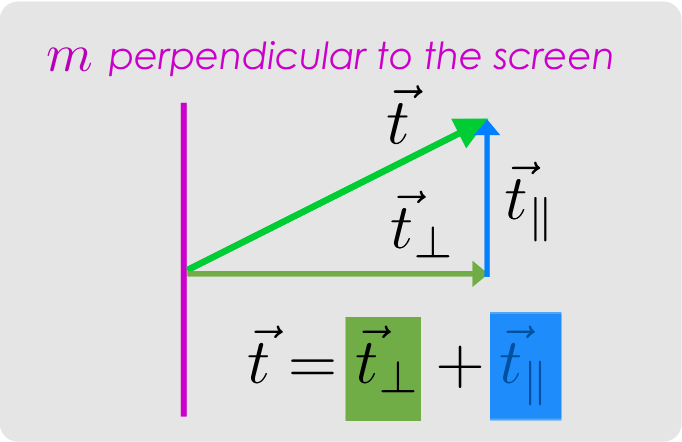
case 3: $m \times \vec{t}$ with $\vec{t}$ oblique / m

Decomposition $\vec{t} = \vec{t}_{\perp} + \vec{t}_{||}$

where $\vec{t}_{\perp}$ & $\vec{t}_{||}$ are the components s $\perp$ & $||$ to m

.

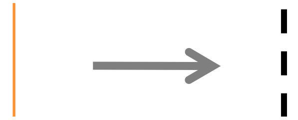




$\vec{t}_{||}$ changes the nature of the **mirror** obtained by considering $\vec{t}_{\perp}$, but only if $\vec{t}_{||}$ **is not** a lattice translation.

⇓

glide plane



Position symmetry: mirror × lattice translation

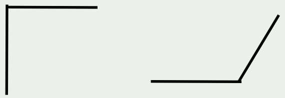
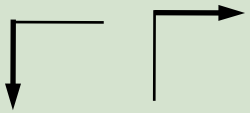
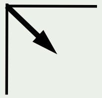
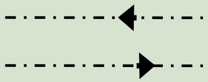
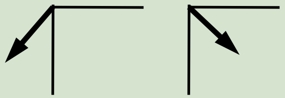
- Mirror m combined with a translation $\vec{t}_{||}$ parallel to m ($\vec{t}_{||}$ **is not** a lattice translation)
- Symmetry element of order 2; associated operation noted $(m, \vec{t}_{||})$

$(m, \vec{t}_{||})^2 = (2\,m, 2\,\vec{t}_{||})$ = identity thus $2\vec{t}_{||} = p\,\vec{t}$ with p = 0 or 1

Axial glide planes

lattice translation	glide	symbol
$\vec{t} = \vec{a}$	$\vec{t}_{\|} = \frac{\vec{a}}{2}$	a
$\vec{t} = \vec{b}$	$\vec{t}_{\|} = \frac{\vec{b}}{2}$	b
$\vec{t} = \vec{c}$	$\vec{t}_{\|} = \frac{\vec{c}}{2}$	c

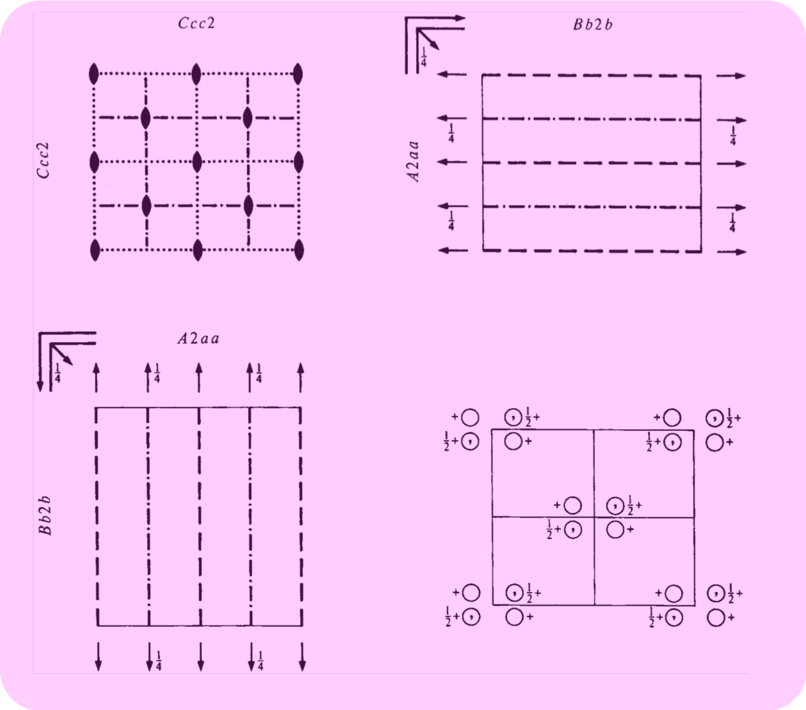
Position symmetry: mirror × lattice translation

Type of plane	Symbol	Translation	Representation	
			normal to the plane of the figure	parallel to the plane of the figure
mirror plane	m	0		
axial glide plane	a or b c	$\vec{a}/2$ or $\vec{b}/2$ $\vec{c}/2$		
diagonal glide plane	n	$(\vec{a} \pm \vec{b})/2$ $(\vec{a} \pm \vec{c})/2$ $(\vec{b} \pm \vec{c})/2$		
diamond-type glide plane	d	$(\vec{a} \pm \vec{b})/4$ $(\vec{a} \pm \vec{c})/4$ $(\vec{b} \pm \vec{c})/4$		

glide planes as space group generators

perp. to [100]

$Ccc2$	C_{2v}^{13}	$mm2$	Orthorhombic
No. 37	$Ccc2$		Patterson symmetry $Cmmm$



Origin on $cc2$

The spacegroup symbol contains 2 glide planes c that we can see on the schemes.

Glide plane of type n are generated by the lattice translation C :

$$\vec{t} = \frac{\vec{a} + \vec{b}}{2}$$

$$c \perp [100] : \quad \vec{t}_{\perp} = \frac{\vec{a}}{2} \qquad \vec{t}_{\parallel} = \frac{\vec{b}}{2}$$

➔ new glide plane n on $\frac{\vec{t}_{\perp}}{2}$

Position symmetry: A_n × lattice translation

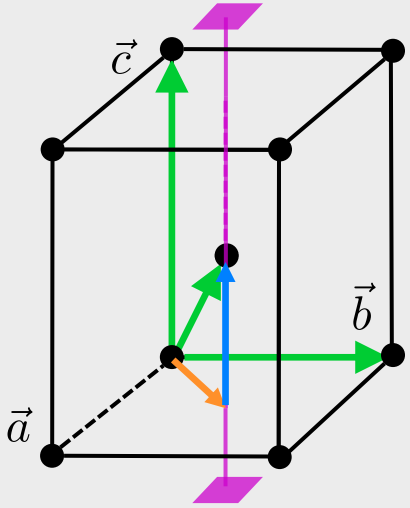
axis A_n × $\vec{t}$

casse 1: $\vec{t} \parallel$ axis $\vec{t} = \vec{c}$

case 2: $\vec{t} \perp$ axis $\vec{t} = \vec{b}$

case 3: $\vec{t}$ oblique / axis $\vec{t} = \frac{\vec{a}+\vec{b}+\vec{c}}{2}$ $\vec{t} = \vec{t}_\perp + \vec{t}_\parallel$

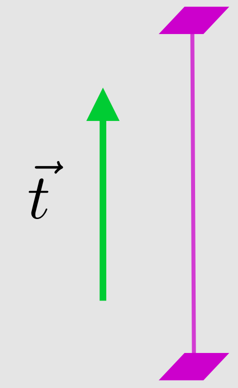
$\vec{t}_\perp$ & $\vec{t}_\parallel$ *are not lattice translations*



