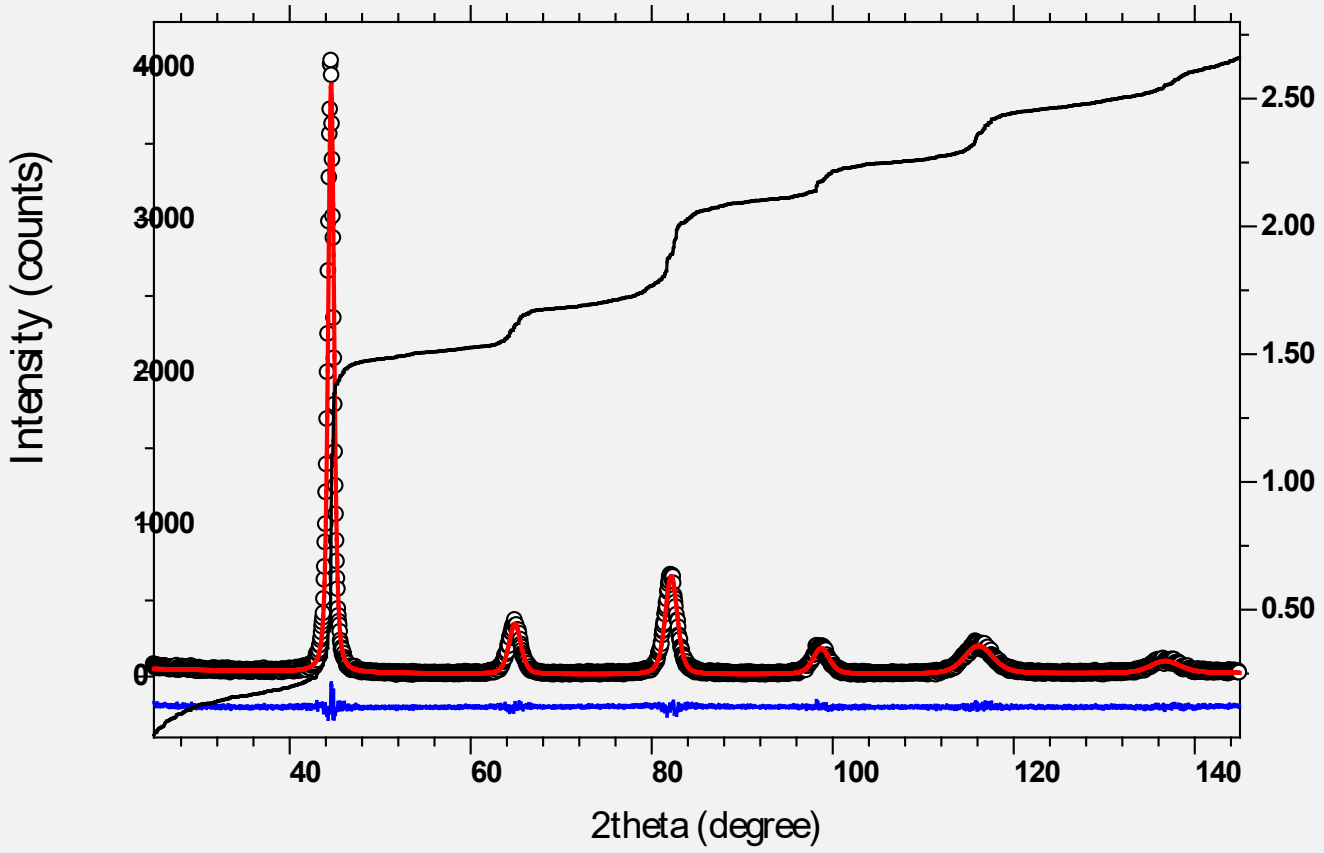

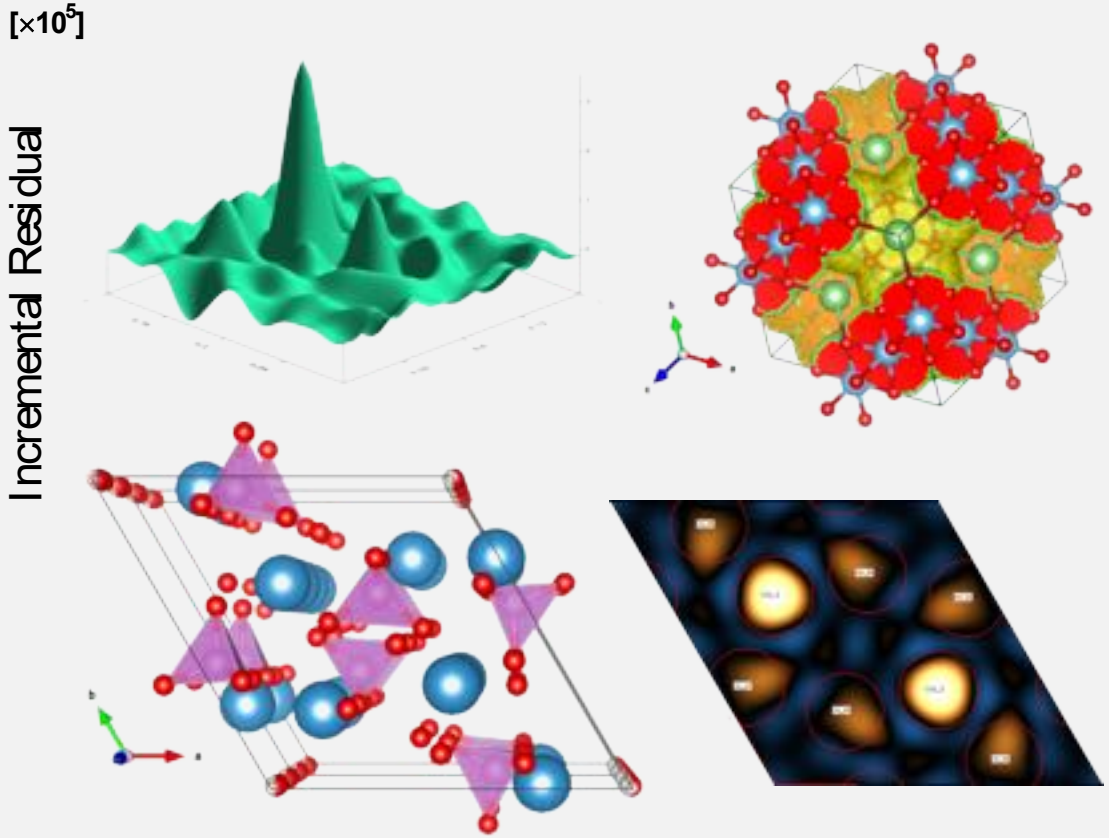

Introduction to Crystallography (Lec-01)

Dr. Maykel T. E. Manawan // UNIVERSITAS PERTAHANAN RI
Dr. Frank Hoffmann // UNIVERSITY OF HAMBURG

Course Materials

- Crystallography
  - Symmetry & crystal system
  - Bravais lattices
  - Point group & space group
  - Miller indices
- Diffraction
  - Diffraction by atom and plane of atoms
  - Miller indices and diffraction
  - Structure Factor
  - Instrumentation
  - X-ray generation
  - Beam path (optics)
    - X-ray monochromatizating
  - Instrument configuration
    - Optimum setup
- Sample Preparation
  - Particle/Crystallite Size
  - Homogeneity
  - Texture/Preferred Orientation
- Data Acquisition
  - Angular Range
  - Step Size
  - Counting Time

Brief overview

- Qualitative Analysis (Identification)
  - Data base
  - Phase Identification
- Quantitative Analysis (Rietveld Analysis)
  - Intensity Equation
  - Profile Function
    - Instrumental function
    - Sample physical function
  - R-indices (How good is good enough)
- Qualitative Analysis
  - Practices with …
    - Sample : mixture of Al2O3, CaF2, Zincite (Quantitative Analysis Round Robin (QARR) sample from International Union for Crystallography (IUCr))
- Quantitative Analysis
  - Practices with …
    - Sample : mixture of Al2O3, CaF2, Zincite (QARR sample from IUCR)
- Advanced Analysis
  - Practices with PM2K (Whole Powder Pattern Modelling) => Microstructure
    - Sample : CeO2 (Size Strain Round Robin (SSRR) sample from IUCR)
  - Practices with Rietan-FP/GSAS/Fullprof/Z-Rietveld => Electron Density
    - Sample : CeO2/Fa-apatite

Software & References

Software:

EVA : https://www.bruker.com/en/products-and-solutions/diffractometers-and-scattering-systems/x-ray-diffractometers/diffrac-suite-software/diffrac-eva.html
Topas : https://www.bruker.com/en/products-and-solutions/diffractometers-and-scattering-systems/x-ray-diffractometers/diffrac-suite-software/diffrac-topas.html

JADE : https://www.icdd.com/mdi-jade/
PDF-4+ : https://www.icdd.com/pdf-4/

QualX2 : http://www.ba.ic.cnr.it/softwareic/qualx/
PowCod : http://www.ba.ic.cnr.it/softwareic/qualx/powcod-download/
GSAS : https://subversion.xray.aps.anl.gov/trac/EXPGUI
Profex : https://www.profex-xrd.org/?page_id=279
PM2K : Matteo.Leoni@unitn.it

References:

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4. Leoni M., Confente T. & Scardi P., *PM2K: a flexible program implementing Whole Powder Pattern Modelling*, Z. Kristallogr. Suppl. 23 (2006) 249-254.
5. Scardi P., Leoni M., *Whole Powder Pattern Modelling*, Acta Crystall. A 58 (2002) 190-200.
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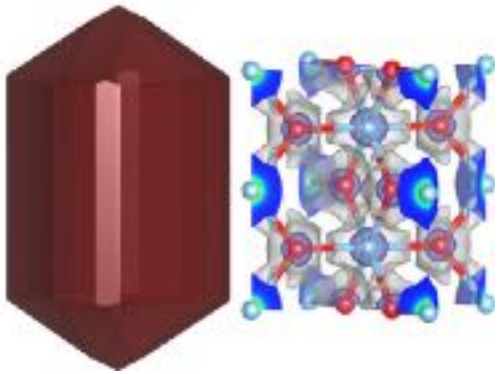
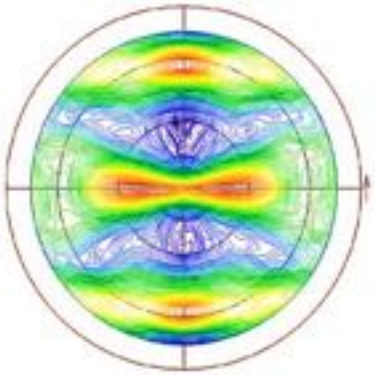
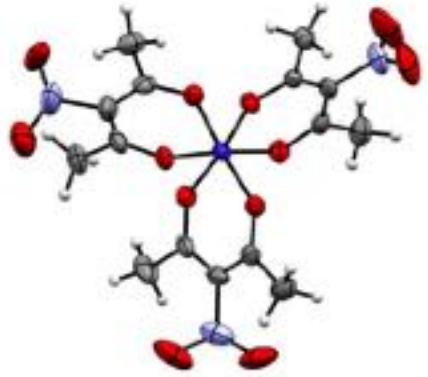
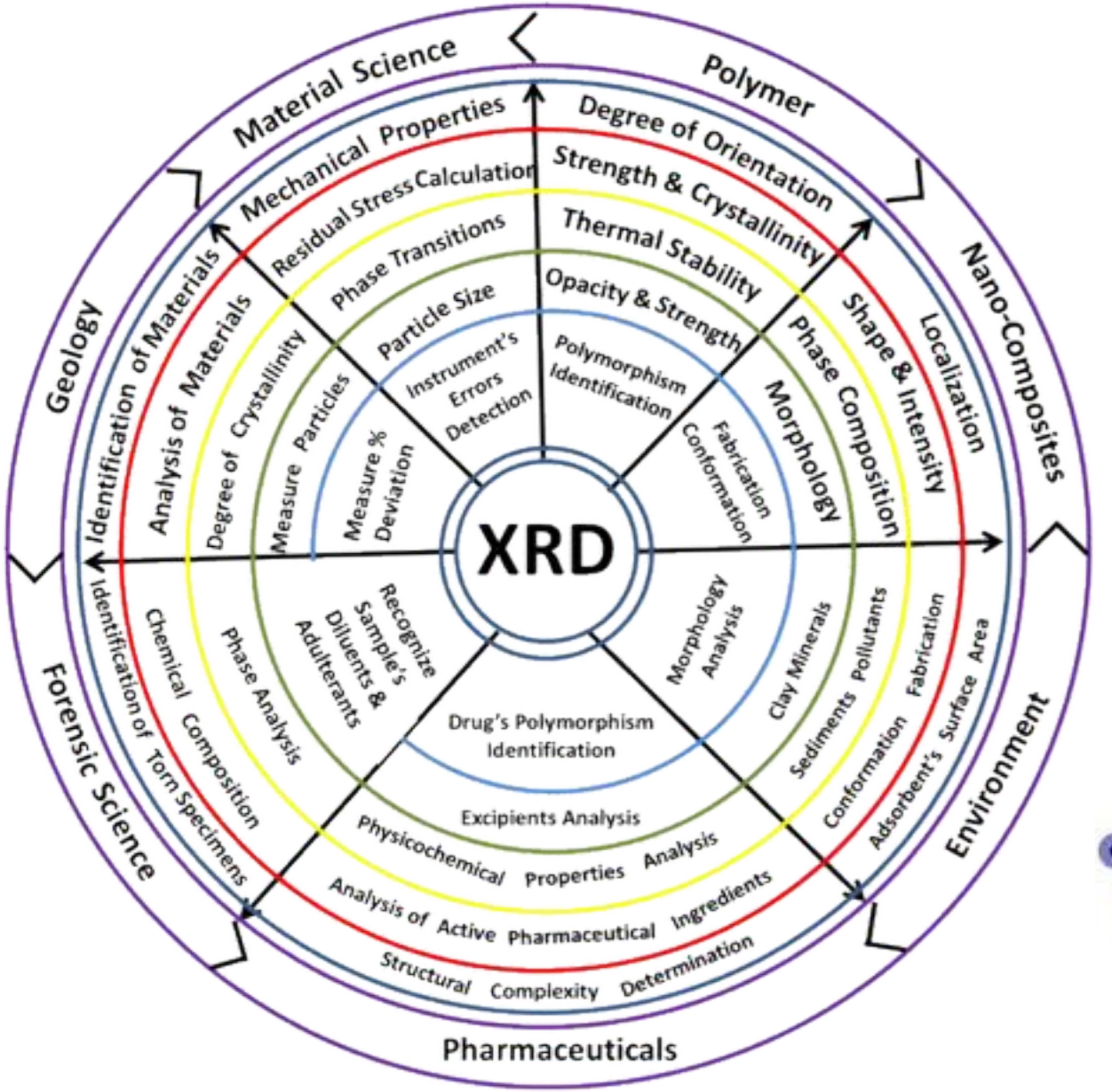
7. Balzar, D., Audebrand, N., Daymond, M. R., Fitch, A., Hewat, A., Langford, J. I., Le Bail, A., Louer, D., Masson, O., McCowan, C. N., Popa, N. C., Stephens, P. W. & Toby, B. H., *Size–strain line-broadening analysis of the ceria round-robin sample*, J. Appl. Cryst. 37 (2004) 911-924.
8. Toby, B., *R factors in Rietveld analysis: How good is good enough?,* Powder Diffraction, 21 (2006) 67-70
9. Cullity, B. D., & Stock, S. R., *Elements of X-ray Diffraction*, Third Edition. Prentice-Hall (2001).

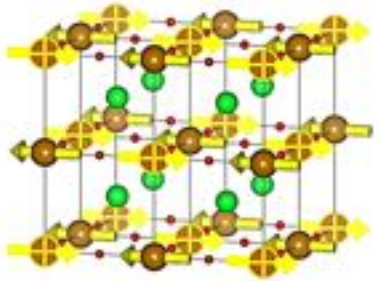
Crystallographer

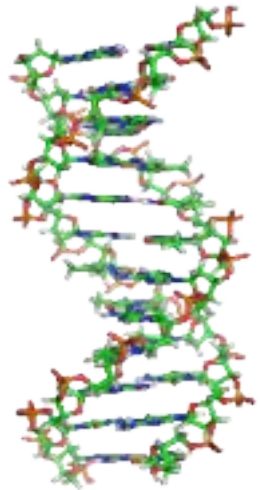


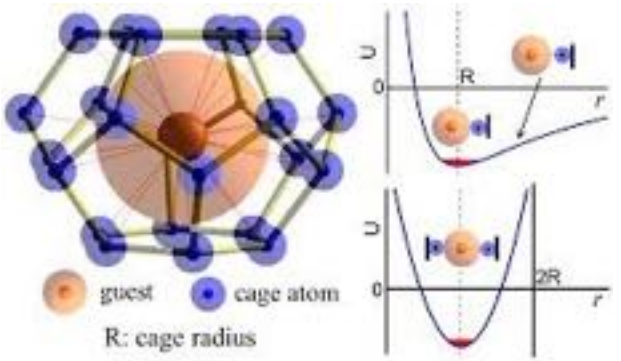








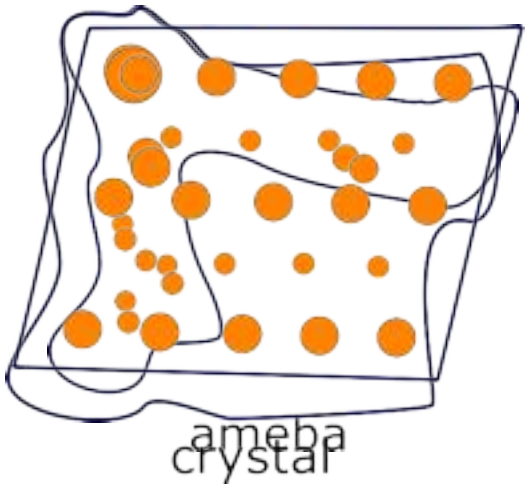




Definition

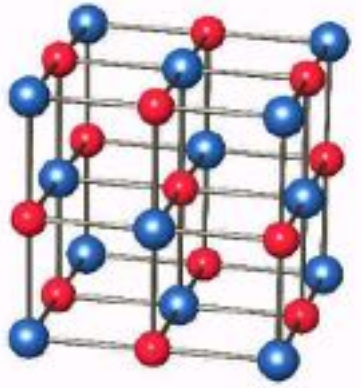
- Definition: Crystals are *homogeneous*, *anisotropic* solid-state bodies, which constituents (atoms, ions, molecules…) are three-dimensional/3D *periodically ordered*.