Position symmetry: A_n × lattice translation

case 1: $A_n \times \vec{t}$ with $\vec{t} \parallel A_n$

example :
$n = 4$



Any axis A_n is infinite

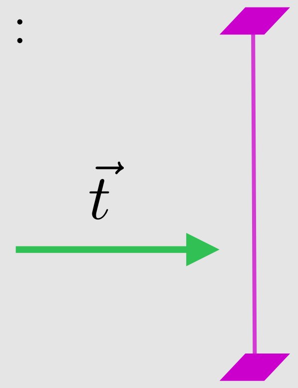
$\vec{t}$ has no effect on it

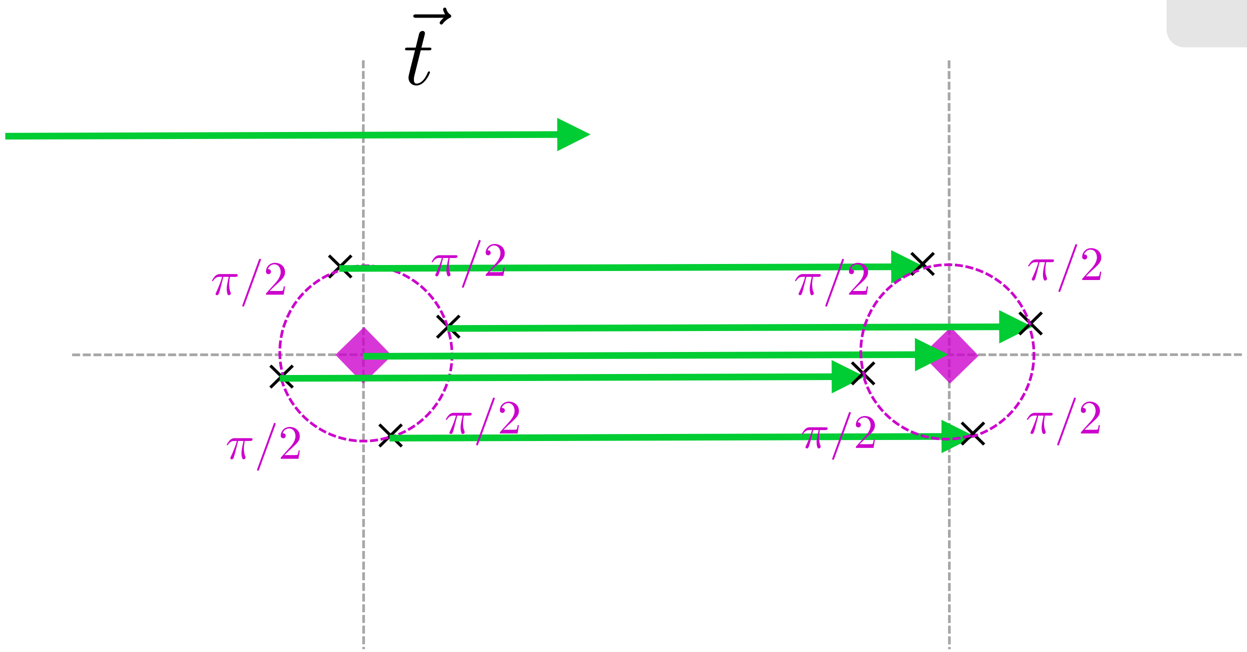
wether $\vec{t}$ is a lattice translation or not