- Solid-state bodies without such a 3D periodic order of its constituents are called amorphous (gels, glasses, wood, plastic….).



aggregate state — solid – liquid – gaseous

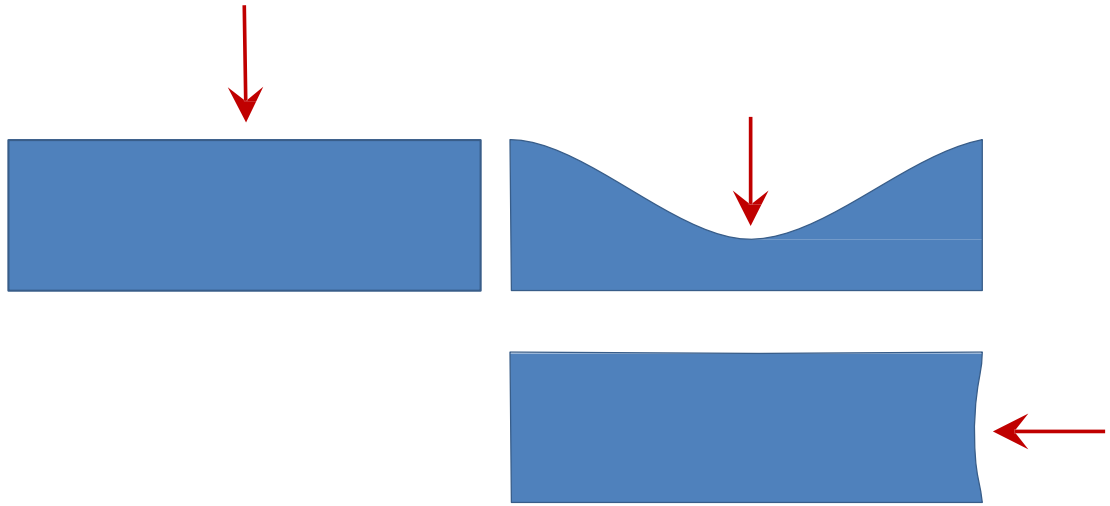
amorphous — crystalline



crystals have a *crystal structure*

Crystals – Anisotropy

- all crystals show anisotropy
  - this means that certain chemical or physical properties are different for different directions, they are directional
- anisotropic properties are, for instance
  - hardness, cleavability
  - elasticity, expansion properties



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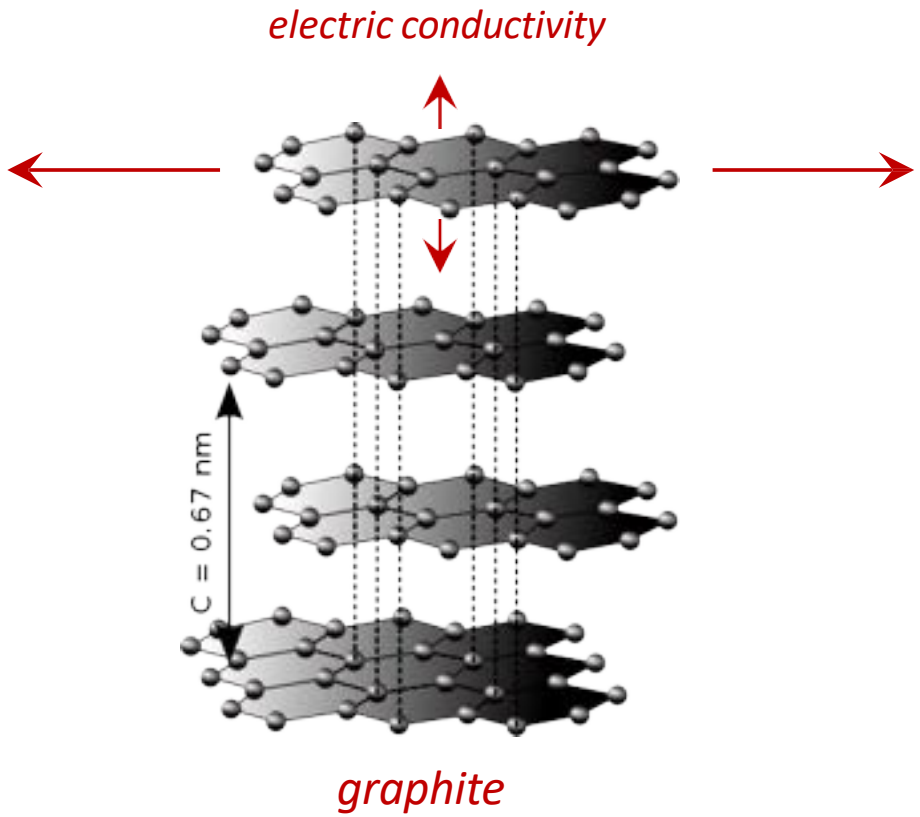
  - electric / thermal conductivity
  - electric polarizability, magnetization



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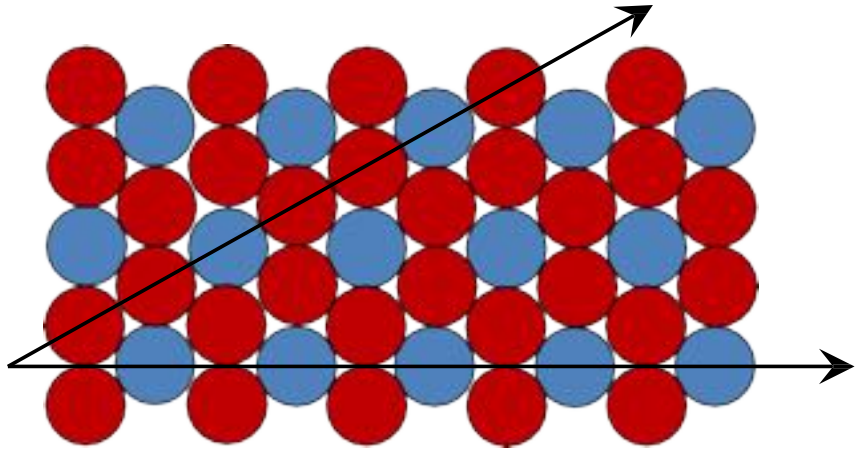
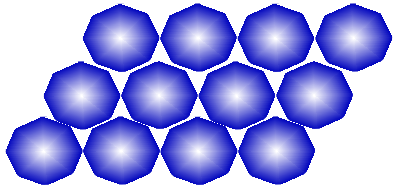
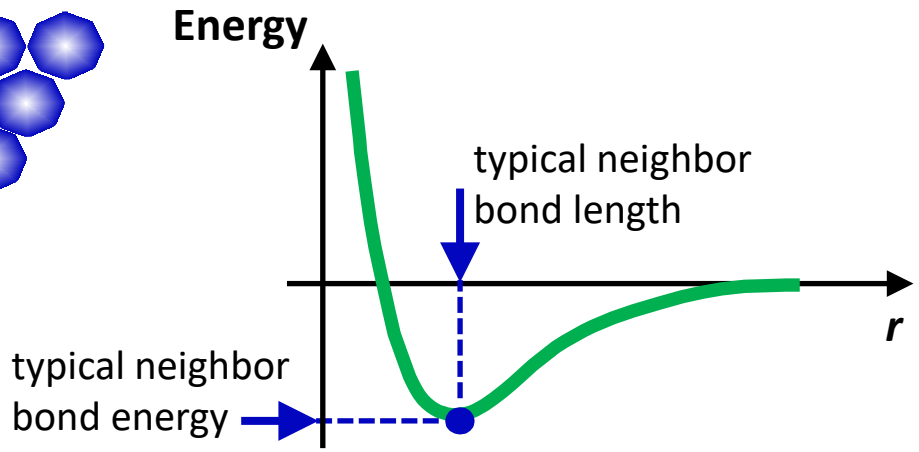


Energy and Packing

❖ Dense, **ordered** packing

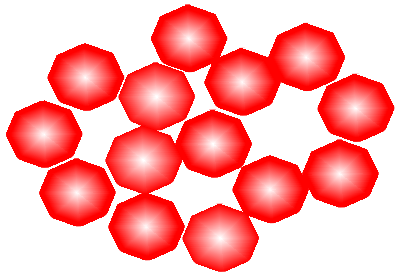


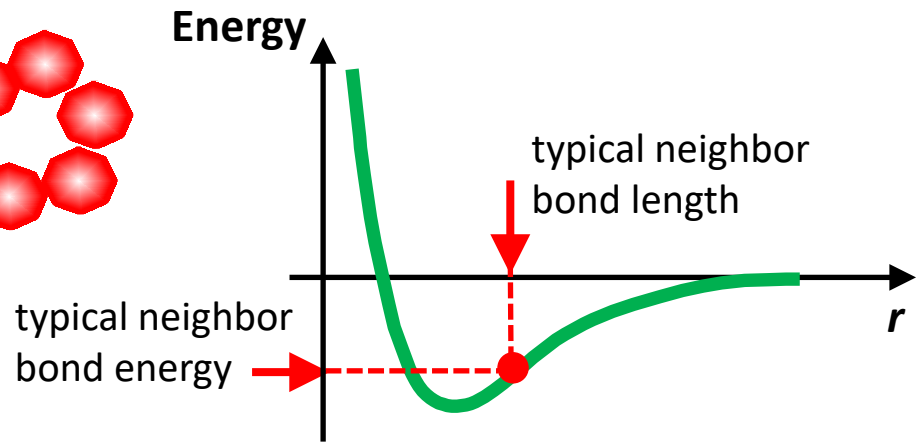


Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of:
  - ➢ metals
  - ➢ many ceramics
  - ➢ some polymers

❖ Non dense, **random** packing



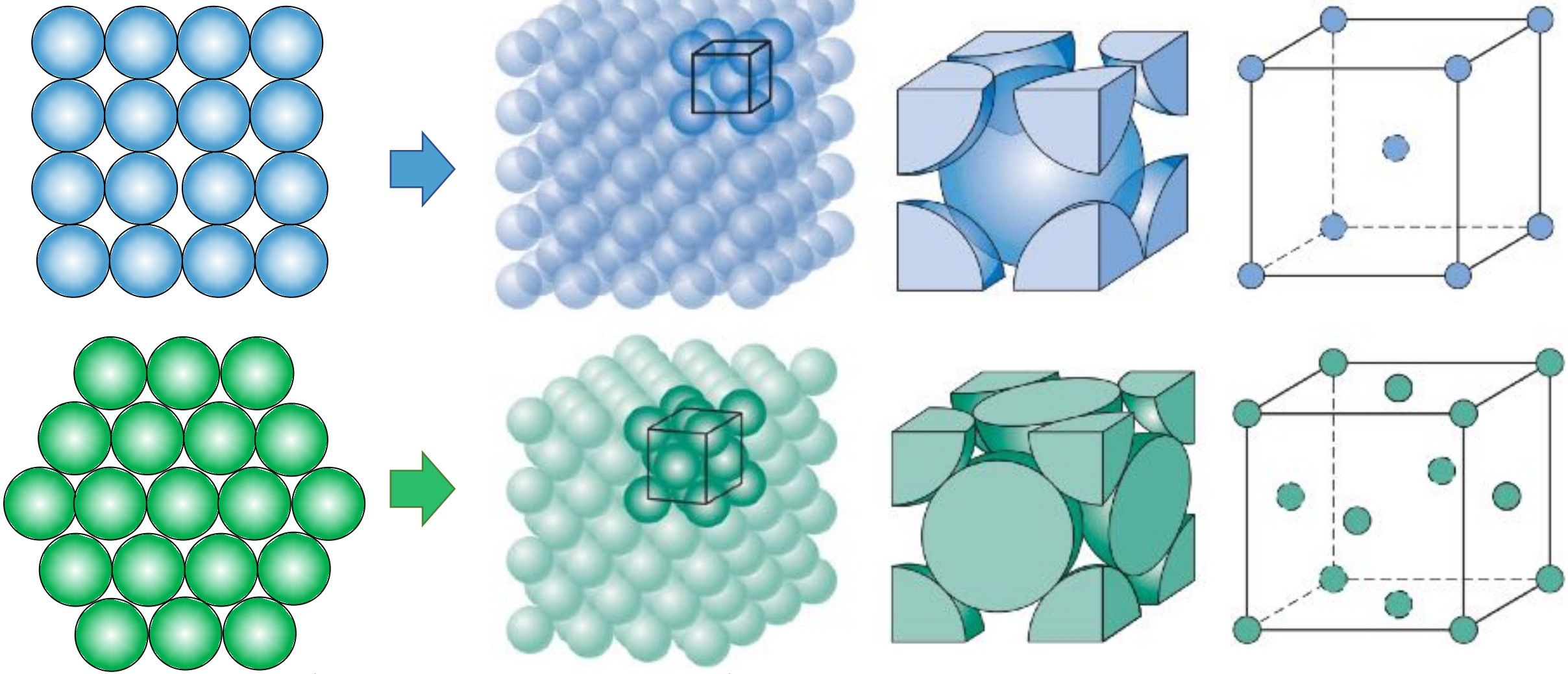


Non-crystalline materials...

- atoms have no periodic packing
- occurs for:
  - ➢ complex structures
  - ➢ rapid cooling

Metallic Crystal Structure

How can we stack metal atoms to minimize empty space?



2-dimensions

3-dimensions

Callister & Rethwisch, 8e.

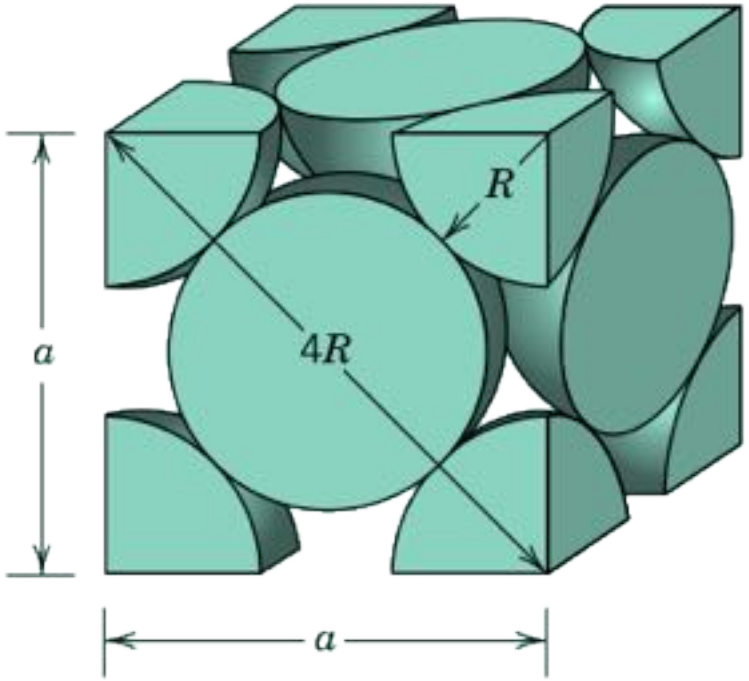
Unit Cell and Packing Factor

- No. of atom in unit cell
  - Cubic: $N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$
  - Hexagonal: $N = N_i + \frac{N_f}{2} + \frac{N_c}{6}$

N_i = the number of interior atoms

N_f = the number of face atoms

N_c = the number of corner atoms



- Atomic Packing Factor

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

$$V_s = N \times V_{ball} = (4)\frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3$$

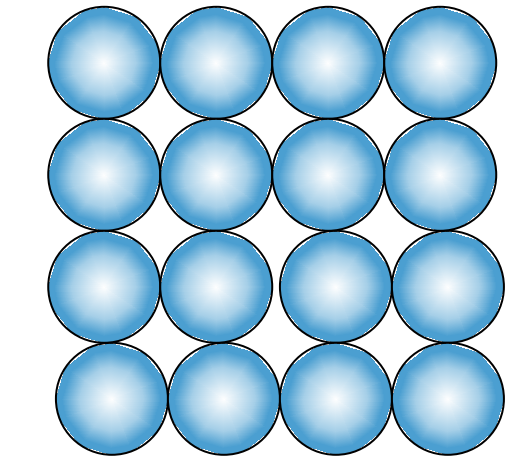
$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

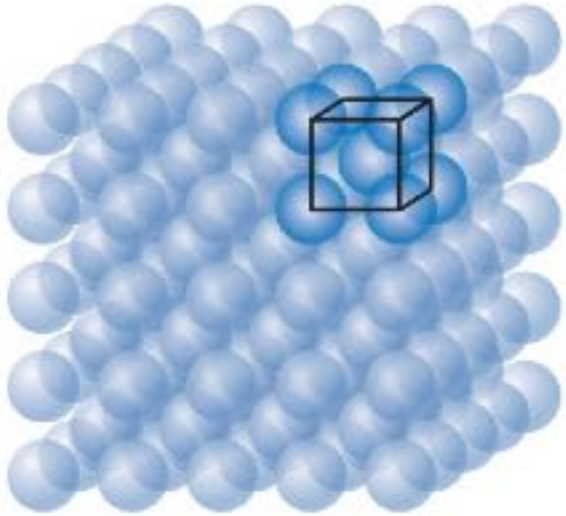
$$APF = \frac{V_s}{V_c} = \frac{(16/3)\pi R^3}{16R^3\sqrt{2}} = 0.74$$

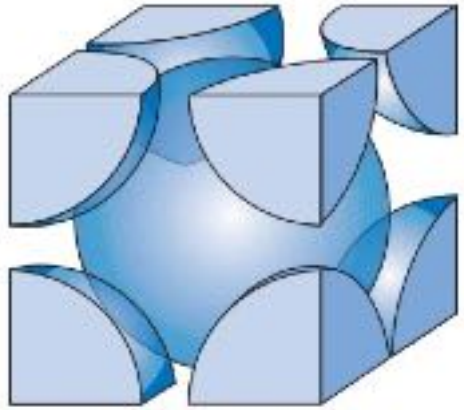
Callister & Rethwisch, 8e.

Metallic Crystal Structure

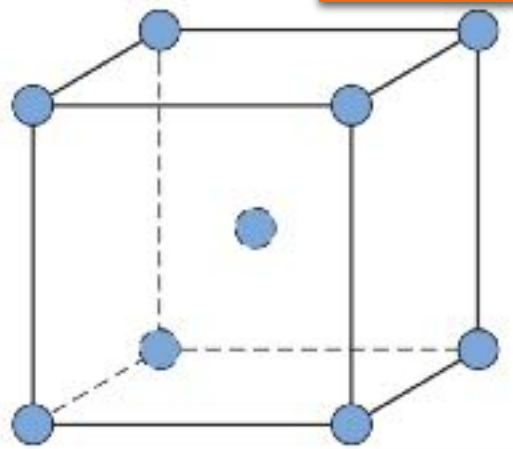
How can we stack metal atoms to minimize empty space?

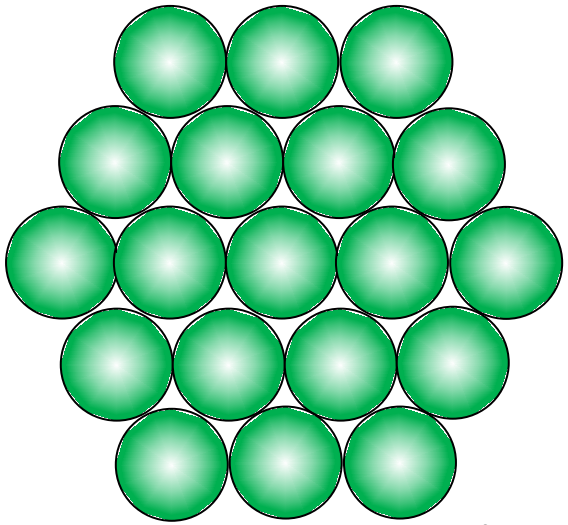


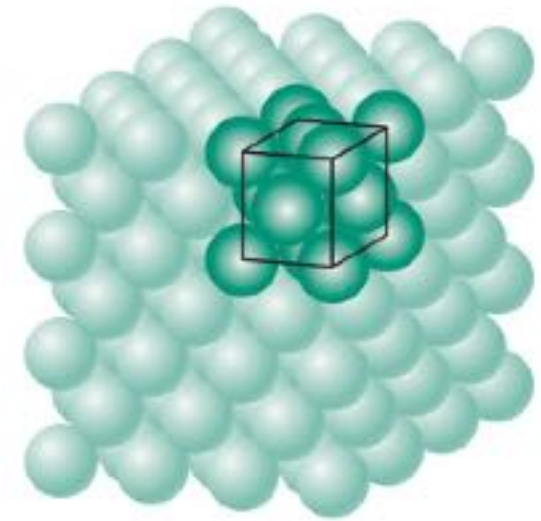


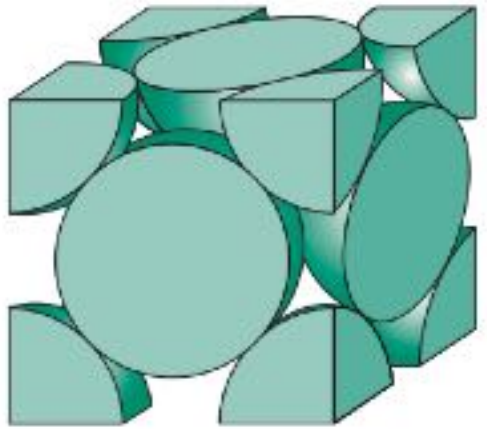


APF = 0.68

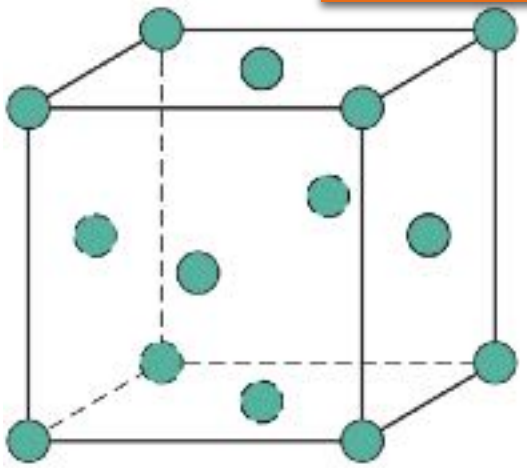








APF = 0.74



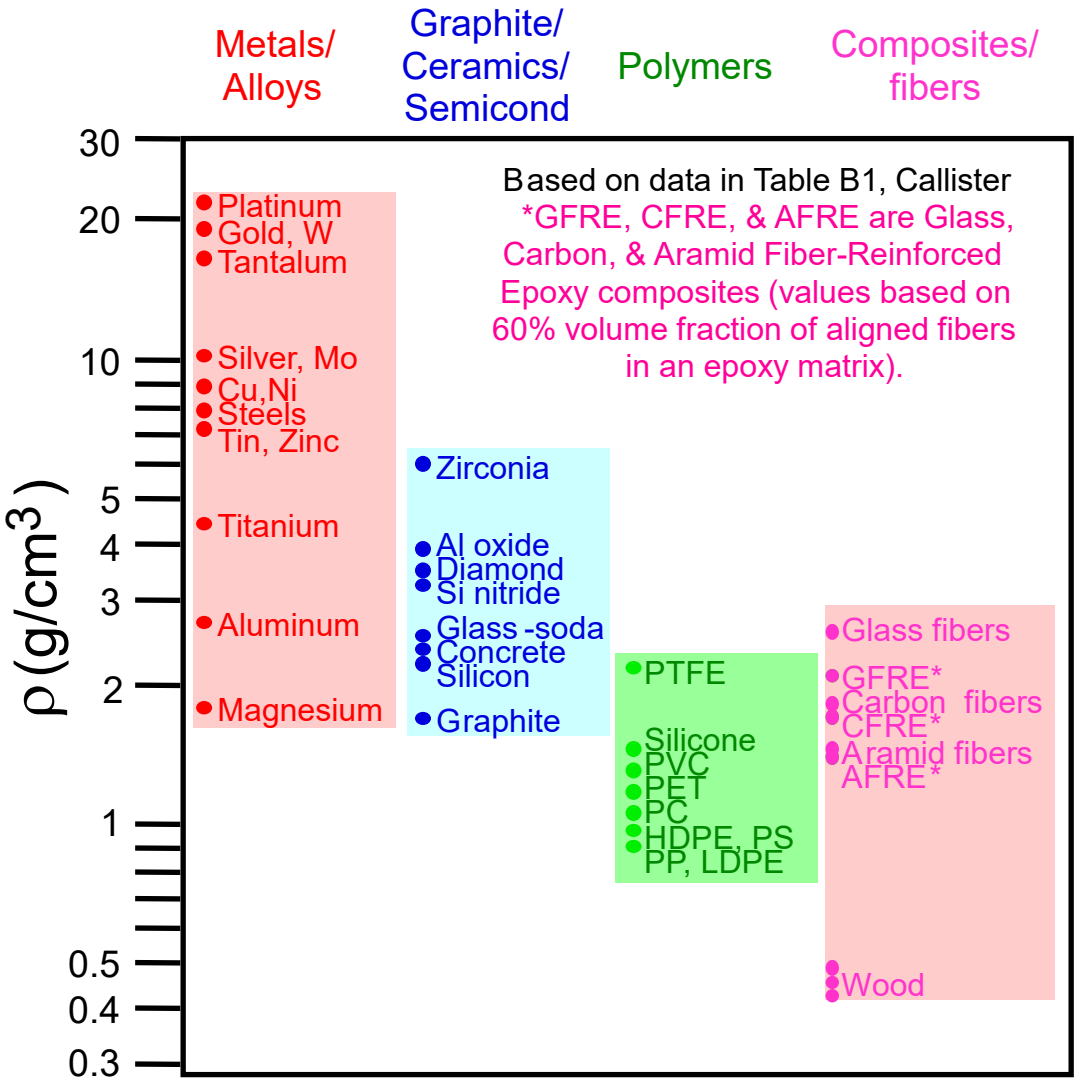
2-dimensions

3-dimensions

Callister & Rethwisch, 8e.

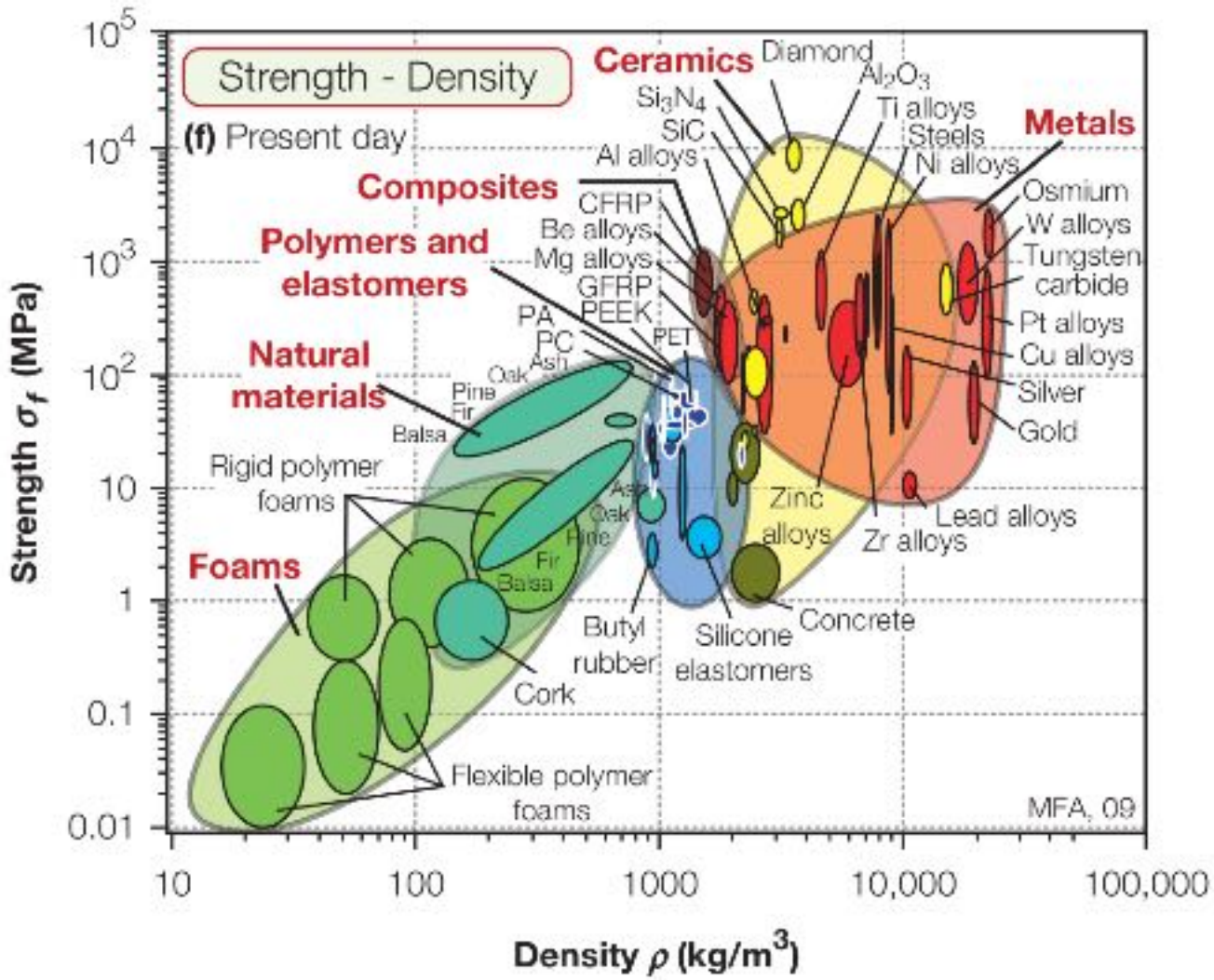
Density and Material Selection

$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$

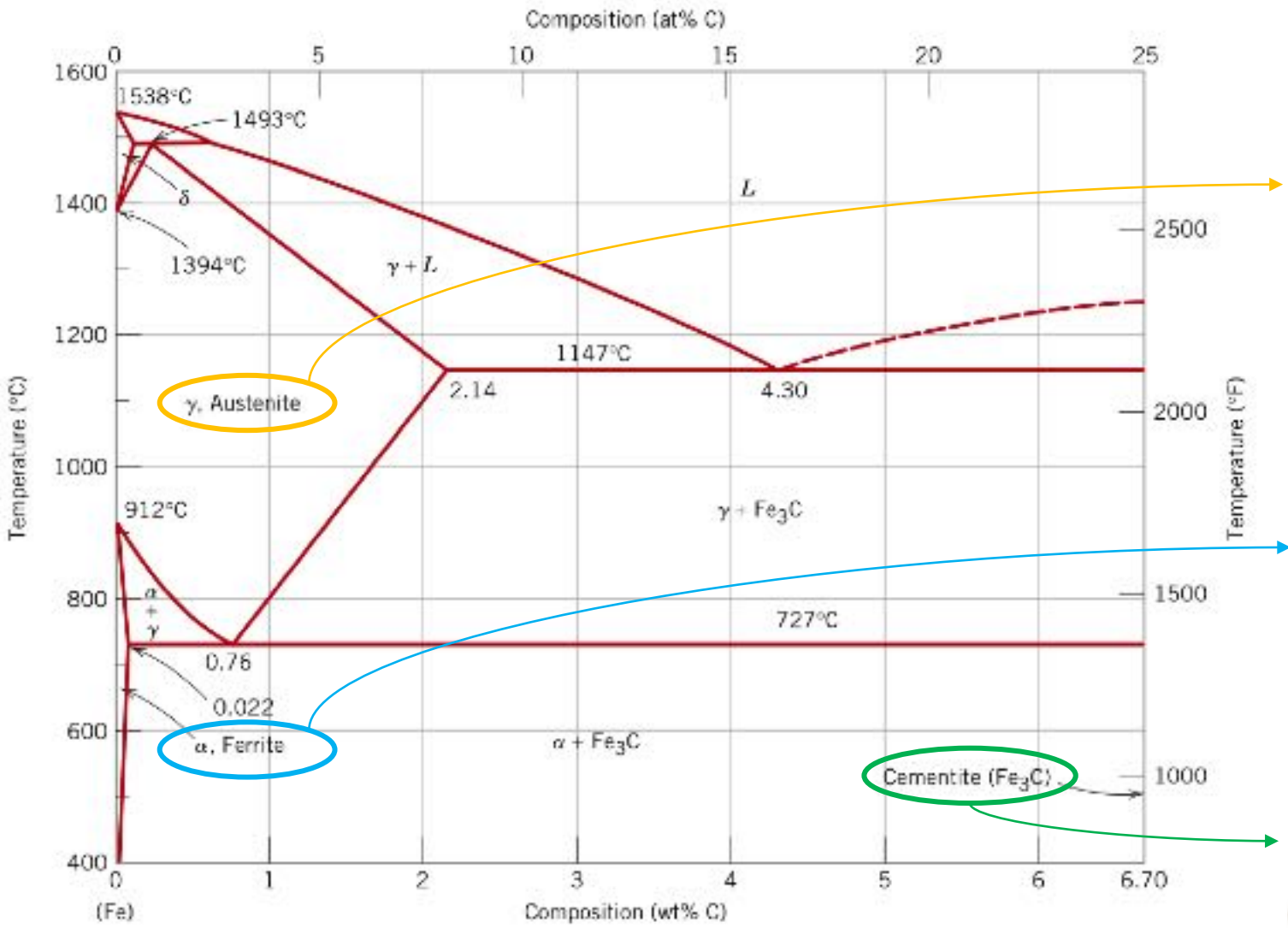


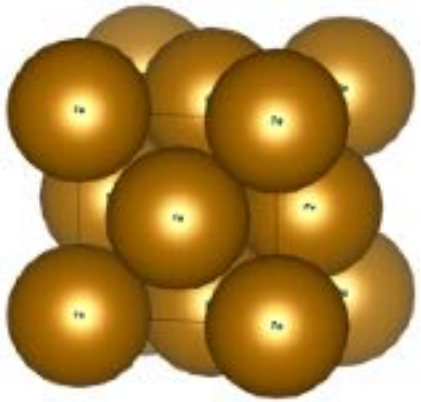
Data from Table B.1, *Callister & Rethwisch, 8e.*