Position symmetry: A_n × lattice translation

case 2: $A_n \times \vec{t}$ with $\vec{t} \perp A_n$

example :
$n = 4$

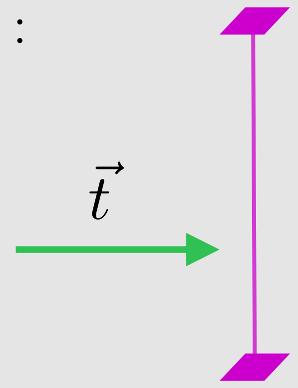


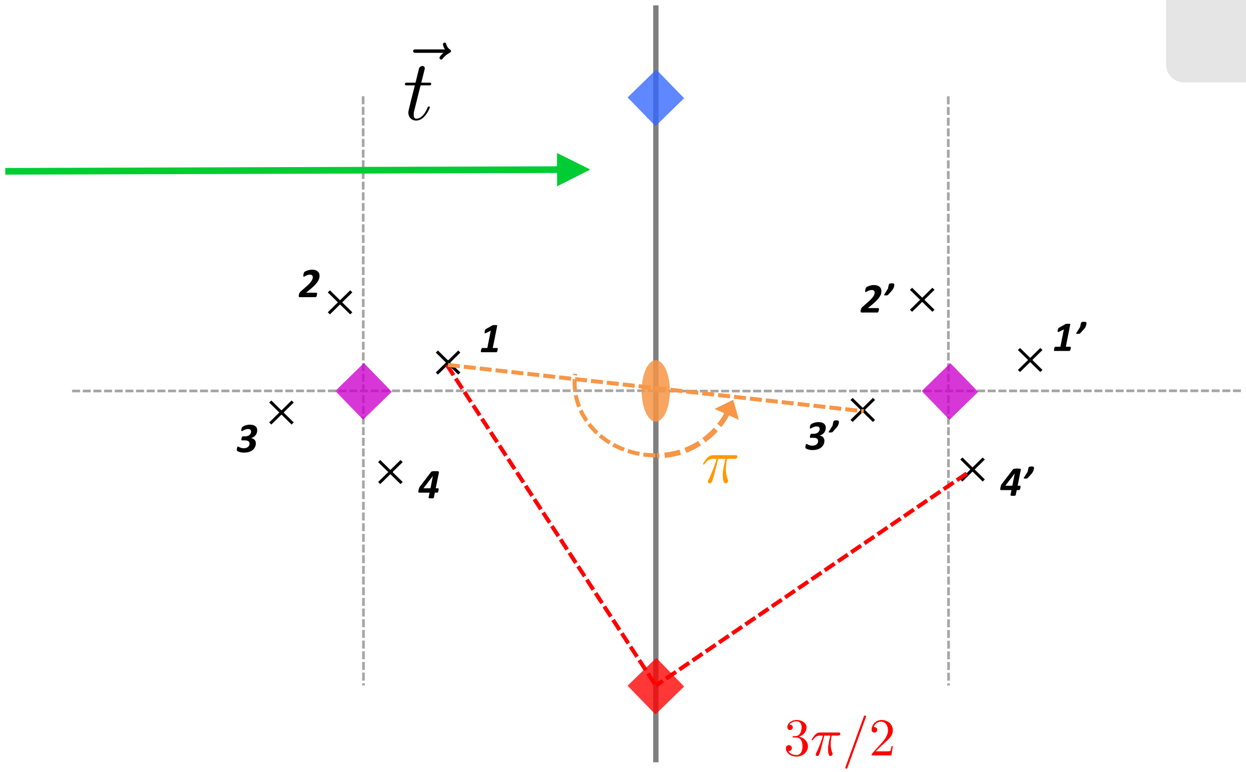


Position symmetry: A_n × lattice translation

case 2: $A_n \times \vec{t}$ with $\vec{t} \perp A_n$

example :
$n = 4$





$1 \longrightarrow 1'$: $\vec{t}$

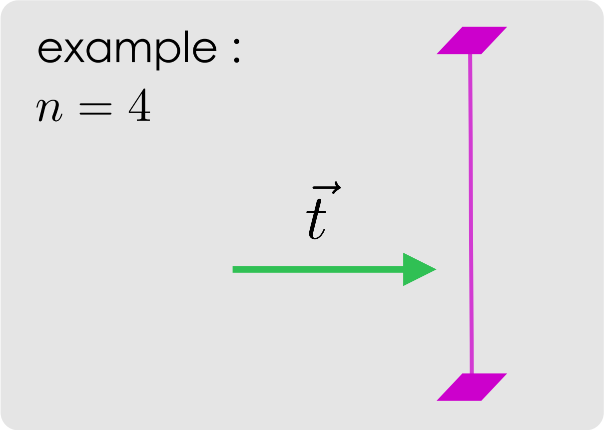
$1 \longrightarrow 2'$: A_4

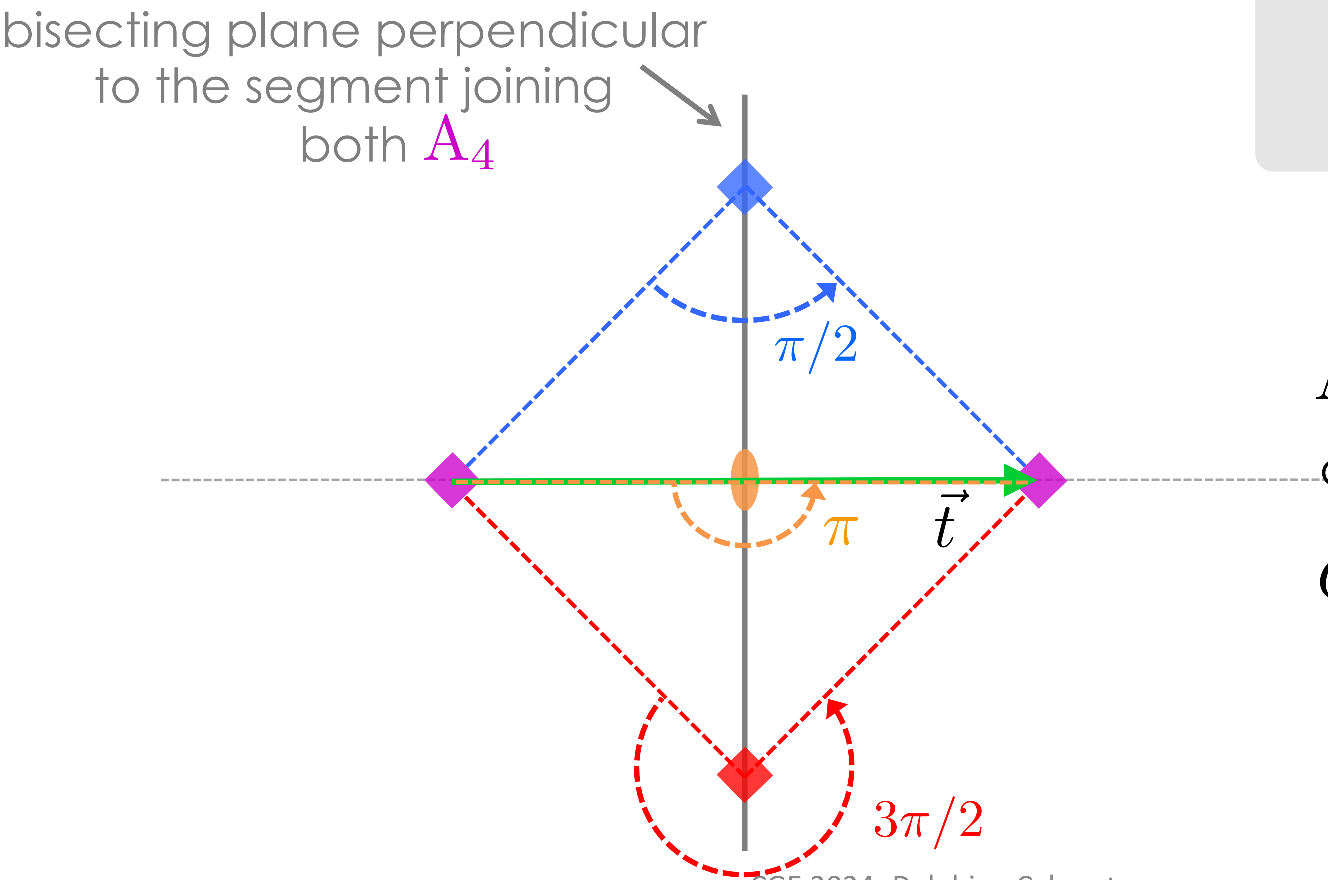
$1 \longrightarrow 3'$: A_2

$1 \longrightarrow 4'$: A_4

Position symmetry: A_n × lattice translation

case 2: $A_n \times \vec{t}$ with $\vec{t} \perp A_n$





A_4 = representation of cyclic group

$$C_4 = (a, a^2, a^3, e)$$

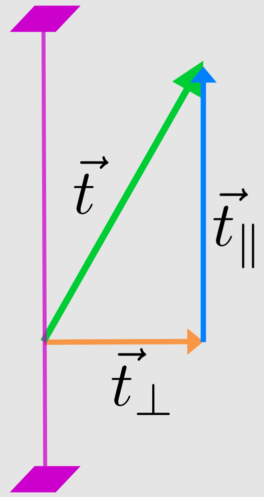
case 3: $A_n \times \vec{t}$ with $\vec{t}$ oblique / A_n

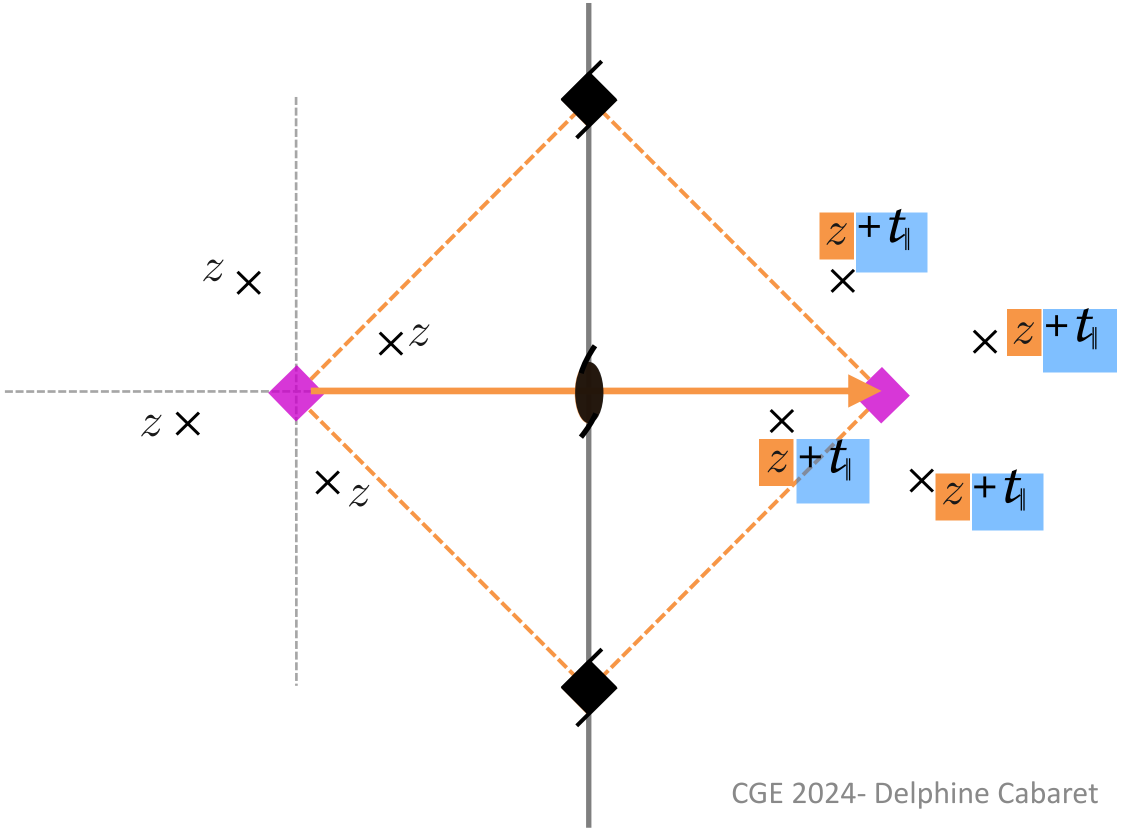
Taking $\vec{t}_{||}$ into account

➔ a component $t_{||}$ to z is added

example :
$n = 4$

$\vec{t} = \vec{t}_{\perp} + \vec{t}_{||}$





Adding $\vec{t}_{||}$ changes the nature of axes A_4 & A_2 obtained by considering $\vec{t}_{\perp}$, if $\vec{t}_{||}$ **is not** a lattice translation.

➔

screw axes

Position symmetry: A_n × lattice translation

case 2: $\mathrm{A}_n \times \vec{t}$ with $\vec{t} \perp \mathrm{A}_n$

In the bisecting plane perpendicular to the segment joining axis A_n and its image by application of translation , $\vec{t}$ appear **new rotation axes** corresponding to operations

$$a^m = \left(m\frac{2\pi}{n} \mid \vec{0} \right)$$

with $m = 1, \ldots, n-1$

Projected in a plane perpendicular to A_n these new rotation axes are located in points of the bisecting plane from which the translation is seen under angle $m\dfrac{2\pi}{n}$

A_n is a representation of cyclic group

$$C_n = (a, a^2, \ldots, a^{n-1}, e)$$

such as $a^n = e$

Position symmetry: screw axis

- Rotation axis A_n of order n combined with translation $\vec{t}_{||}$ parallel to A_n
- Associate operation noted $\left(\frac{2\pi}{n}, \vec{t}_{||}\right)$

Question: In **a crystal lattice** such as $\mathrm{A}_n \parallel \vec{c}$, which vectors $\vec{t}_{||}$ are possible?

$$\left(\frac{2\pi}{n}, \vec{t}_{||}\right)^n = (2\pi, n\vec{t}_{||})$$ = identity

thus $n\vec{t}_{||} = p\vec{c}$ with p an integer

so $\vec{t}_{||} = \frac{p\vec{c}}{n}$ where $p = 0, ..., n-1$

$p = 0 \Rightarrow \vec{t}_{||} = \vec{0}$

$p = 1 \Rightarrow \vec{t}_{||} = \frac{\vec{c}}{n}$

$p = 2 \Rightarrow \vec{t}_{||} = \frac{2\vec{c}}{n}$

$p = 3 \Rightarrow \vec{t}_{||} = \frac{3\vec{c}}{n}$

...

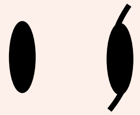
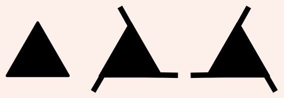
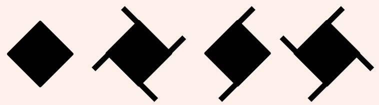
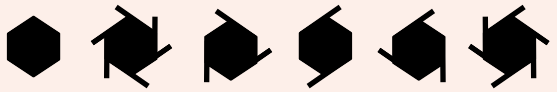
$p = n-1 \Rightarrow \vec{t}_{||} = \frac{(n-1)\vec{c}}{n}$

Position symmetry: screw axis

- Rotation axis A_n of order n combined with translation $\vec{t}_{||}$ parallel to A_n ($\vec{t}_{||}$ **is not** lattice translation)
- Associate operation noted $\left(\frac{2\pi}{n}, \vec{t}_{||}\right)$

➡ **Question:** In **a crystal lattice** such as $\mathrm{A}_n \parallel \vec{c}$, which vectors $\vec{t}_{||}$ are possible?

$\left(\frac{2\pi}{n}, \vec{t}_{||}\right)^n = (2\pi, n\vec{t}_{||})$ = identity thus $n\vec{t}_{||} = p\vec{c}$ with p an integer

A_n order	1	2		3			4				6					
Translation	0	0	$\frac{\vec{c}}{2}$	0	$\frac{\vec{c}}{3}$	$\frac{2\vec{c}}{3}$	0	$\frac{\vec{c}}{4}$	$\frac{2\vec{c}}{4}$	$\frac{3\vec{c}}{4}$	0	$\frac{\vec{c}}{6}$	$\frac{2\vec{c}}{6}$	$\frac{3\vec{c}}{6}$	$\frac{4\vec{c}}{6}$	$\frac{5\vec{c}}{6}$
Hermann-Mauguin symbol	1	2	2_1	3	3_1	3_2	4	4_1	4_2	4_3	6	6_1	6_2	6_3	6_4	6_5
Representation																

Position symmetry: screw axis

axis A_n $\times$ $\vec{t}$

case 1: $\vec{t} \parallel$ axis → no effect

case 2: $\vec{t} \perp$ axis → **new rotation axes** in the bisecting plane perpendicular to the segment joining axis A_n and its image by application of $\vec{t}$

case 3: $\vec{t}$ oblique / axis $\vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$

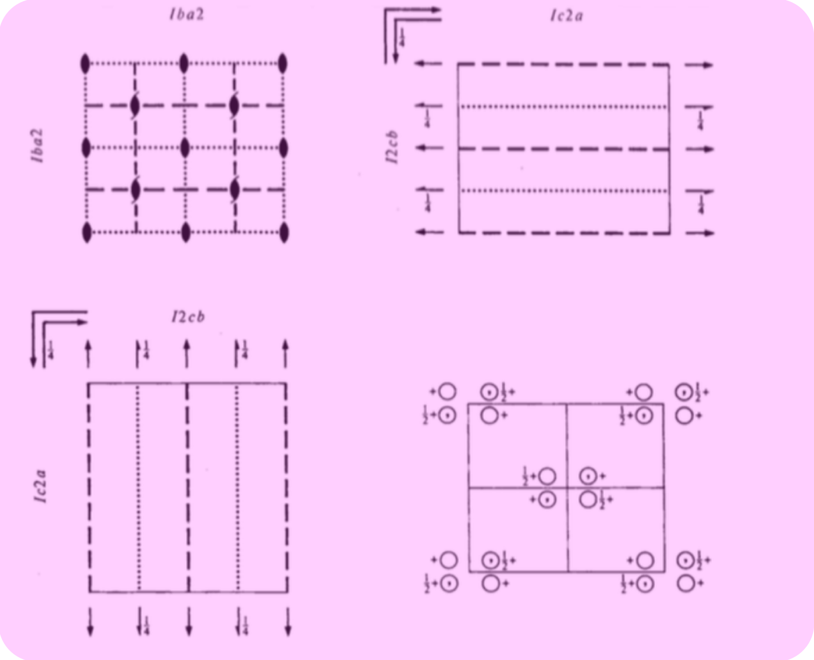
→ **Change of the new axes nature** if $\vec{t}_{\parallel}$ is not a lattice translation

Position symmetry: screw axis

//[001]

International Tables for Crystallography (2006). Vol. A, Space group 45, pp. 258–259.

*Iba*2	C_{2v}^{21}	*mm*2	Orthorhombic
No. 45	*Iba*2		Patterson symmetry *Immm*



Origin on *cc*2

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,*z*	(3) *a* *x*,¼,*z*	(4) *b* ¼,*y*,*z*

For (½,½,½)+ set

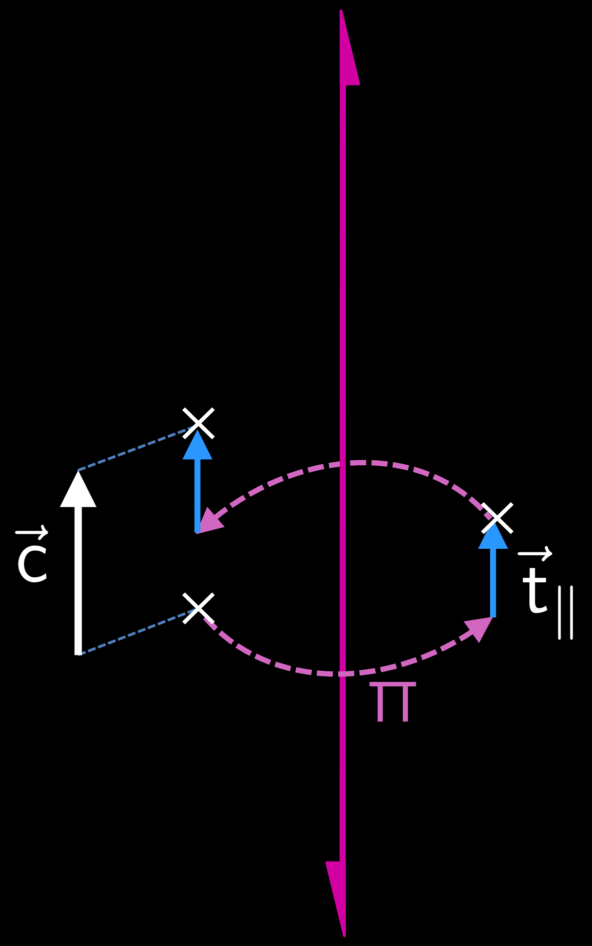
(1) *t*(½,½,½)	(2) 2(0,0,½) ¼,¼,*z*	(3) *c* *x*,0,*z*	(4) *c* 0,*y*,*z*

Screw axes 2_1 are generated by the lattice translation I:

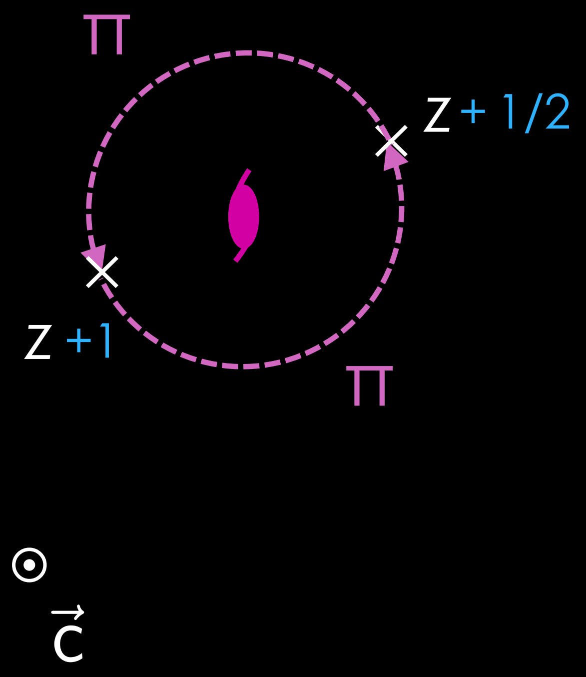
$$\frac{\vec{a}+\vec{b}+\vec{c}}{2}$$

$$\vec{t}_{\perp} = \frac{\vec{a}+\vec{b}}{2} \qquad \vec{t}_{\parallel} = \frac{\vec{c}}{2}$$