Materials Selection in Mechanic Ashby - Chart



Phase Diagram of Fe-Fe3C





Crystal System: Cubic
Space Group: Fm-3m (225)
Aspect: -
Author's Unit Cell ▼

a: 3.61 Å	α: -	Volume: 47.05 Å³	c/a: -
b: -	β: -	Z: 4.00	a/b: -
c: -	γ: -	MolVol: 11.76	c/b: -

Calculated Density: 7.884 g/cm³ | Melting Point: Stable between 1
Measured Density: - | Color: -
Structural Density: 7.883 g/cm³

Crystal System: Cubic
Space Group: Im-3m (229)
Aspect: -
Author's Unit Cell ▼

a: 2.86840(2) Å	α: -	Volume: 23.60 Å³	c/a: -
b: -	β: -	Z: 2.00	a/b: -
c: -	γ: -	MolVol: 11.80	c/b: -

Calculated Density: 7.859 g/cm³ | Melting Point: -
Measured Density: - | Color: -
Structural Density: 7.86 g/cm³

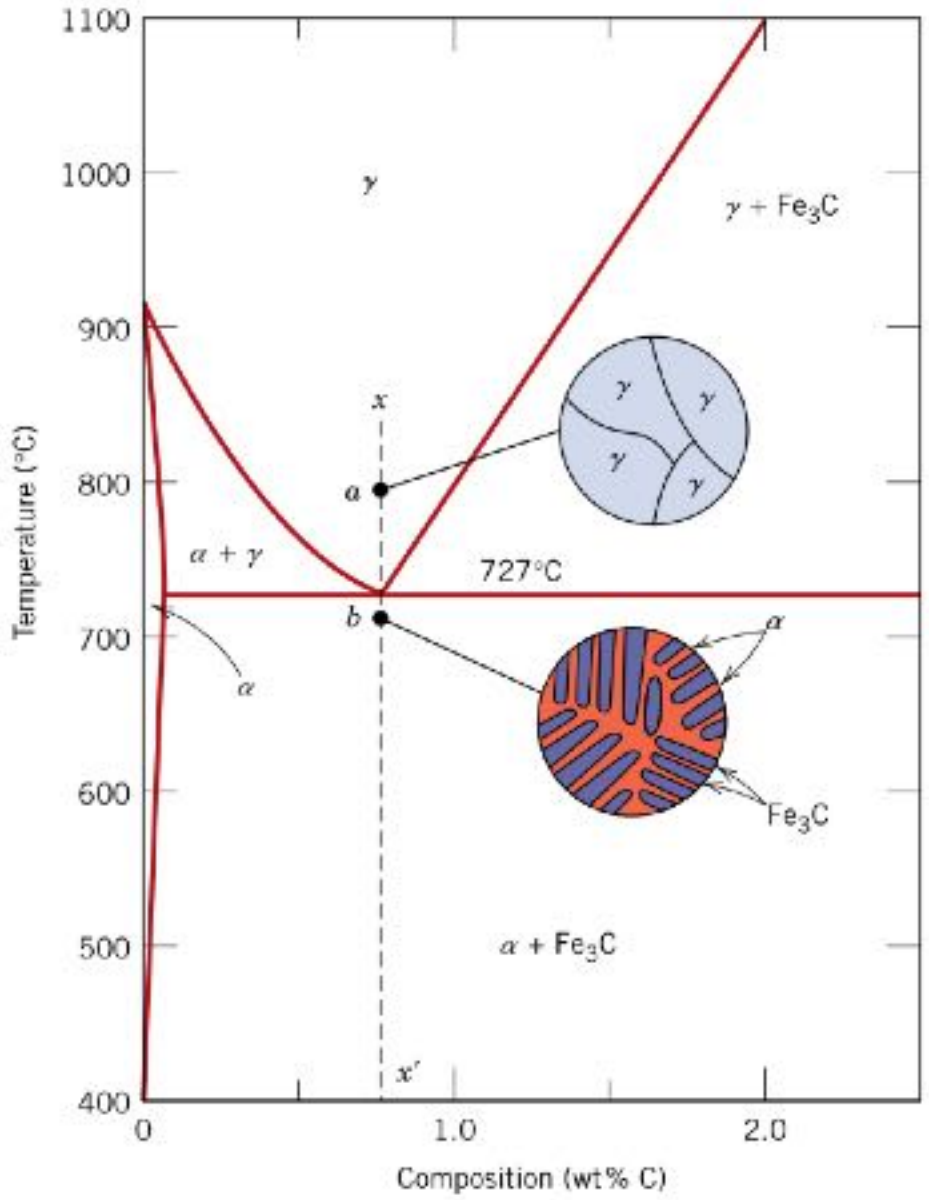
Crystal System: Tetragonal
Space Group: I4/mmm (139)
Aspect: -
Author's Unit Cell ▼

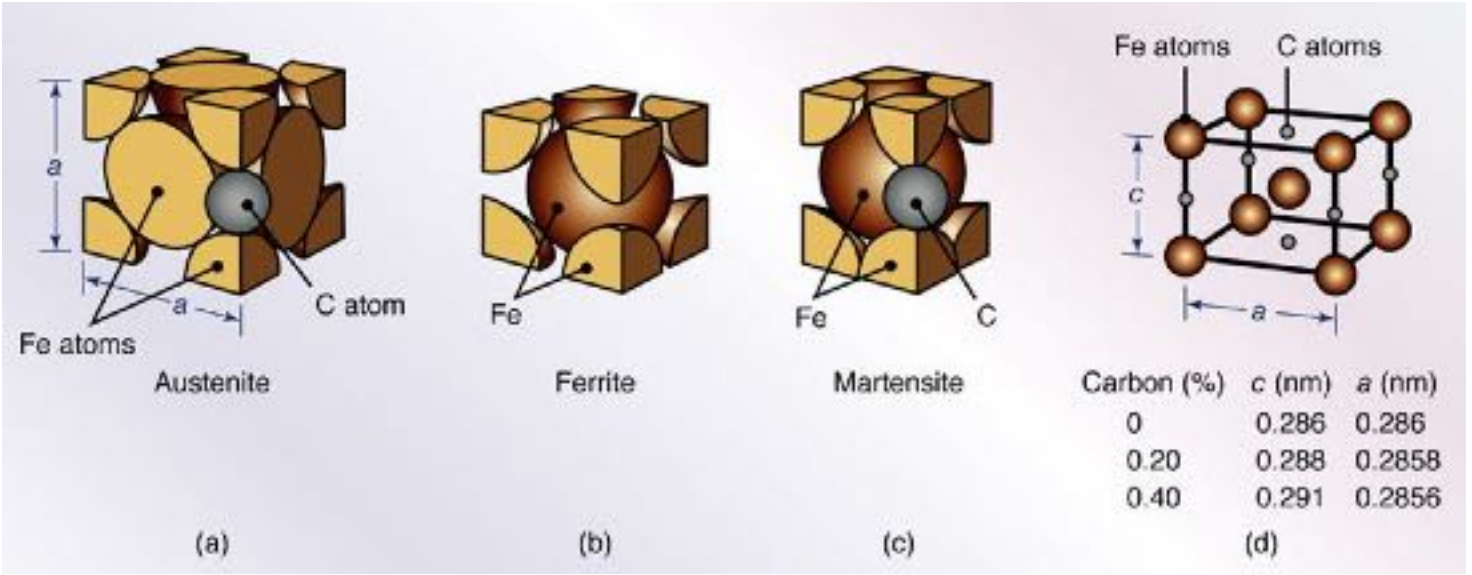
a: 2.8232(22) Å	α: -	Volume: 22.86 Å³	c/a: 1.016
b: -	β: -	Z: 2.00	a/b: -
c: 2.8678(2) Å	γ: -	MolVol: 11.43	c/b: -

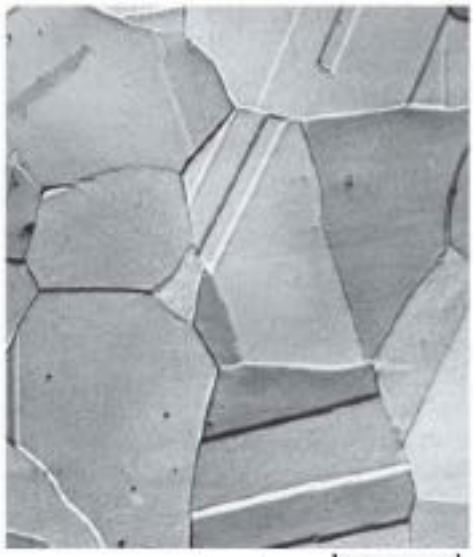
Calculated Density: 8.142 g/cm³ | Melting Point: -
Measured Density: - | Color: -
Structural Density: 8.14 g/cm³

Adapted from Binary Alloy Phase Diagrams, 2nd edition, Vol. 1, T. B. Massalski (Editor-in-Chief), 1990.

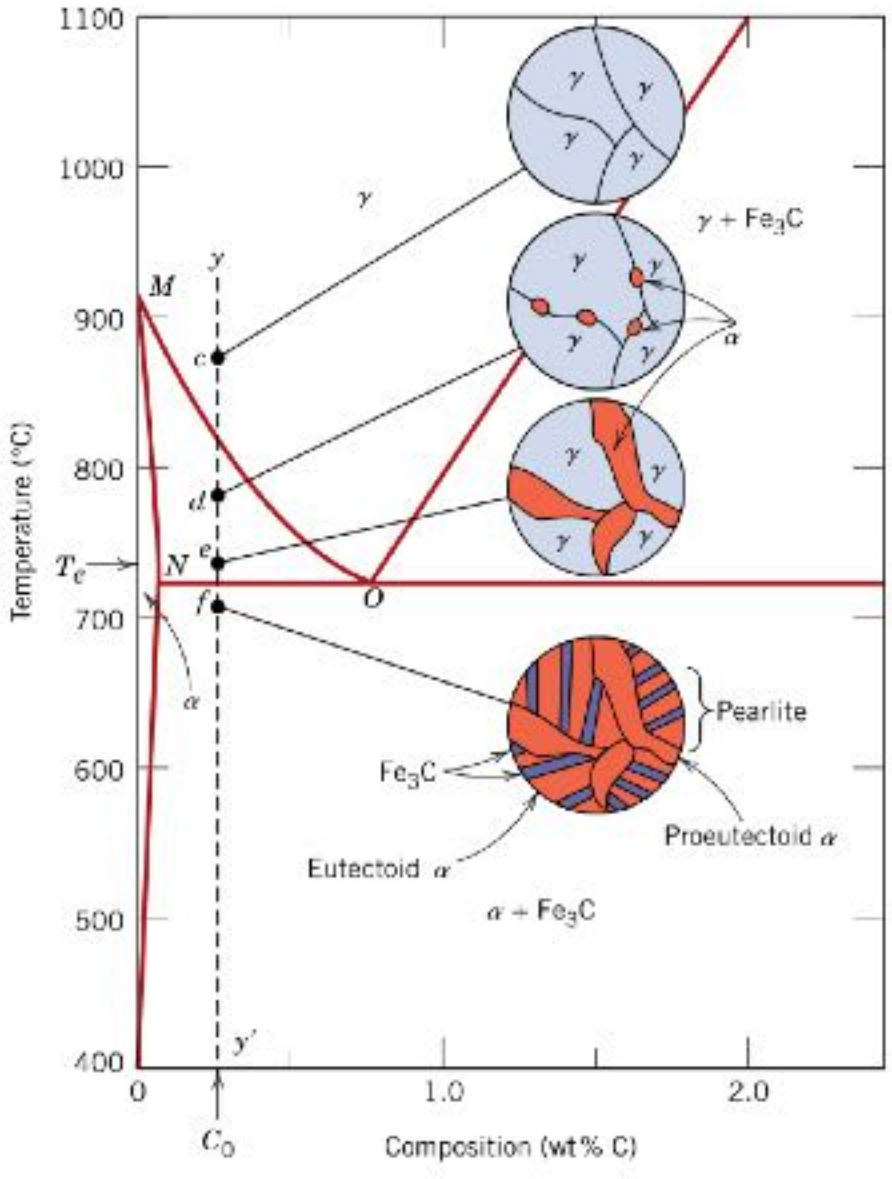
Phase Diagram of Steel

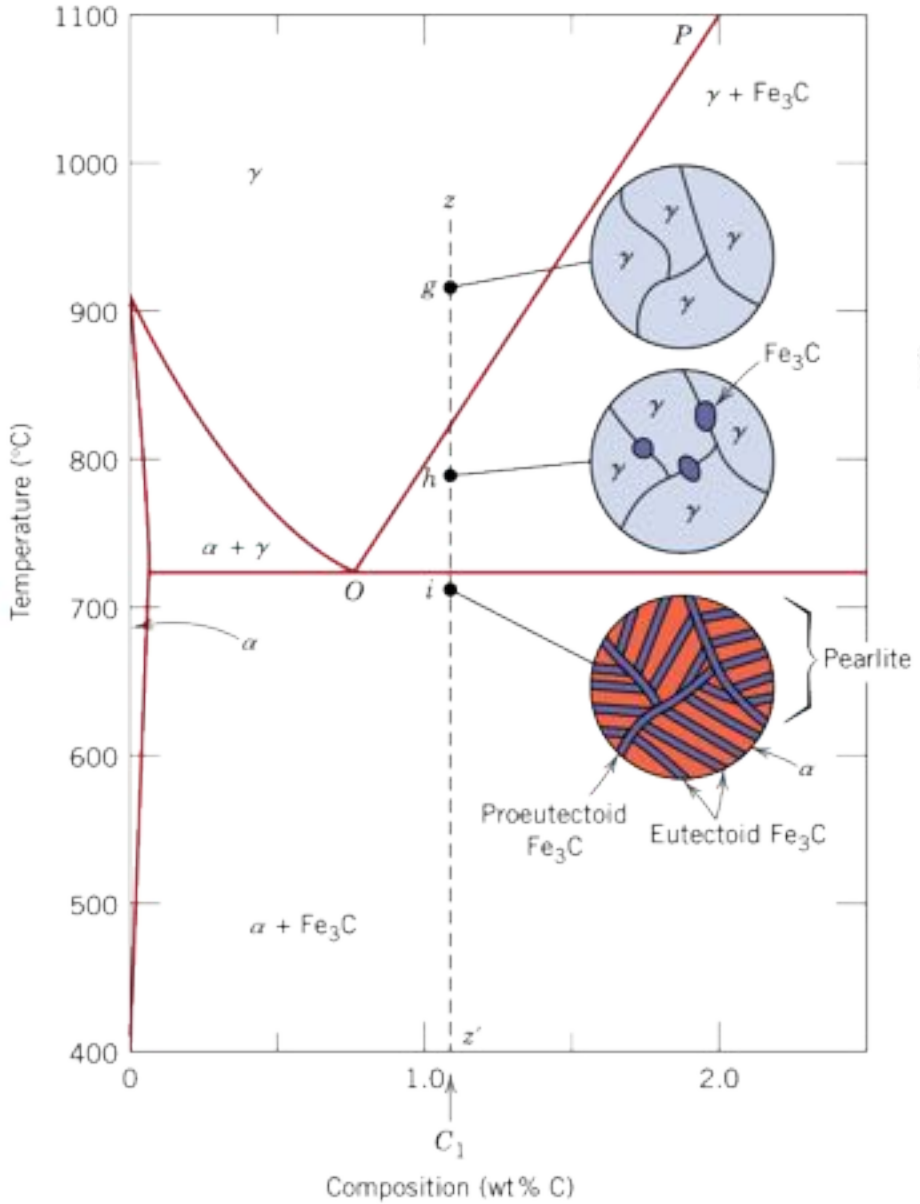


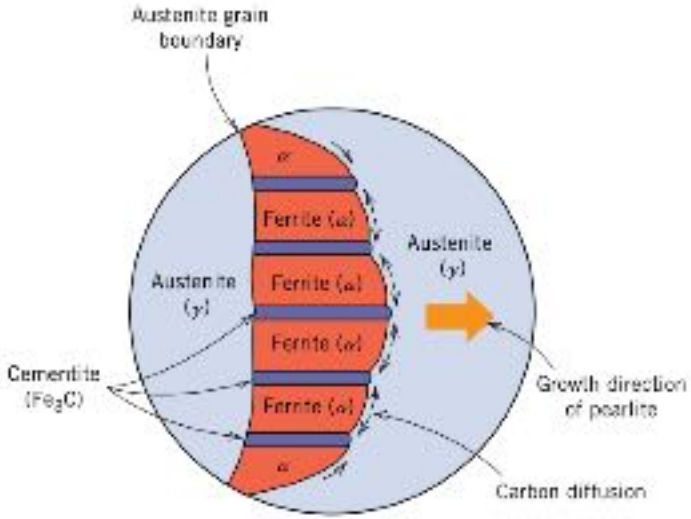


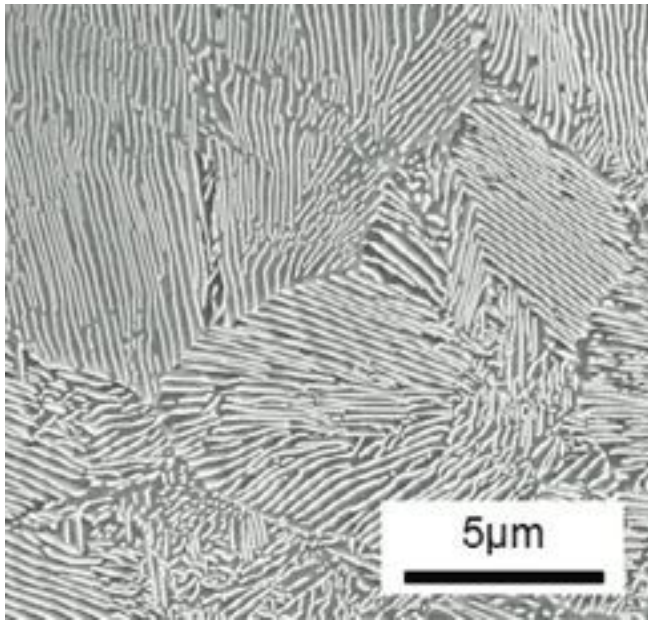


Pearlite Structure

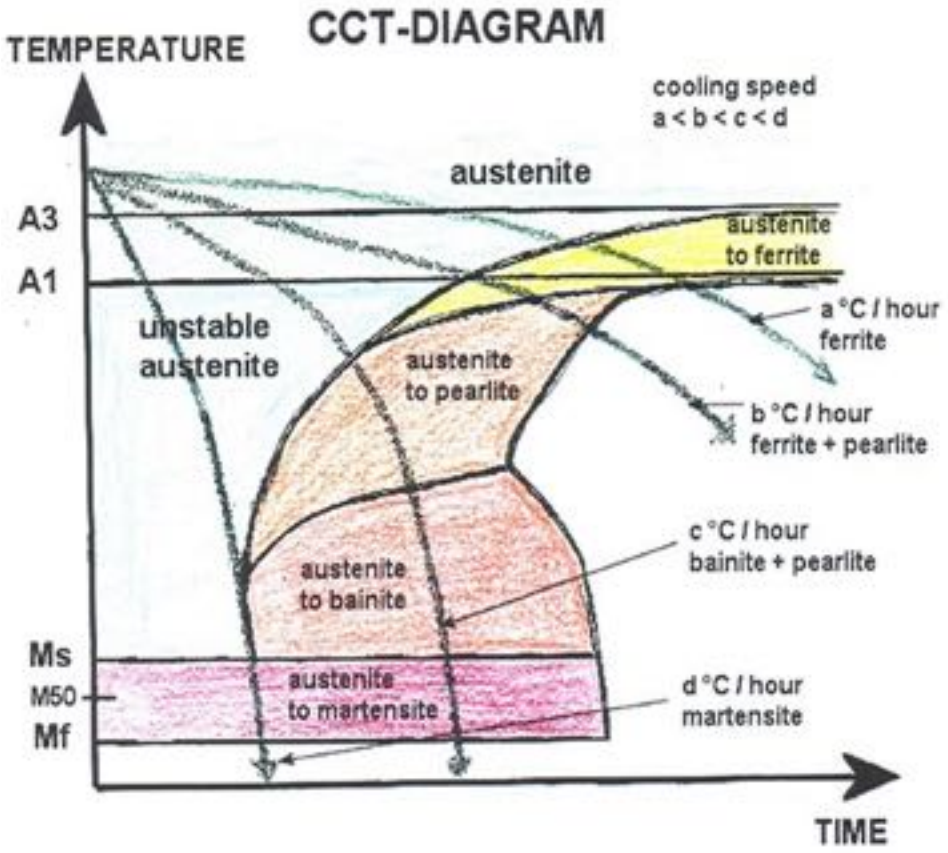








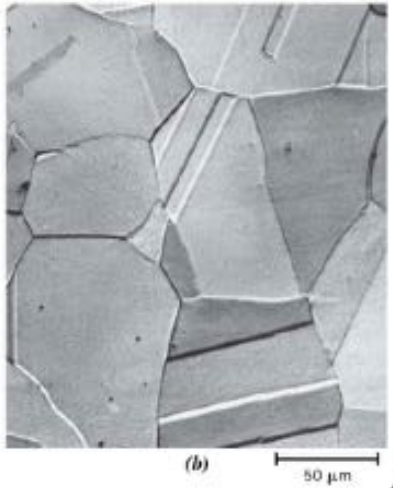
Steel processing as f(t)

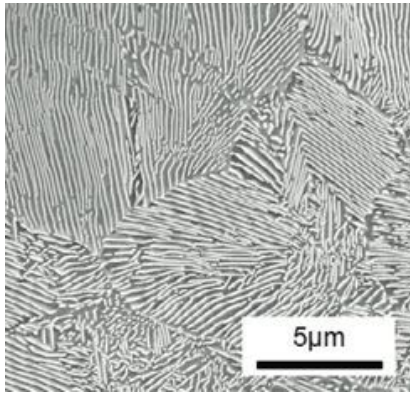


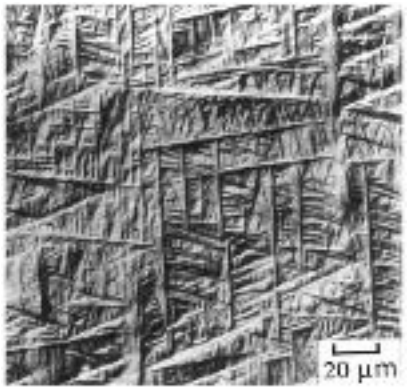
Strength

Ductility

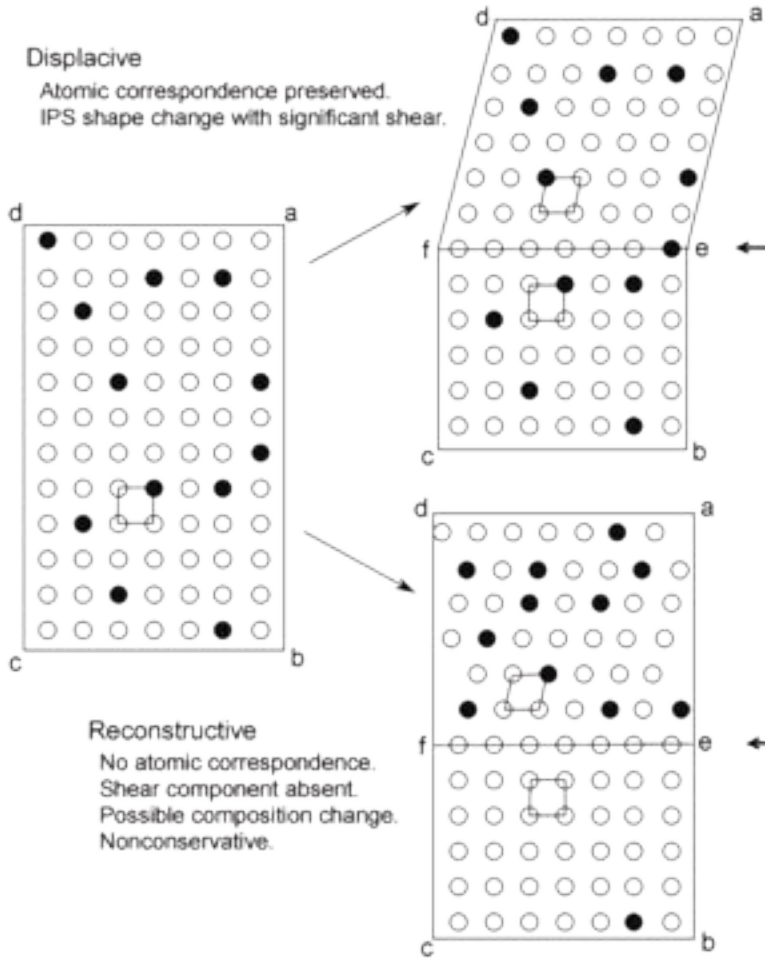
Martensite
tempered **Martensite**
Bainite
Fine **Pearlite**
Coarse **Perlite**





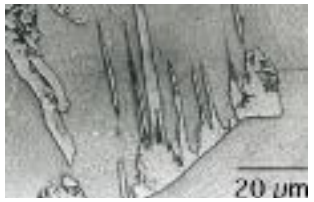


Atomic Mechanisms of Transformation



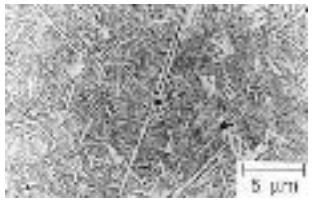
DISPLACIVE

Invariant-plane strain shape deformation with large shear component. No Iron substitutional solute diffusion. Thin plate shape



WIDMANSTATTEN FERRITE

Carbon diffusion during para-equilibrium nucleation & growth



BAINITE & ACICULAR FERRITE

Carbon diffusion during para-equilibrium nucleation. No diffusion during growth

MARTENSITE

Diffusionless nucleation & growth

RECONSTRUCTIVE

Diffusion of all atoms during nucleation and growth. Sluggish below 850 K.

ALLOTRIOMORPHIC FERRITE

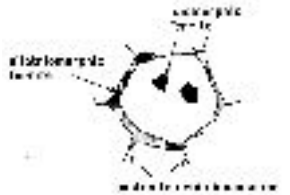
(Shape doesn't reflect its symmetry)

IDIOMORPHIC FERRITE

(Shape some relation to crystallographic symmetry)

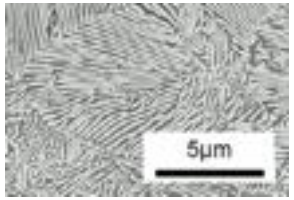
MASSIVE FERRITE

No change in bulk composition



PEARLITE

Cooperative growth of ferrite and cementite



Soil and Soil Dynamics

Rocks

Minerals

Weathering

Physical

Chemical

Biosphere

Atmosphere

Hydrosphere

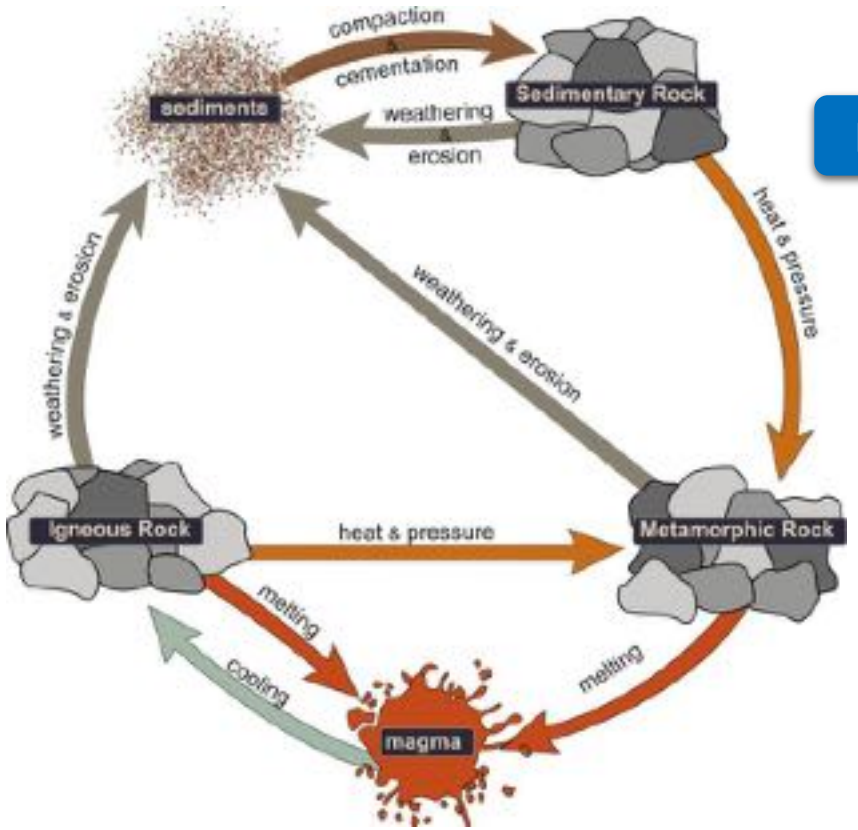
Time

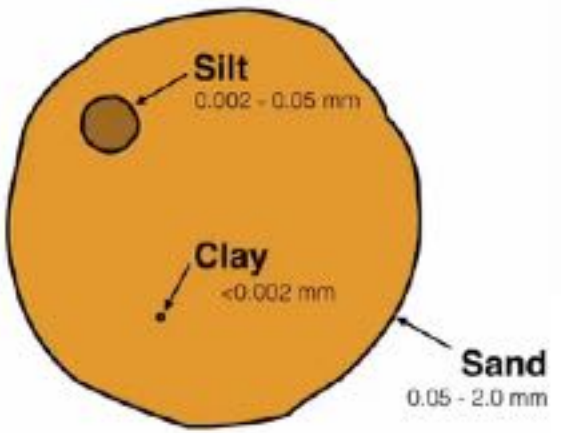
Soil

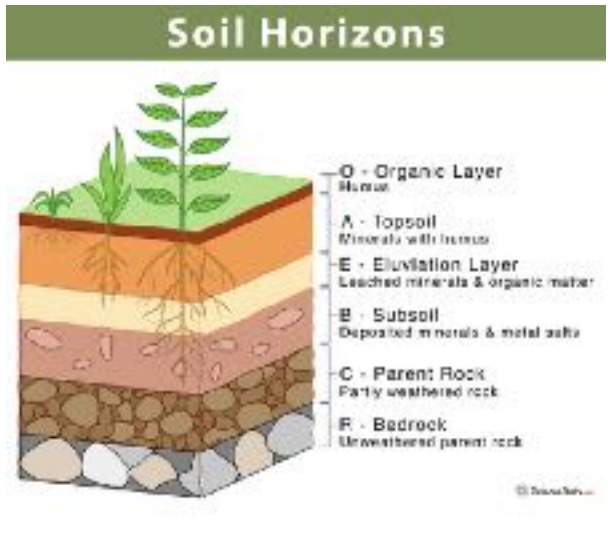
Types

Particle Size

Porosity

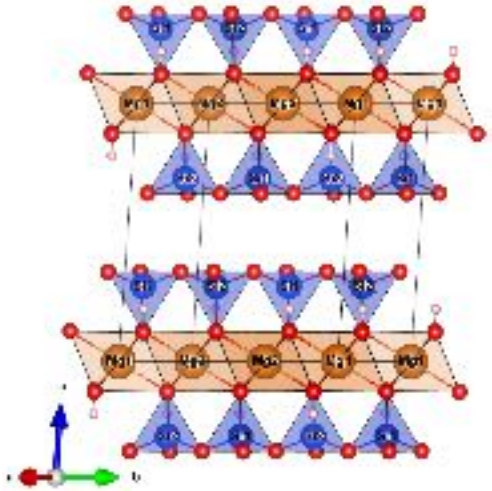






Mineral Physical Properties

Talc, $Mg_3Si_4O_{10}(OH)_2$



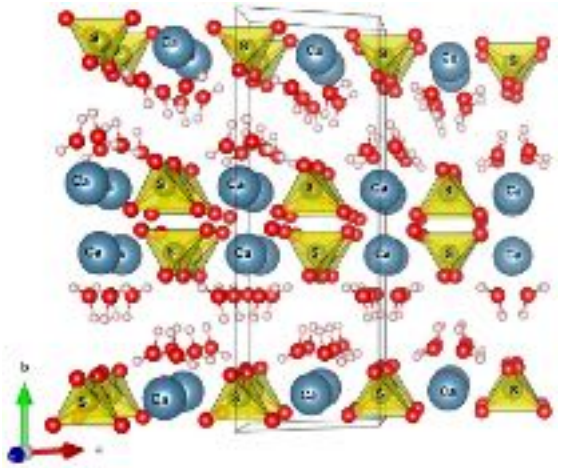
Crystal System: Triclinic (Anorthic)
Space Group: C-1 (2)
Aspect: -

Author's Unit Cell ▼

a: 5.290(3) Å	α: 90.46(5)°	Volume: 453.77 Å³		c/a: 1.788	
b: 9.173(5) Å	β: 98.68(5)°	Z: 2.00		a/b: 0.577	
c: 9.460(5) Å	γ: 90.09(5)°	MolVol: 226.88		c/b: 1.031	

Calculated Density: 2.776 g/cm³	Melting Point: -
Measured Density: -	Color: -
Structural Density: 2.775 g/cm³	

Gypsum, $CaSO_4(H_2O)_2$



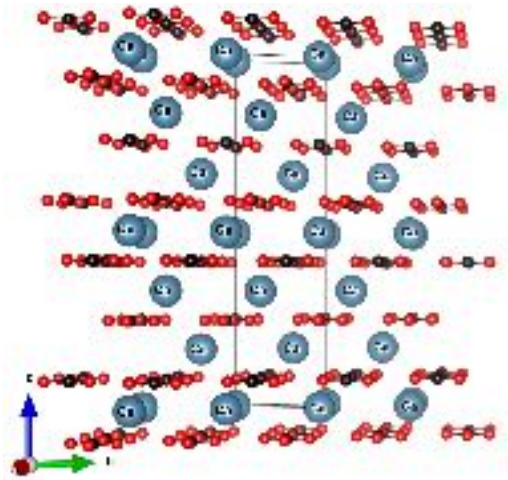
Crystal System: Monoclinic
Space Group: I2/c (15)
Aspect: -