Screw axis $2_1 \parallel \vec{c}$

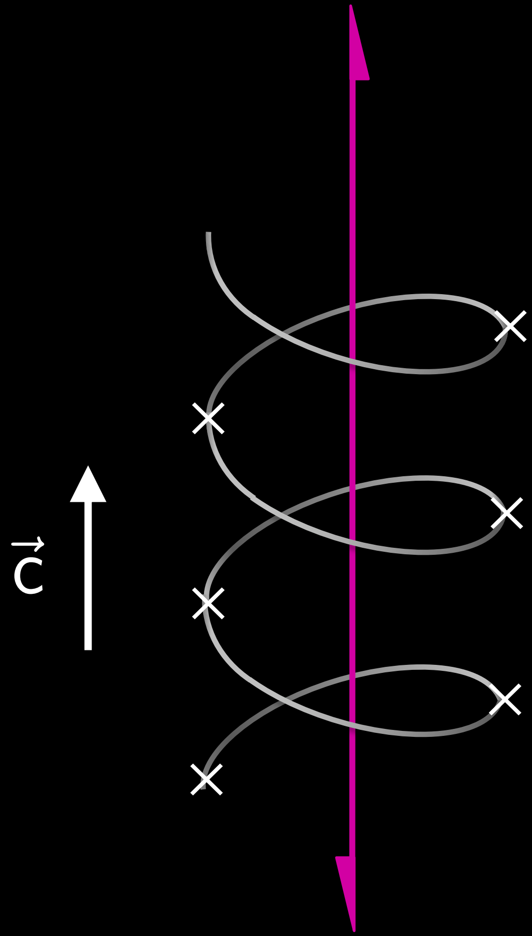


in the plane of the screen



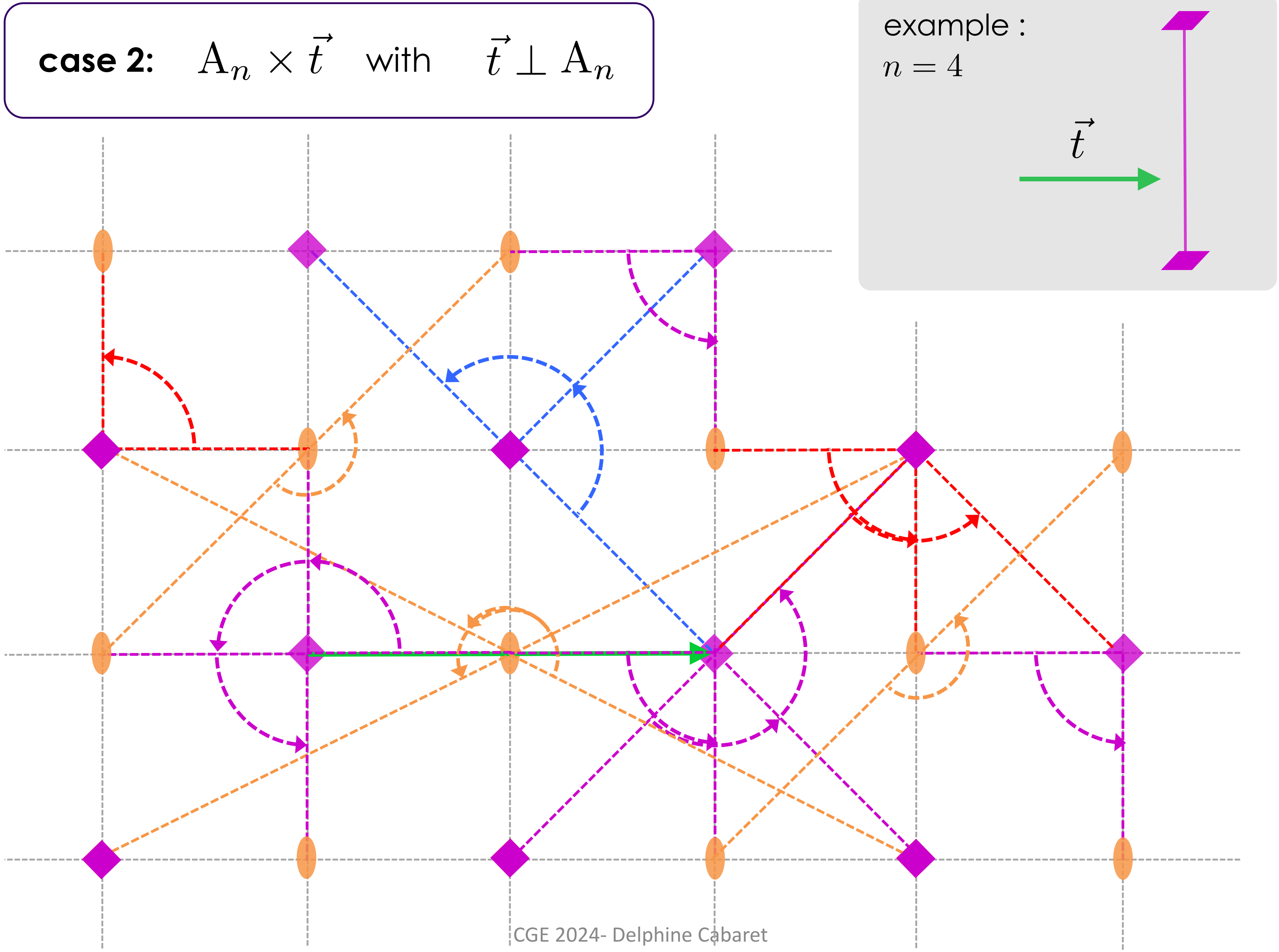
normal to the plane of the screen

Screw axis $2_1 \parallel \vec{c}$



case 2: $A_n \times \vec{t}$ with $\vec{t} \perp A_n$

example :
$n = 4$

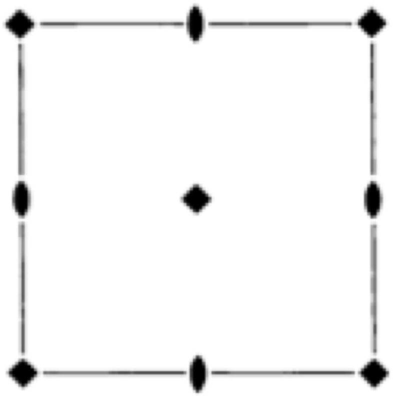


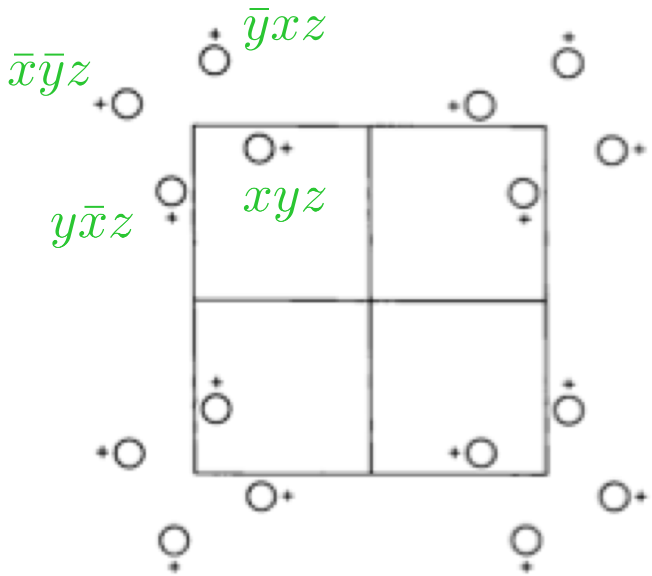
example of 1-generator point group

1st space group of point group C_4

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

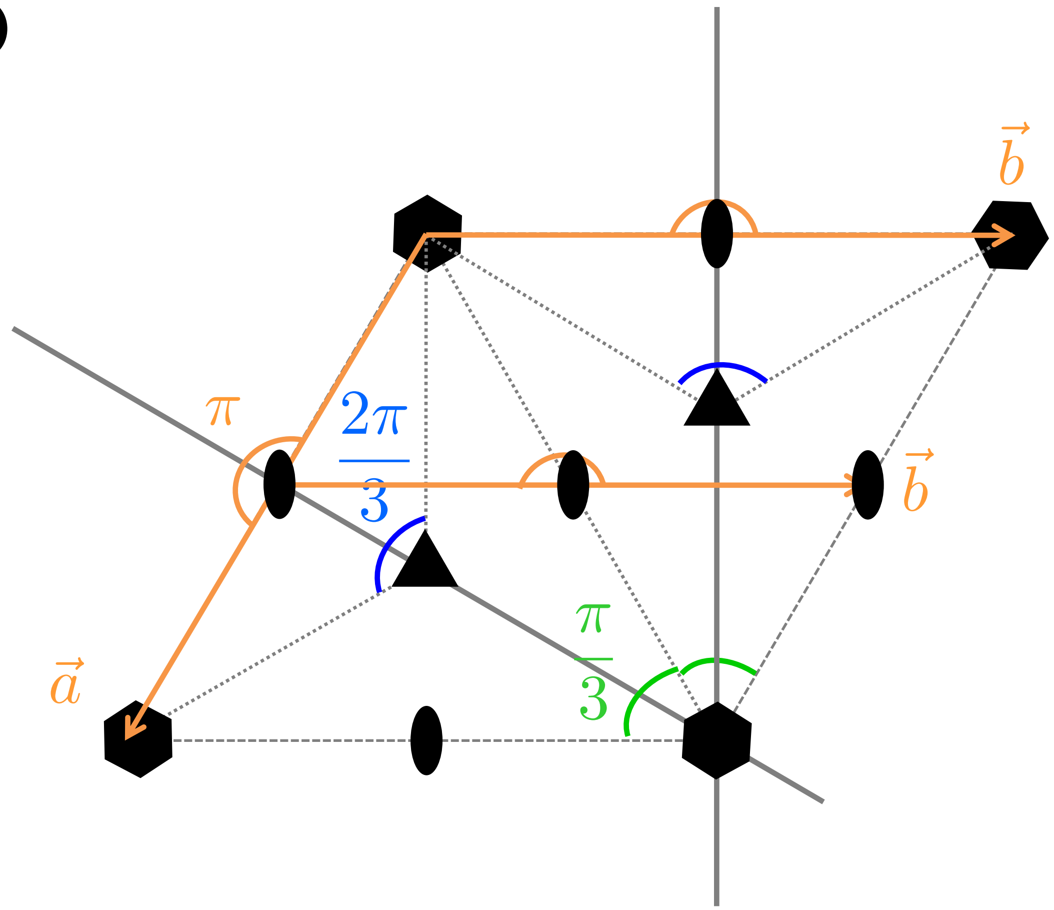
***P*4**	C_4^1	4	Tetragonal
No. 75	*P*4		Patterson symmetry *P*4/*m*





example of 1-generator point group

$P\ 6$



13 – Space groups

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

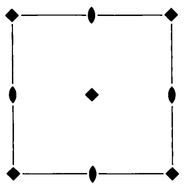
$P4$ | C_4^1 | 4 | Tetragonal
No. 75 | $P4$ | | Patterson symmetry $P4/m$

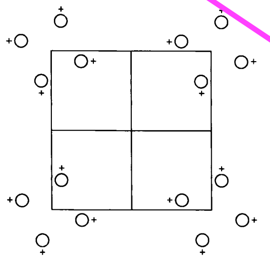
name (symbol) & number of the space group

Schönflies symbol

crystal system

corresponding point group





origin choice
(drawings and positions)

≢ motif
- The symmetry-independent part of the structure
- A rational fraction of the unit cell (related to the other part of the unit cell by space group symmetry operations)

Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	c	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $h+k=2n$
1	b	4 . .	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 . .	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2$ (3) 1; 2
IIa none
IIb [2] $P4_2$ ($\mathbf{c}' = 2\mathbf{c}$) (77); [2] $F4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4$, 79)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4$ ($\mathbf{c}' = 2\mathbf{c}$) (75); [2] $C4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4$, 75)

Minimal non-isomorphic supergroups

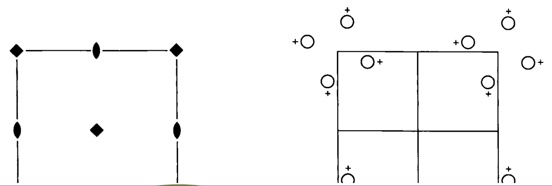
I [2] $P4/m$ (83); [2] $P4/n$ (85); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4cc$ (103); [2] $P4nc$ (104)
II [2] $I4$ (79)

 332

13 – Space groups

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

$P4$	C_4^1	4	Tetragonal
No. 75	$P4$		Patterson symmetry $P4/m$



Positions

Multiplicity,	Wyckoff letter,	Site symmetry	Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	c	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $h+k=2n$