Author's Unit Cell ▼

a: 5.680(8) Å	α: -	Volume: 494.61 Å³		c/a: 1.148	
b: 15.180(9) Å	β: 118.38(33)°	Z: 4.00		a/b: 0.374	
c: 6.520(8) Å	γ: -	MolVol: 123.65		c/b: 0.430	

Calculated Density: 2.312 g/cm³	Melting Point: -
Measured Density: -	Color: -
Structural Density: 2.258 g/cm³	

Calcite, $CaCO_3$



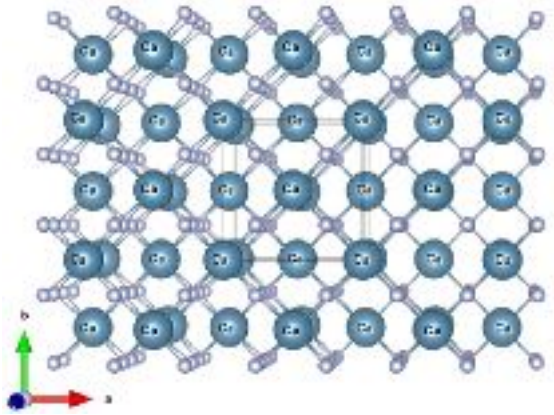
Crystal System: Rhombohedral
Space Group: R-3c (167)
Aspect: -

Author's Unit Cell ▼

a: 4.989 Å	α: -	Volume: 367.78 Å³		c/a: 3.420	
b: -	β: -	Z: 6.00		a/b: -	
c: 17.062 Å	γ: -	MolVol: 61.30		c/b: -	

Calculated Density: 2.711 g/cm³	Melting Point: -
Measured Density: 2.71 g/cm³	Color: Colorless
Structural Density: -	

Fluorite, CaF_2



Crystal System: Cubic
Space Group: Fm-3m (225)
Aspect: -

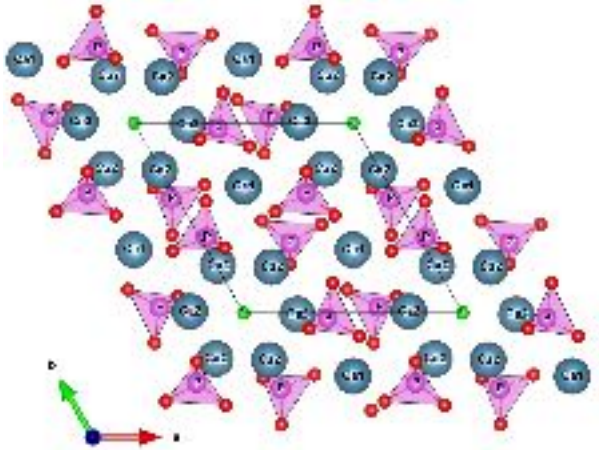
Author's Unit Cell ▼

a: 5.453 Å	α: -	Volume: 162.15 Å³		c/a: -	
b: -	β: -	Z: 4.00		a/b: -	
c: -	γ: -	MolVol: 40.54		c/b: -	

Calculated Density: 3.198 g/cm³	Melting Point: -
Measured Density: 3.18 g/cm³	Color: Various
Structural Density: -	

Mineral Physical Properties

Apatite, $Ca_{10}(PO_4)_6(OH,F,Cl)_2$

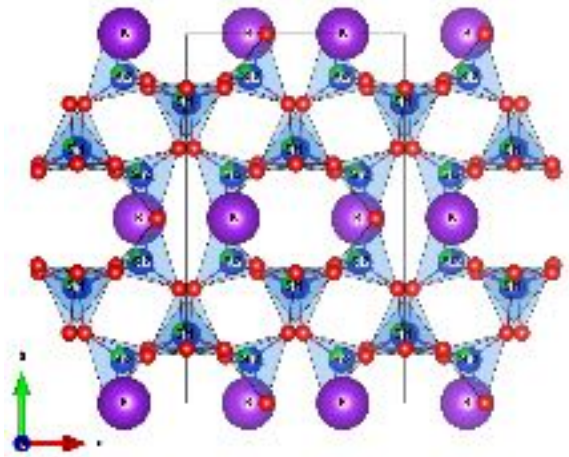


Crystal System: Hexagonal
Space Group: P63/m (176)
Aspect: -
Author's Unit Cell ▼

a: 9.418 Å	α: -	Volume: 528.80 Å³		c/a: 0.731	
b: -	β: -	Z: 2.00		a/b: -	
c: 6.884 Å	γ: -	MolVol: 264.40		c/b: -	

Calculated Density: 3.155 g/cm³		Melting Point: -	
Measured Density: 3.08 g/cm³		Color:	Green, bluish green,
Structural Density: -			

Orthoclase, $KAlSiO_3$

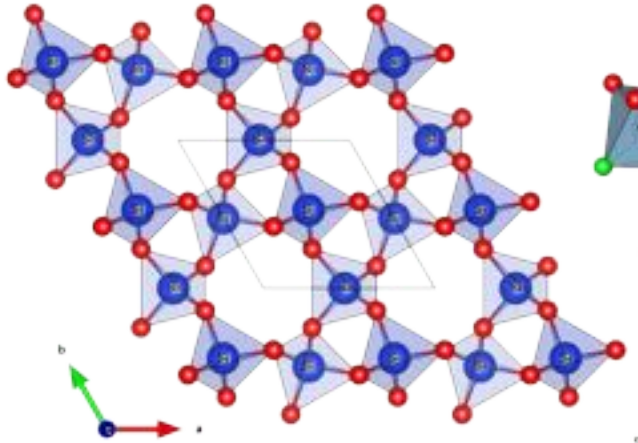


Crystal System: Monoclinic
Space Group: C2/m (12)
Aspect: -
Author's Unit Cell ▼

a: 8.556 Å	α: -	Volume: 719.18 Å³		c/a: 0.842	
b: 12.98 Å	β: 116°	Z: 4.00		a/b: 0.659	
c: 7.205 Å	γ: -	MolVol: 179.79		c/b: 0.555	

Calculated Density: 2.571 g/cm³		Melting Point: -	
Measured Density: 2.6 g/cm³		Color:	-
Structural Density: -			

Quartz, SiO_2

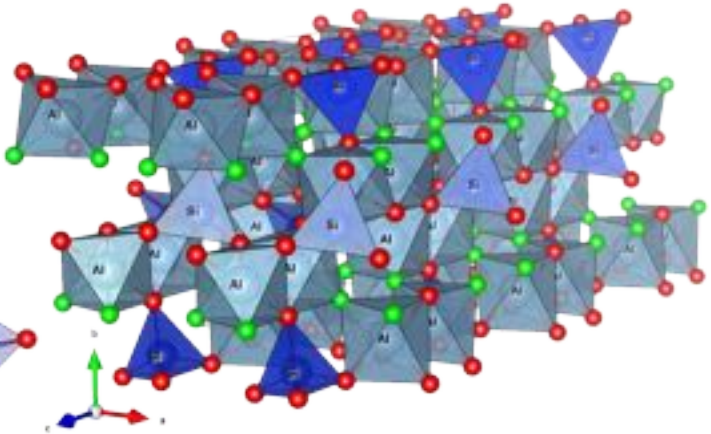


Crystal System: Hexagonal
Space Group: P3221 (154)
Aspect: -
Author's Unit Cell ▼

a: 4.91344(4) Å	α: -	Volume: 113.01 Å³		c/a: 1.100	
b: -	β: -	Z: 3.00		a/b: -	
c: 5.40524(8) Å	γ: -	MolVol: 37.67		c/b: -	

Calculated Density: 2.649 g/cm³		Melting Point: -	
Measured Density: 2.66 g/cm³		Color:	White
Structural Density: -			

Topaz, $Al_2SiO_4(F,OH)_2$



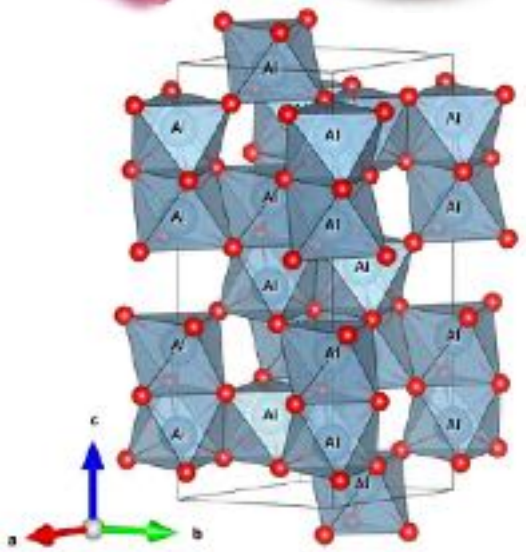
Crystal System: Orthorhombic
Space Group: Pbnm (62)
Aspect: -
Author's Unit Cell ▼

a: 4.649 Å	α: -	Volume: 343.10 Å³		c/a: 1.806	
b: 8.792 Å	β: -	Z: 4.00		a/b: 0.529	
c: 8.394 Å	γ: -	MolVol: 85.78		c/b: 0.955	

Calculated Density: 3.558 g/cm³		Melting Point: -	
Measured Density: -		Color:	Colorless
Structural Density: -			

Mineral Physical Properties

Corundum, Al_2O_3

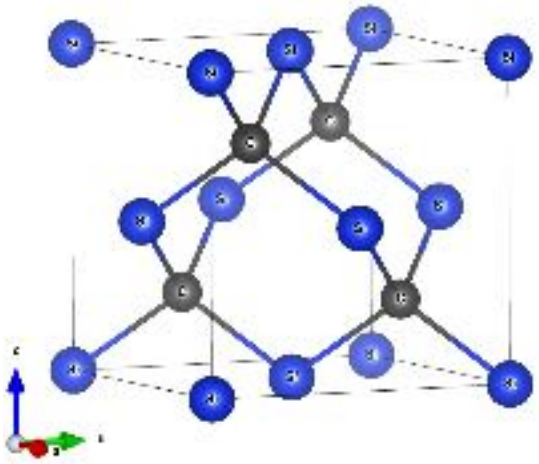


Crystal System: Rhombohedral
Space Group: R-3c (167)
Aspect: -
Author's Unit Cell ▼

a: 4.7587(1) Å	α: -	Volume: 254.81 Å³	c/a: 2.730
b: -	β: -	Z: 6.00	a/b: -
c: 12.9929(3) Å	γ: -	MolVol: 42.47	c/b: -

Calculated Density: 3.987 g/cm³	Melting Point: -
Measured Density: -	Color: -
Structural Density: -	

Moissanite, SiC

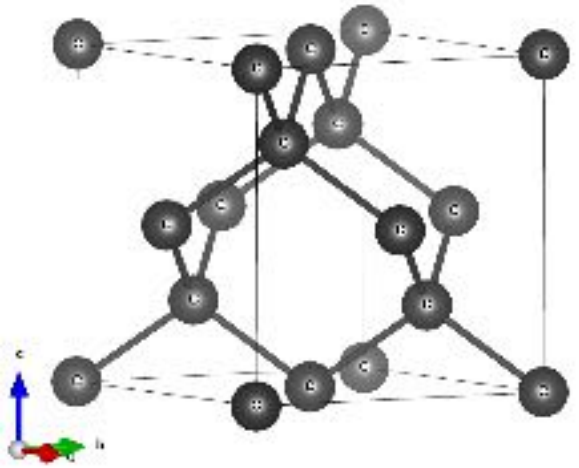


Crystal System: Cubic
Space Group: F-43m (216)
Aspect: -
Author's Unit Cell ▼

a: 4.3589 Å	α: -	Volume: 82.82 Å³	c/a: -
b: -	β: -	Z: 4.00	a/b: -
c: -	γ: -	MolVol: 20.70	c/b: -

Calculated Density: 3.216 g/cm³	Melting Point: -
Measured Density: -	Color: Greenish yellow
Structural Density: -	

Diamond, C



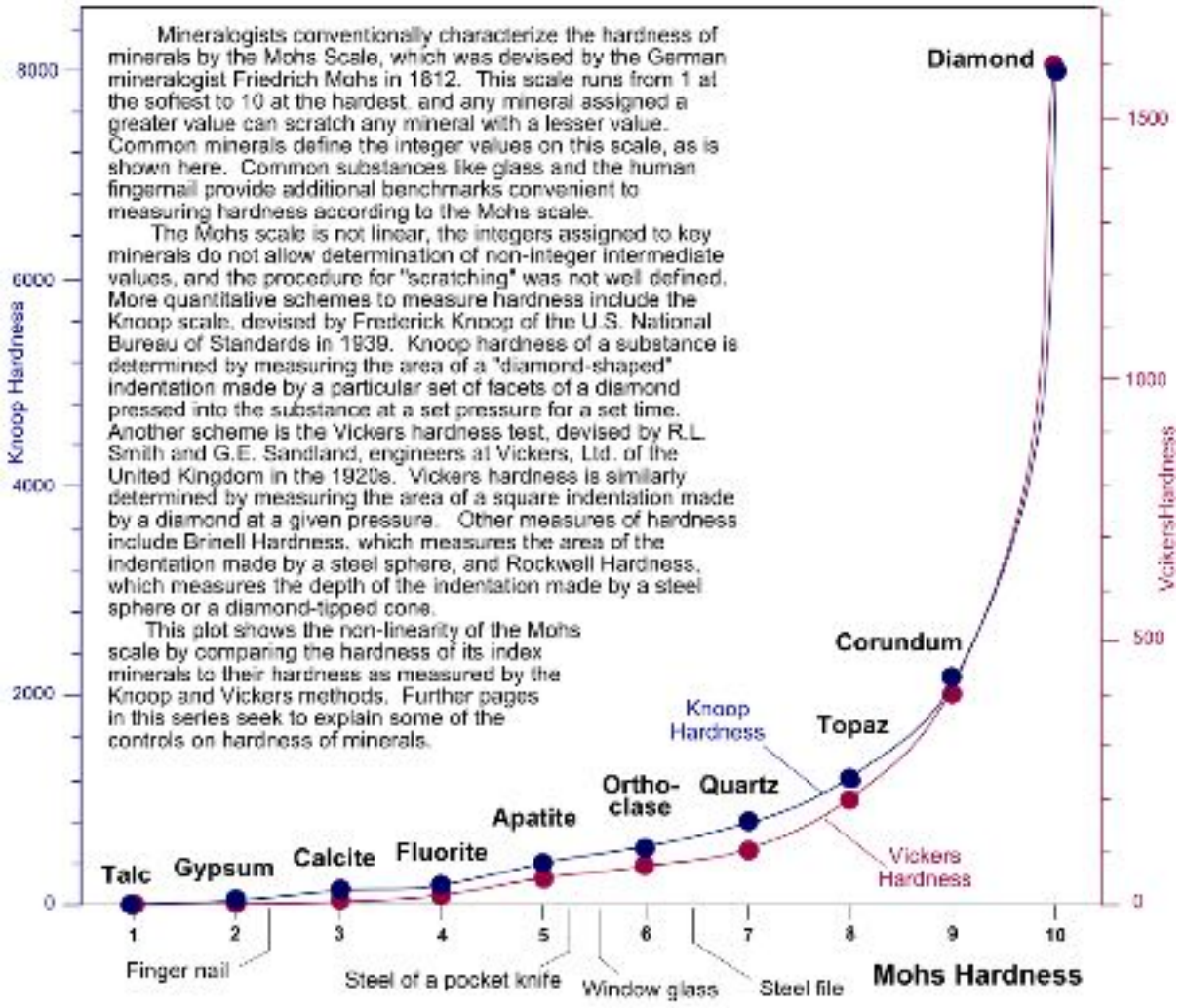
Crystal System: Cubic
Space Group: Fd-3m (227)
Aspect: -
Author's Unit Cell ▼

a: 3.56712(5) Å	α: -	Volume: 45.39 Å³	c/a: -
b: -	β: -	Z: 8.00	a/b: -
c: -	γ: -	MolVol: 5.67	c/b: -

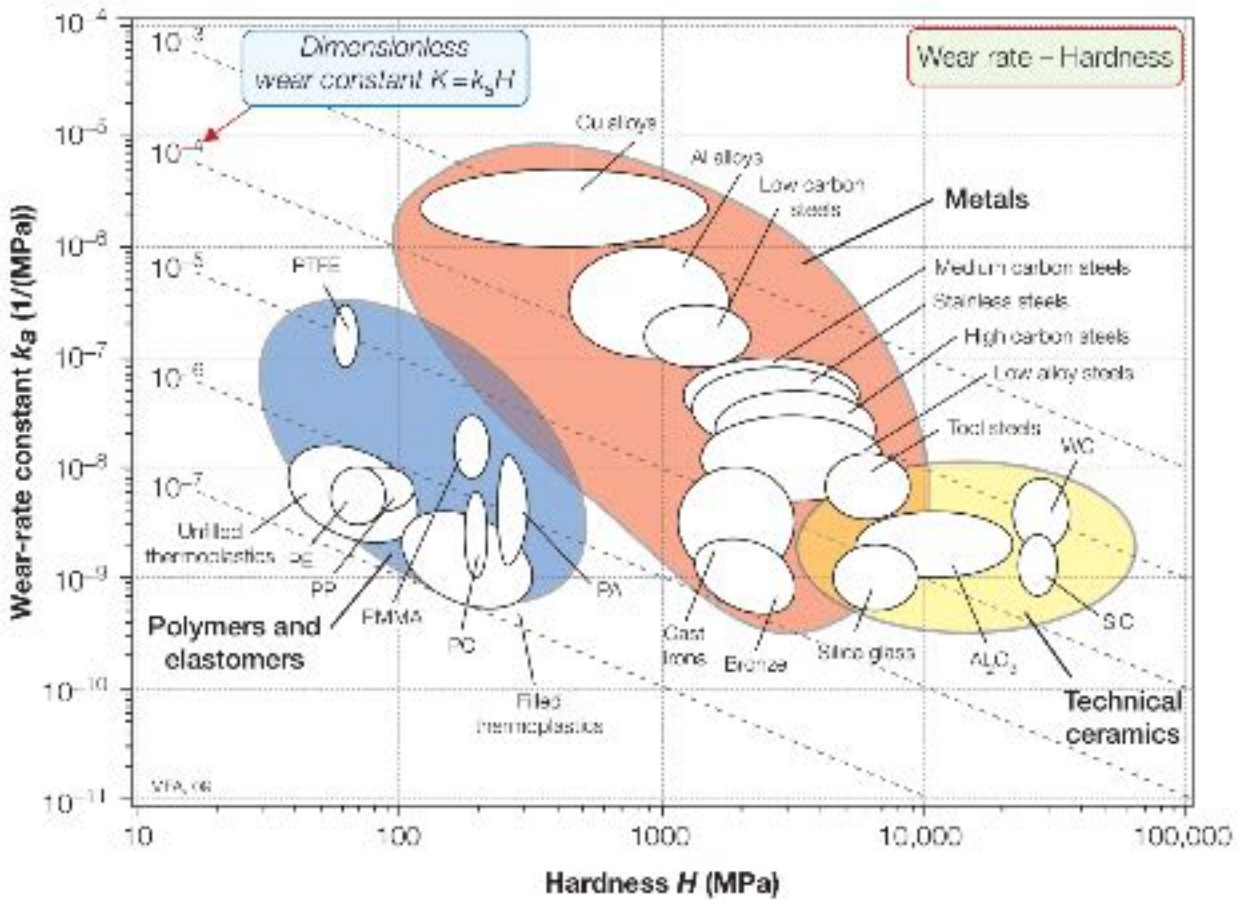
Calculated Density: 3.515 g/cm³	Melting Point: -
Measured Density: -	Color: -
Structural Density: 3.515 g/cm³	

Hardnes and Material Selection

Hardness of Minerals



Materials Selection in Mechanic Ashby - Chart



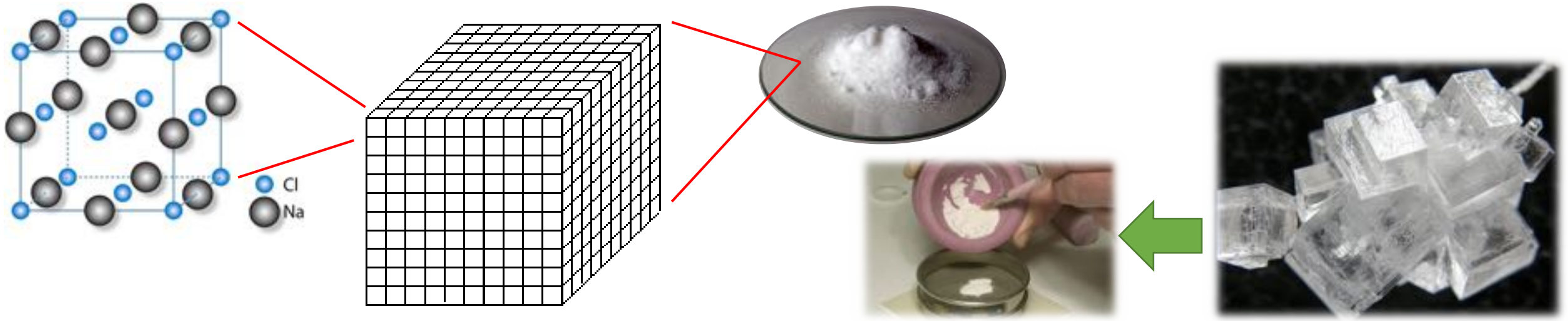
Crystals and Symmetry

Imagine…

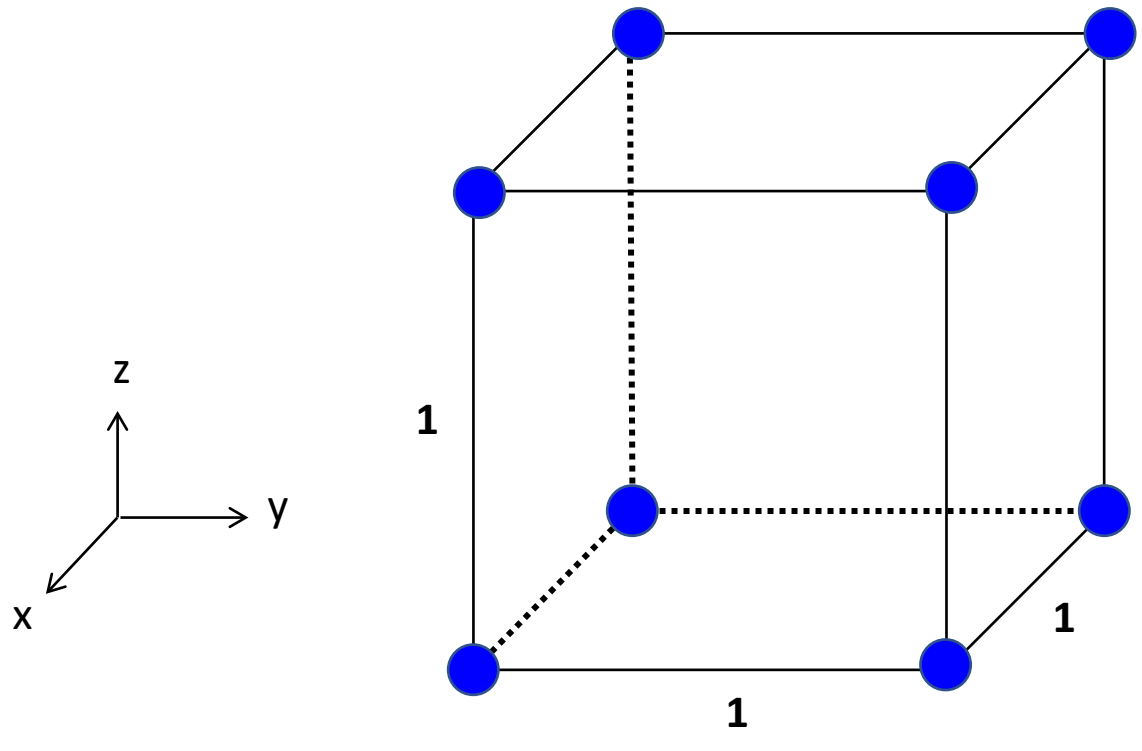
- having to describe an infinite crystal with an **infinite number of atoms**
- or even a **finite crystal**, with some **10^{20} atoms**

Sounds horrible?... Well, there's **symmetry** to help you out! Instead of an infinite number of atoms, you only need to describe the contents of **one-unit cell**, the structural repeating motif…

- and life could be even easier, if there are **symmetry** elements present inside the **unit cell**!
- you only need to describe the **asymmetric unit** if this is the case