1	b	4 . .	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 . .	$0,0,z$				no extra conditions

cf. diffraction cours

Symmetry of special projections
Along [001] $p4$ — $\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Along [100] $p1m1$ — $\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Along [110] $p1m1$ — $\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$

multiplicity: number of equivalent positions équivalentes within the unit cell for a given Wyckoff position

Maximal non-isomorphic subgroups
I [2] $P2$ (3) 1; 2
IIa none

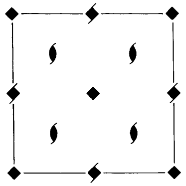
Wyckoff letter: identifies the atomic positions, in alphabetic order,
from the most symmetric (bottom) to the general position without symmetry (top)

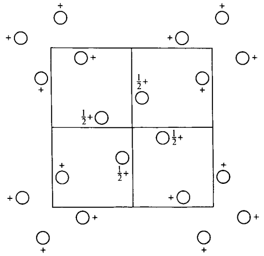
point group of the site (sub-group of the crystal point group)

13 – Space groups

International Tables for Crystallography (2006). Vol. A, Space group 79, pp. 336–337.

$I4$	C_4^5	4	Tetragonal
No. 79	$I4$		Patterson symmetry $I4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$;

Symmetry operations

For (0,0,0)+ set
(1) 1 (2) 2 0,0,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$

CONTINUED No. 79 $I4$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	b	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $l=2n$
2	a	4 . .	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$\frac{1}{2},\frac{1}{2})$

...west index

...$2\mathbf{b}$, $\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (79)

...mm (107); [2] $I4cm$ (108)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+			
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
4	b	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$		
2	a	4 . .	$0,0,z$			

336 337

comparison between space groups *P*3 & *R*3

crystallographic point group 3

rhombohedral axes
→ lattice R

space group: R 3 (n° 146)

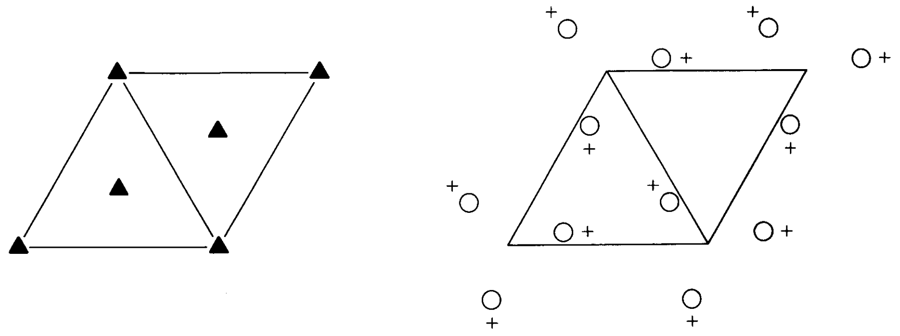
hexagonal axes
→ lattice P

space group: P 3 (n° 143)

comparison between space groups *P*3 & *R*3

$P3$ $\quad C_3^1 \quad$ 3 $\quad$ Trigonal

No. 143 $\quad P3 \quad$ Patterson symmetry $P\bar{3}$



Origin on 3

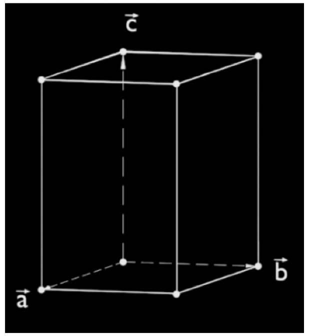
Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\quad \frac{1}{2},0,0$ $\quad \frac{2}{3},\frac{1}{3},0$ $\quad \frac{1}{3},\frac{2}{3},0$ $\quad 0,\frac{1}{2},0$

$0,0,1$ $\quad \frac{1}{2},0,1$ $\quad \frac{2}{3},\frac{1}{3},1$ $\quad \frac{1}{3},\frac{2}{3},1$ $\quad 0,\frac{1}{2},1$

Symmetry operations

(1) 1 $\quad$ (2) 3^+ $0,0,z$ $\quad$ (3) 3^- $0,0,z$



CONTINUED $\quad$ No. 143 $\quad P3$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	*d*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
						Special: no extra conditions
1	*c*	3 . .	$\frac{2}{3},\frac{1}{3},z$			
1	*b*	3 . .	$\frac{1}{3},\frac{2}{3},z$			
1	*a*	3 . .	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $P1$ (1) 1

IIa none

IIb [3] $P3_2$ ($\mathbf{c}' = 3\mathbf{c}$) (145); [3] $P3_1$ ($\mathbf{c}' = 3\mathbf{c}$) (144); [3] $R3$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{a}+2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (146); [3] $R3$ ($\mathbf{a}' = 2\mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (146)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3$ ($\mathbf{c}' = 2\mathbf{c}$) (143); [3] $H3$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3$, 143)

Minimal non-isomorphic supergroups

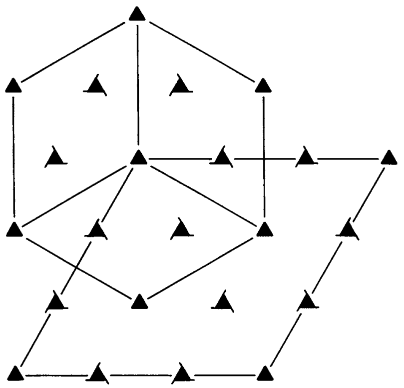
I [2] $P\bar{3}$ (147); [2] $P312$ (149); [2] $P321$ (150); [2] $P3m1$ (156); [2] $P31m$ (157); [2] $P3c1$ (158); [2] $P31c$ (159); [2] $P6$ (168); [2] $P6_3$ (173); [2] $P\bar{6}$ (174)

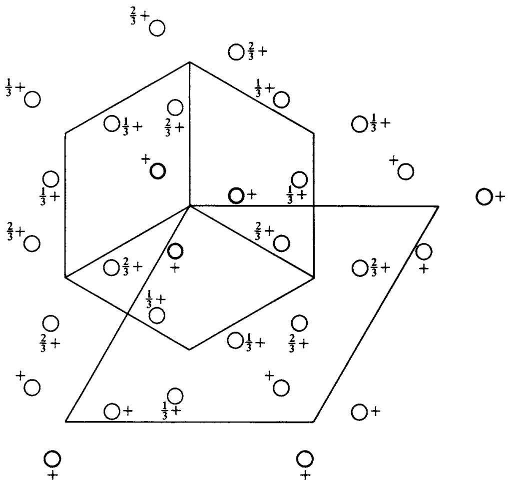
II [3] $R3$ (obverse) (146); [3] $R3$ (reverse) (146)

comparison between space groups $P3$ & $R3$

$R3$	C_3^4	3	Trigonal
No. 146	$R3$		Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin on 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{3}$ $\frac{1}{2},0,\frac{1}{3}$ $\frac{2}{3},\frac{1}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3},\frac{1}{3}$ $0,\frac{1}{2},\frac{1}{3}$

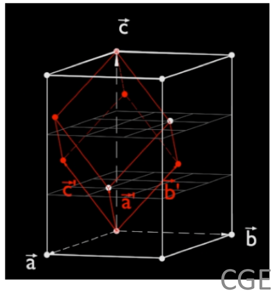
Symmetry operations

For $(0,0,0)+$ set
(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set
(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ (2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$ (3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set
(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ (2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$ (3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$

conventionnel setting



CONTINUED No. 146 $R3$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$

9 b 1 (1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$

General:
$hkil$: $-h+k+l=3n$
$hki0$: $-h+k=3n$
$hh\overline{2h}l$: $l=3n$
$h\bar{h}0l$: $h+l=3n$
$000l$: $l=3n$
$h\bar{h}00$: $h=3n$

3 a 3 . $0,0,z$

Special: no extra conditions

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1+
IIa [3] $P3_2$ (145) 1; $2+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; $3+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
[3] $P3_1$ (144) 1; $2+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $3+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
[3] $P3$ (143) 1; 2; 3
IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (146); [4] $R3$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (146)

Minimal non-isomorphic supergroups

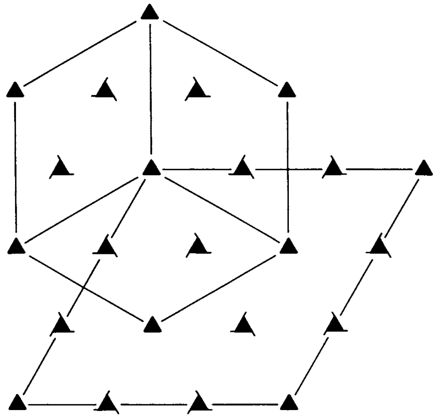
I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)
II [3] $P3$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (143)

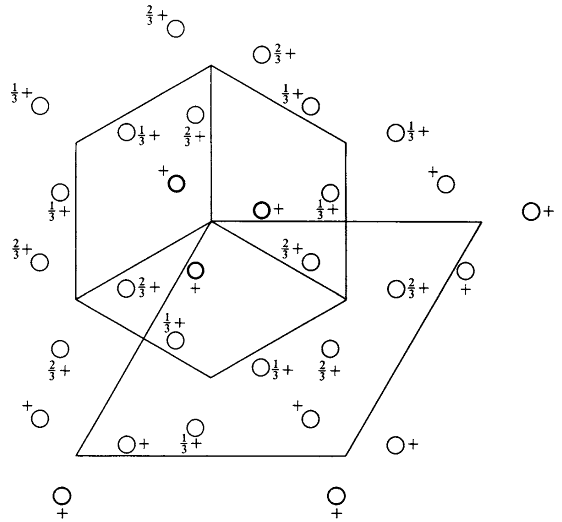
comparison between space groups *P*3 & *R*3

$R3$ | C_3^4 | 3 | Trigonal

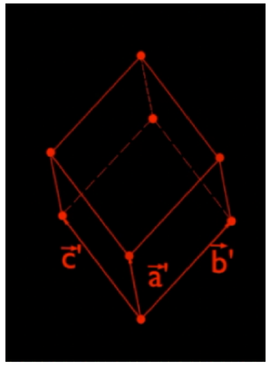
No. 146 | $R3$ | Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes



Origin on 3

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $z \le \min(x,y)$

Vertices 0,0,0 1,0,0 1,1,0 0,1,0 1,1,1

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x

CONTINUED No. 146 $R3$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
3 b 1	(1) x,y,z (2) z,x,y (3) y,z,x	no conditions
		Special: no extra conditions
1 a 3 .	x,x,x	

Symmetry of special projections

Along [111] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1

IIa none

IIb [3] $P3_2$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b}, \mathbf{b}'=\mathbf{b}-\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (145); [3] $P3_1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b}, \mathbf{b}'=\mathbf{b}-\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (144);
[3] $P3$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b}, \mathbf{b}'=\mathbf{b}-\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (143)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}$) (146); [4] $R3$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (146)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198);
[4] $I2_13$ (199)

II [3] $P3$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (143)

come back to example 3 of the "*Objectives*"

PHYSICAL REVIEW B **78**, 195103 (2008)

X-ray linear dichroism in cubic compounds: The case of Cr^{3+} in $MgAl_2O_4$

Amélie Juhin,[1,*] Christian Brouder,[1] Marie-Anne Arrio,[1] Delphine Cabaret,[1] Philippe Sainctavit,[1] Etienne Balan,[1,2] Amélie Bordage,[1] Ari P. Seitsonen,[1] Georges Calas,[1] Sigrid G. Eeckhout,[3] and Pieter Glatzel[3]

mechanical properties.[13] In $MgAl_2O_4$ spinel ($Fd\bar{3}m$ space-group symmetry), Al^{3+} cations occur at octahedral sites, which exhibit D_{3d} (or $\bar{3}m$) symmetry and build chains aligned along the six twofold axis of the cubic structure.[14]

?

Extract of the space-group table of spinel

$Fd\bar{3}m$	O_h^7	$m\bar{3}m$	Cubic
No. 227	$F\ 4_1/d\ \bar{3}\ 2/m$		Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 2

2 possible choices for the origin : the 2nd, when it exists, corresponds to the position of inversion center

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+\quad(\frac{1}{2},0,\frac{1}{2})+\quad(\frac{1}{2},\frac{1}{2},0)+$

h,k,l permutable

General:

Mult.	Wyckoff	Site sym.							Reflection conditions
192	i	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$			hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$			
			(9) y,z,x	(10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$			$0kl$: $k+l=4n$ and $k,l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$			
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$			hhl : $h+l=2n$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z},\bar{y},\bar{x}$			$h00$: $h=4n$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$			
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$			
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) x,z,y	(44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$			
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$	(46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) z,y,x			
									Special: as above, plus
96	h	..2	$0,y,\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{1}{2},\bar{y}+\frac{3}{4},y+\frac{1}{4}$			no extra conditions
			$\bar{y},0,y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{4}$	$y+\frac{3}{4},\frac{1}{4},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{1}{2},\bar{y}+\frac{3}{4}$			
			$y,\bar{y},0$	$\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{1}{4}$	$\bar{y}+\frac{3}{4},y+\frac{1}{4},\frac{1}{2}$			
			$0,\bar{y},y$	$\frac{1}{4},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{1}{2},y+\frac{1}{4},\bar{y}+\frac{3}{4}$			
			$y,0,\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y+\frac{3}{4}$	$\bar{y}+\frac{1}{4},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{1}{2},y+\frac{1}{4}$			
			$\bar{y},y,0$	$y+\frac{3}{4},y+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{4}$	$y+\frac{1}{4},\bar{y}+\frac{3}{4},\frac{1}{2}$			
96	g	..m	x,x,z	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{2}$	$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{z}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4}$			no extra conditions
			z,x,x	$z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$	$\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$			
			x,z,x	$\bar{x}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$			
			$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$			
			$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$			
			$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$z+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{z}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z},\bar{x},\bar{x}$			
48	f	2.mm	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{1}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{1}{8},\frac{5}{8},\bar{x}+\frac{3}{4}$	hkl : $h=2n+1$
			$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\bar{x}+\frac{1}{2},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\bar{x}+\frac{1}{2}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$	or $h+k+l=4n$
32	e	.3m	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$					no extra conditions
			$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$					
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$					
			$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$					
16	d	.$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$			hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	.$\bar{3}m$	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			
8	b	$\bar{4}3m$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{1}{8}$					hkl : $h=2n+1$ or $h+k+l=4n$
8	a	$\bar{4}3m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{3}{8}$					

To take a fresh look at all these concepts…

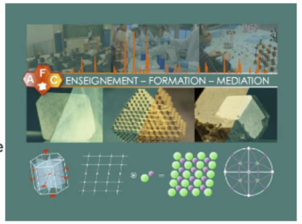
Association Française de Cristallographie

Association ▼ **Adhésion** **Connexion** **Cristallographie**

L'axe transverse Enseignement de la Cristallographie

L'objectif de cet axe est multiple :

- Promouvoir l'enseignement de la cristallographie en France
- Diffuser auprès d'un large public des ressources pédagogiques
- Informer sur les différentes événements en lien avec l'enseignement de la cristallographie



Vous êtes

étudiant-e de licence et master

et vous cherchez

des cours
des ouvrages
des conférences
des logiciels

doctorant-e, ingénieur-e, chercheur-e, enseignant-e du supérieur

et vous cherchez

une formation
une école
un manuel
un logiciel

élève ou enseignant-e du secondaire

et vous cherchez

une vidéo pédagogique
de la documentation

curieux de découvrir le monde des cristaux et la cristallographie

et vous cherchez

de la documentation et des vidéos accesibles à tous

To take a fresh look at all these concepts…

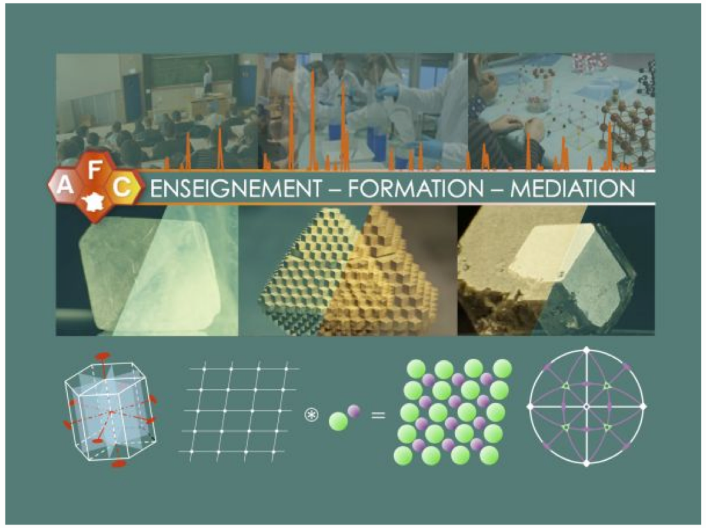
Association Française de Cristallographie

Association ▼ Adhésion Connexion Cristallographie

Vous êtes doctorant-e, ingénieur-e, chercheur-e, enseignant-e du supérieur

Vous cherchez :

- Une formation ou école sur la cristallographie
- Des cours en ligne (vidéos et autres)
- Des manuels de référence
- Des conférences filmées
- Un logiciel gratuit pour visualiser des structures cristallines



To take a fresh look at all these concepts…

Les capsules éducatives de Frank Hoffmann

Il s'agit d'un ensemble de 54 vidéos, en langue anglaise, conçu dans le cadre d'un MOOC, intitulé "The fascination and Crystals and Symmetry", qui a été diffusé sur la plateforme Iversity. Elles sont désormais accessibles sur la chaîne YouTube de Frank Hoffmann. Nous en donnons ici une liste, classés par chapitre, qui sont au nombre de 7 :

Chapitre 1 : Introduction to Crystals and Crystal Systems

Chapitre 2 : Crystal Systems, Fractional Coordinates, and Morphology of Crystals

Chapitre 3 : The World of Symmetry, Crystal classes and Plane groups

Chapitre 4 : Glide planes, Screw axes and Space groups

Chapitre 5 : Quasicrystals and Real Crystal Structures (in 3D)

Chapitre 6 : Metal-Organic Frameworks (MOF) and Networks

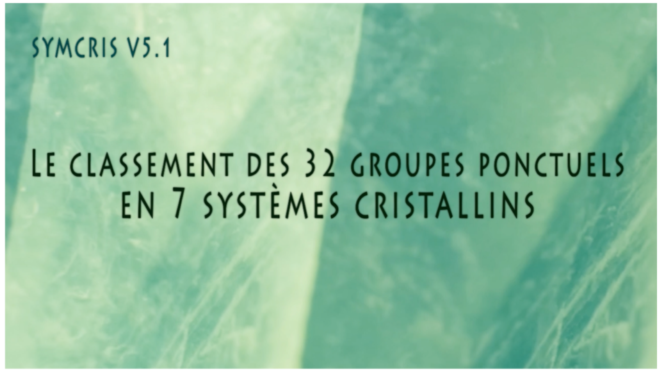
Chapitre 7 : Practising Topology Determination, Tilings

Chapter 1: Introduction to Crystals and Crystal Systems		
Trailer	Unit 1.0	1 min
Crystal and Structures - Powers of Ten	Unit 1.1	7 min
Crystallographic poetry	Unit 1.2a	3 min
Systematization and course overview	Unit 1.2b	5 min
Definition of Crystals and Anisotropy	Unit 1.3	8 min
The Correspondence Principle (I)	Unit 1.4	6 min
The Correspondence Principle (II)	Unit 1.5	4 min
The formation of Snowflakes	Unit 1.6	3 min
The concept of Unit Cell	Unit 1.7	7 min
The seven Crystal Systems	Unit 1.8	10 min
Crystal = lattice + motif	Unit 1.9	5 min
Chapter 2: Crystal Systems, Fractional Coordinates, and Morphology of Crystals	Back to Chapter list	
Visiting the Mineralogical Museum of Hamburg	Unit 2.1	4 min

Les capsules éducatives de Michel Evain

Développées en trois thèmes (cristallographie géométrique, solide cristallin et diffraction), ces capsules vidéo de 3 à 19 minutes chacune constitue une ressource visuelle, didactique, complète et idéale pour comprendre l'organisation de la matière cristalline et des notions élémentaires de cristallographie.

To take a fresh look at all these concepts…



Cours en ligne SYMCRIS : Ensemble de 24 vidéos (dont 6 en cours de finalisation) sur YouTube (ou moodle SU)