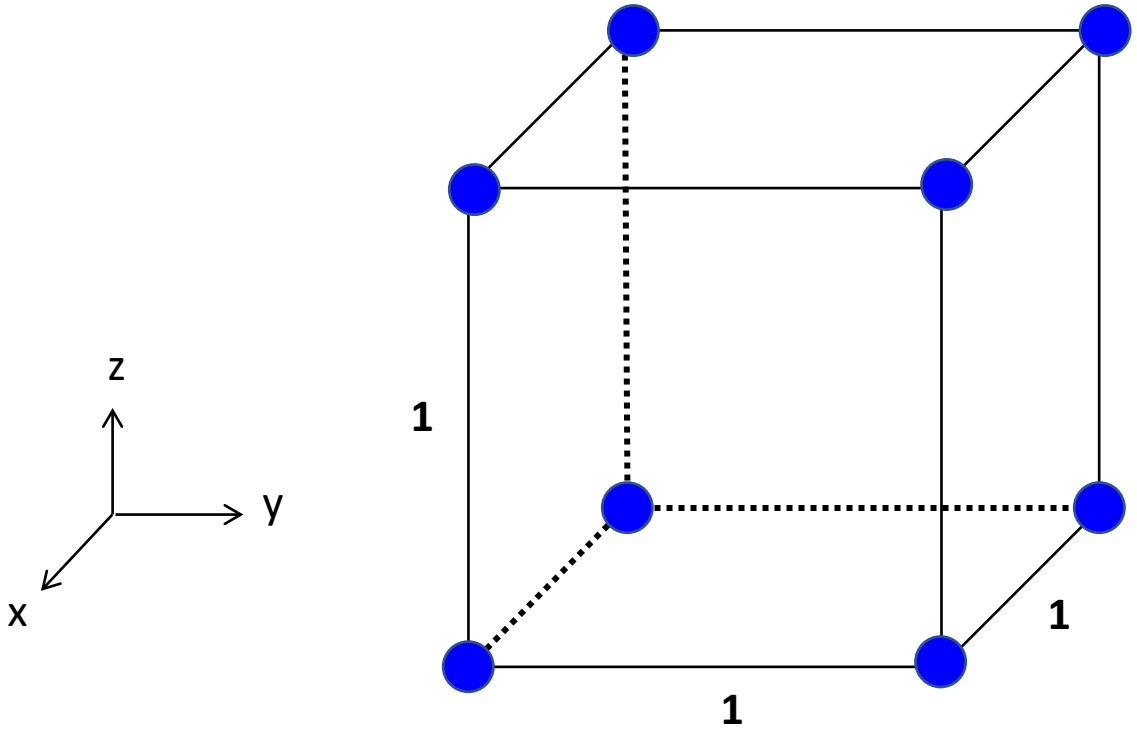
Without Symmetry



1,1,1
0,1,1
1,0,1
0,0,1
1,1,0
0,1,0
1,0,0
0,0,0

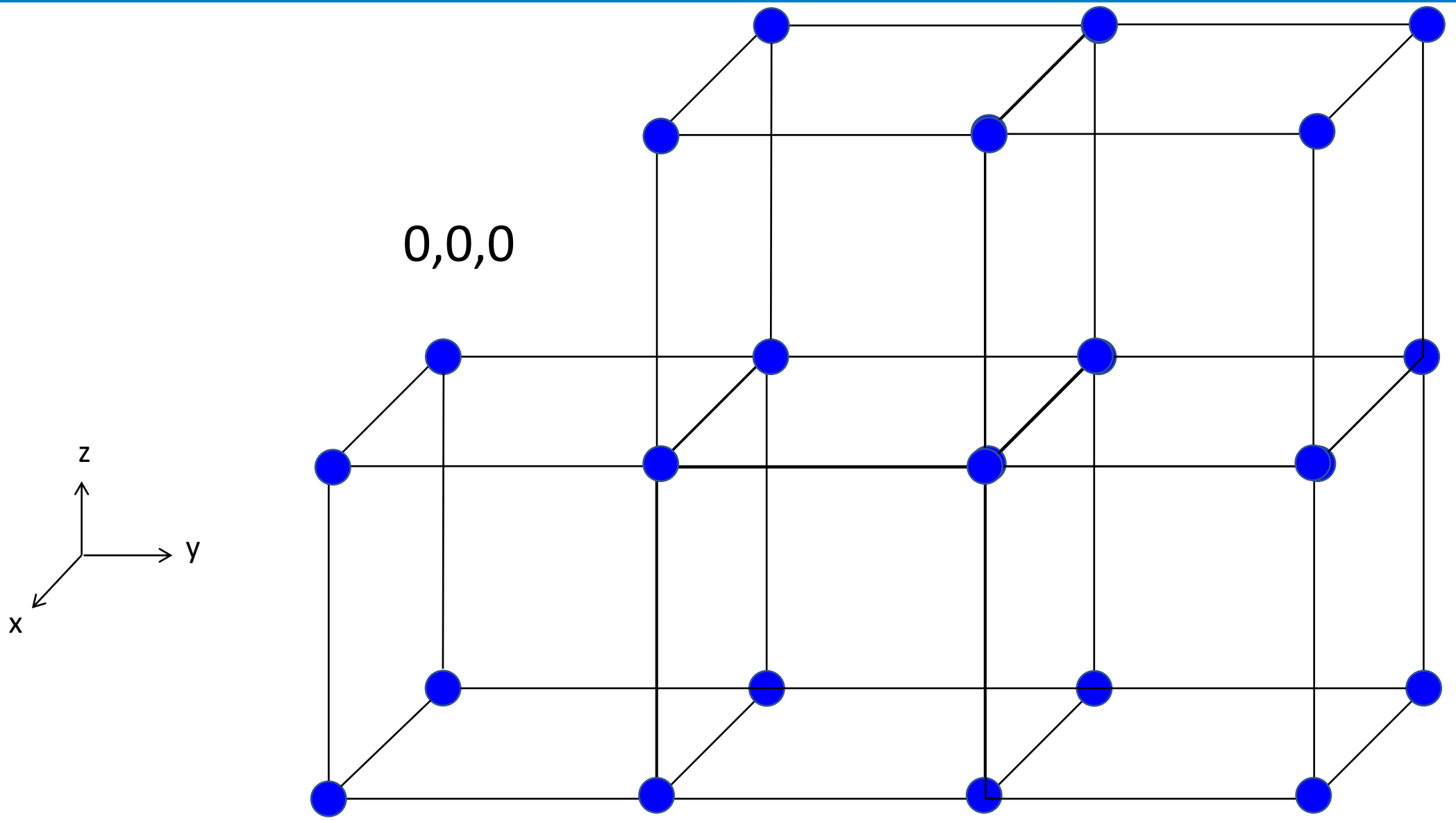
atom or molecule

With Symmetry



0,0,0

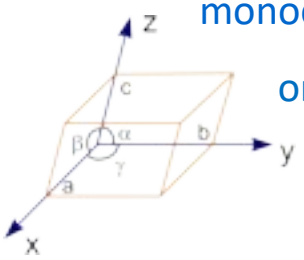
With Symmetry



Systematization

triclinic

monoclinic



orthorhombic

tetragonal

trigonal

unit cell

hexagonal

crystal system

cubic

point group

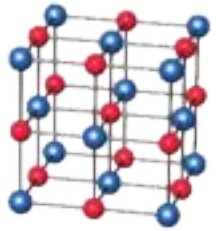
crystal class

spacegroup

base

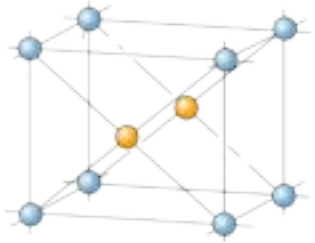
lattice

motif



primitive

face-centered



Bravais lattices

body-centered

2,3,4,6-fold axis of rotation

symmetry elements

1-bar

6-bar

inversion centre

tetrahedral holes

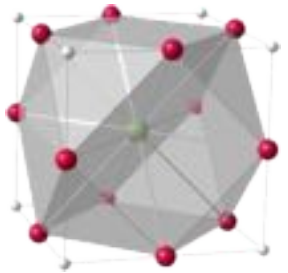
octahedral holes

coordination polyhedra

cube, prism, rhombic dodecahedron

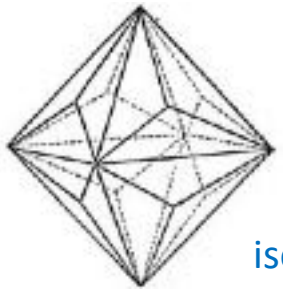
edge-connected

corner-connected



morphology

variety



habitus

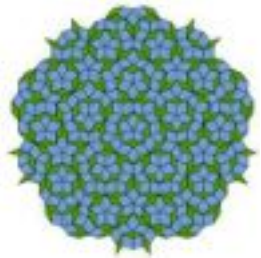
crystal faces

isotypic

Miller indices

hkl values

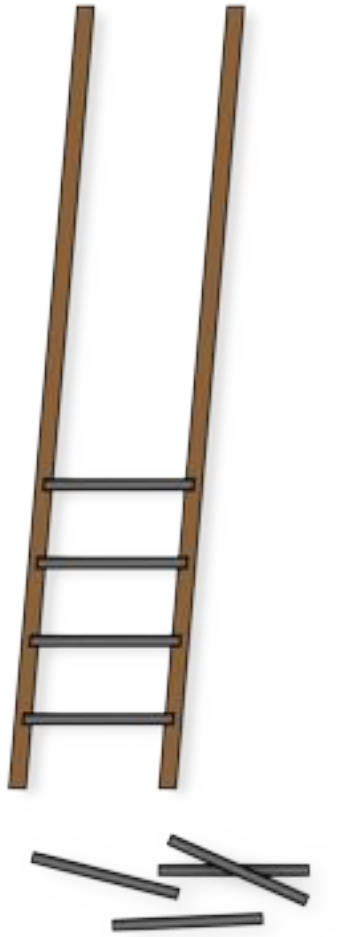
(111) lattice plane families



quasicrystal

~~quasi-crystalline~~

Systematization of Crystal Structures



1. Step: Crystal Systems

metric + symmetry of the UC

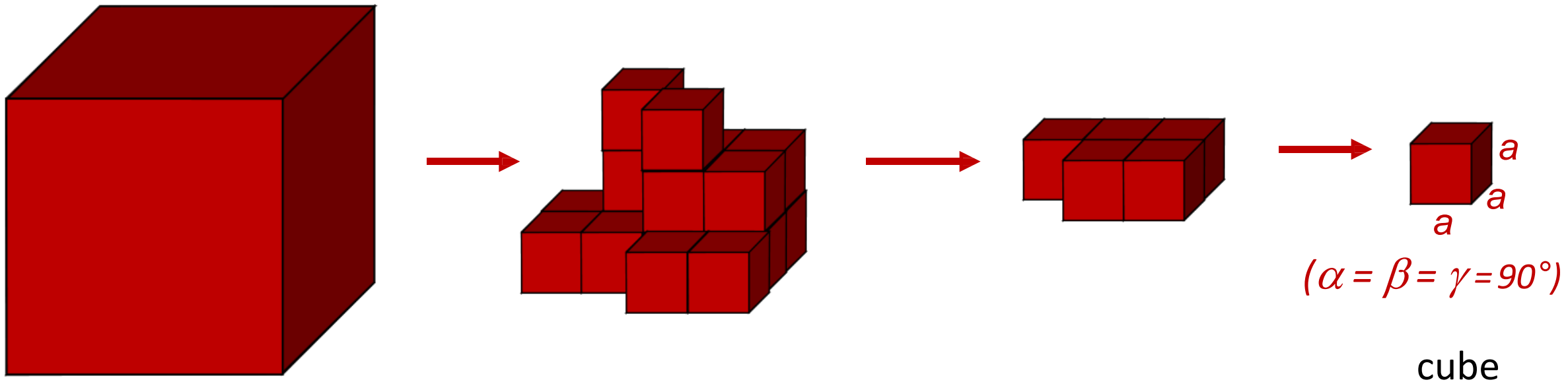
The Concept of the Unit Cell

Task

Divide a space/volume into *identical* building blocks

use only blocks that are *geometrically regular*

use only *a single sort* of blocks



cube

cube

Source: Frank Hoffmann

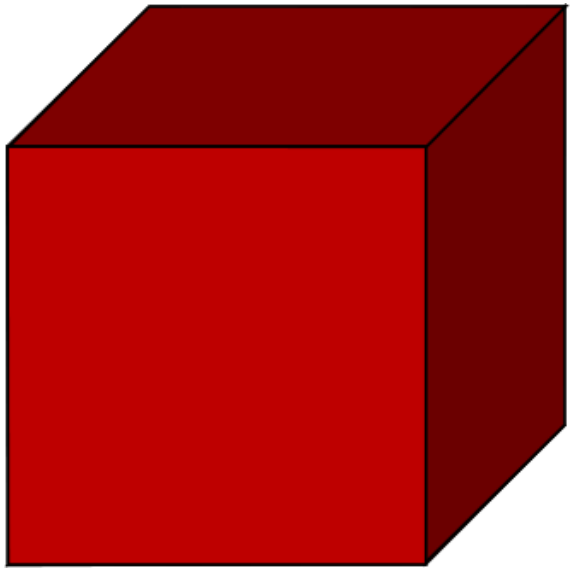
The Concept of the Unit Cell

Task

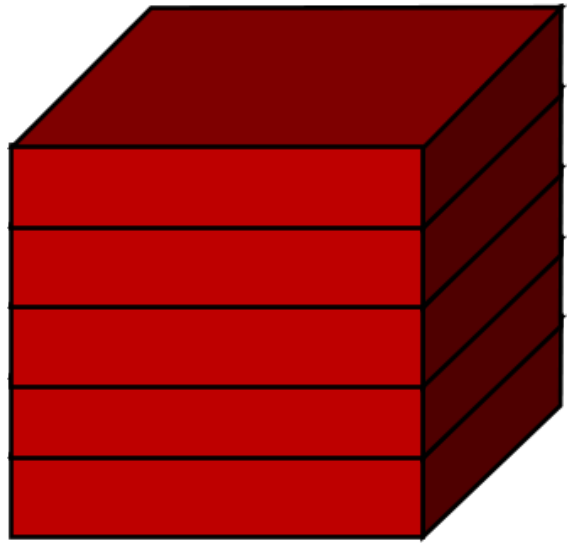
Divide a space/volume into *identical* building blocks

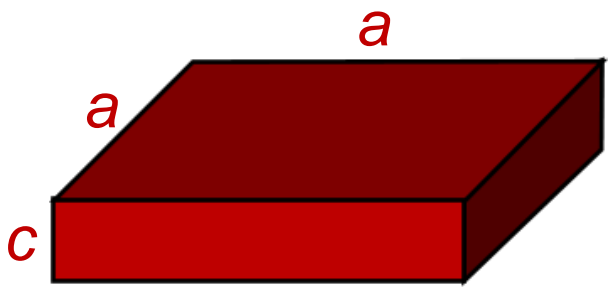
use only blocks that are *geometrically regular*

use only *a single sort* of blocks



cube





$(\alpha = \beta = \gamma = 90°)$

square plate

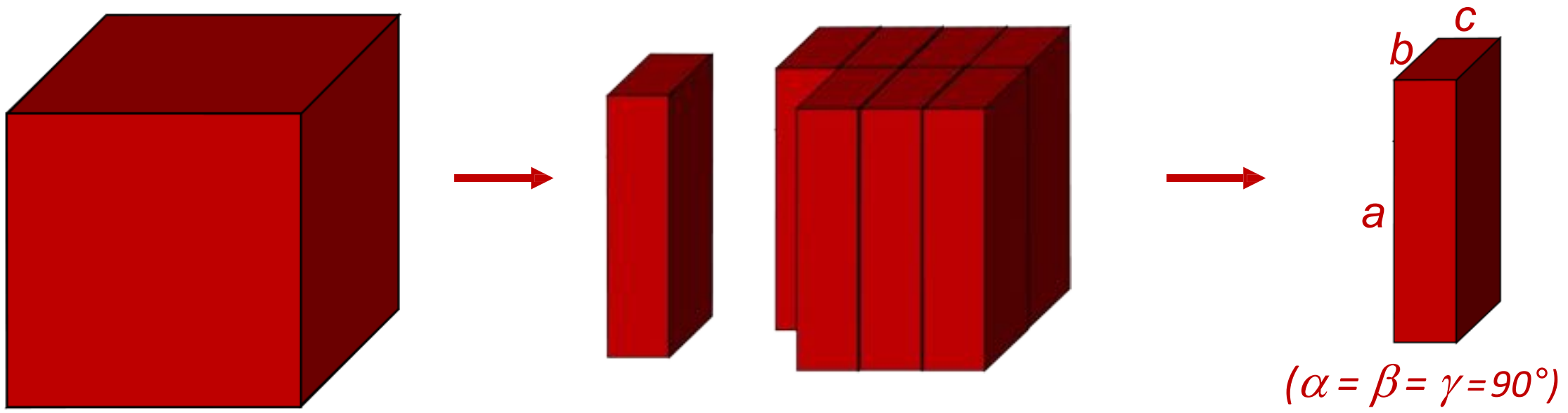
The Concept of the Unit Cell

Task

Divide a space/volume into *identical* building blocks

use only blocks that are *geometrically regular*

use only *a single sort* of blocks



cube

rectangular prism

Source: Frank Hoffmann

The Concept of the Unit Cell

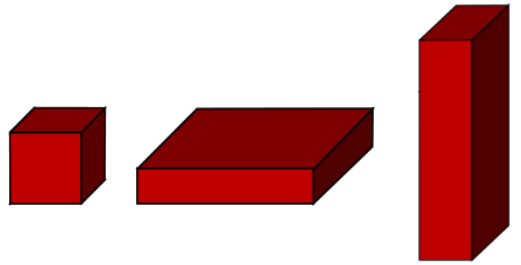
Task

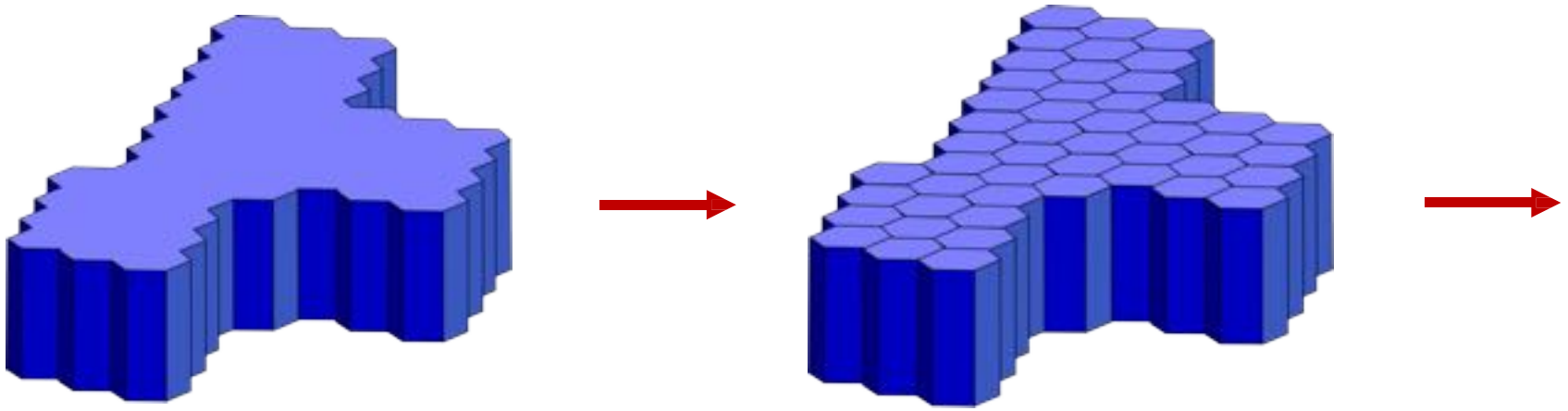
Divide a space/volume into *identical* building blocks

use only blocks that are *geometrically regular*

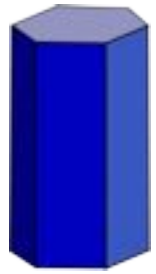
use only *a single sort* of blocks

6 faces
hexahedra





8 faces



Source: Frank Hoffmann

The Concept of the Unit Cell

Task

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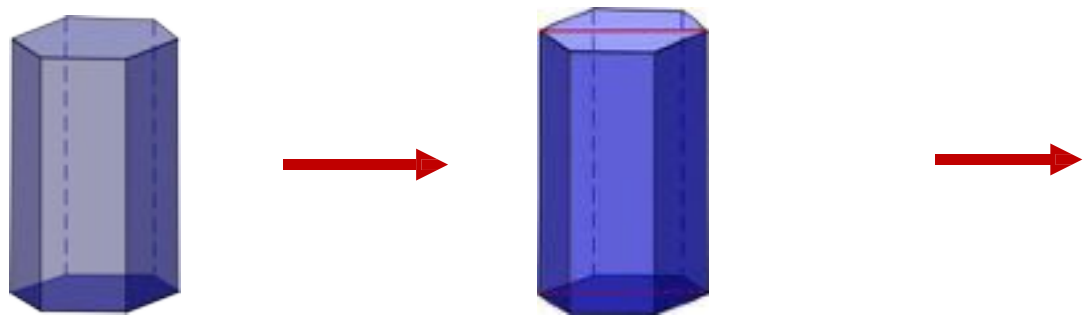

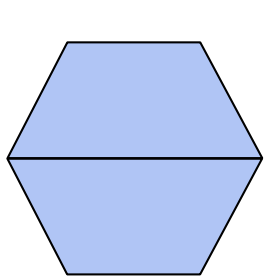

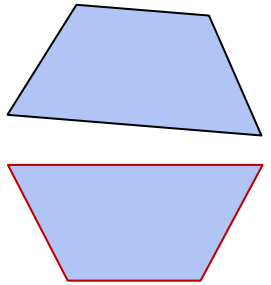

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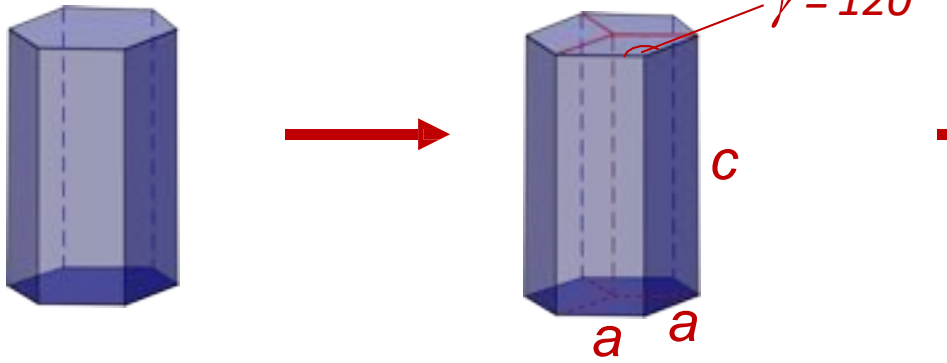
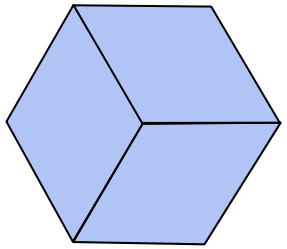
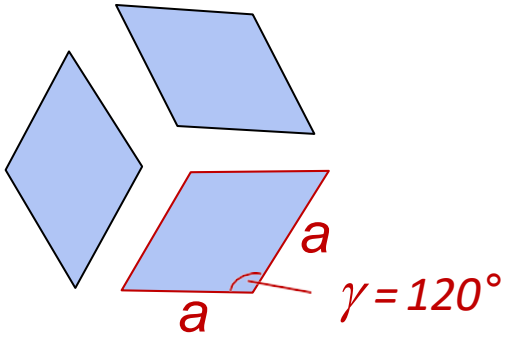
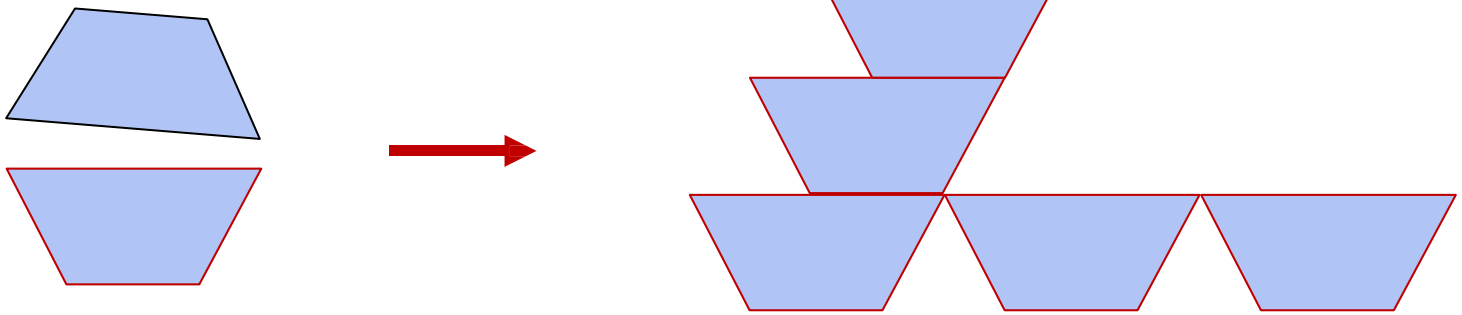




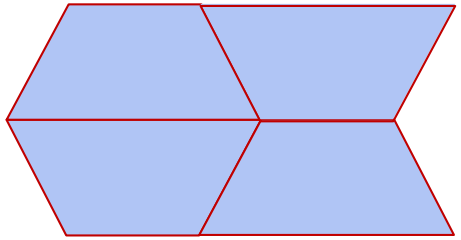


Source: Frank Hoffmann

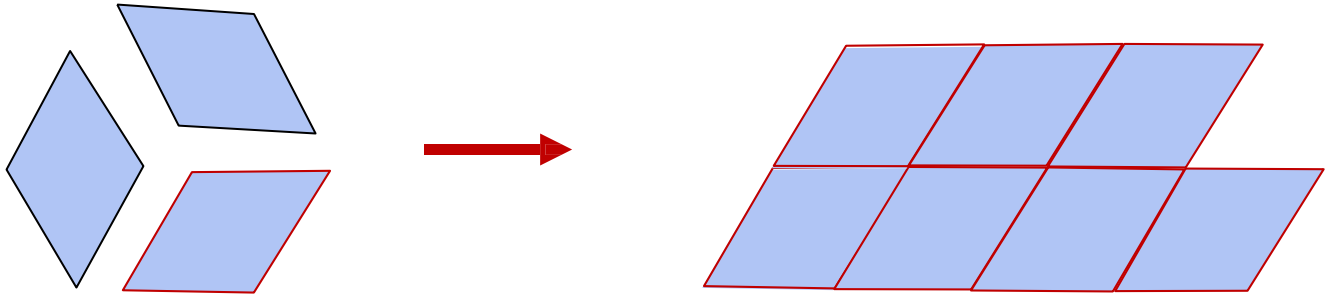
The Concept of the Unit Cell



voids
not completely space-filling



completely space-filling
but two orientations



no voids
completely space-filling

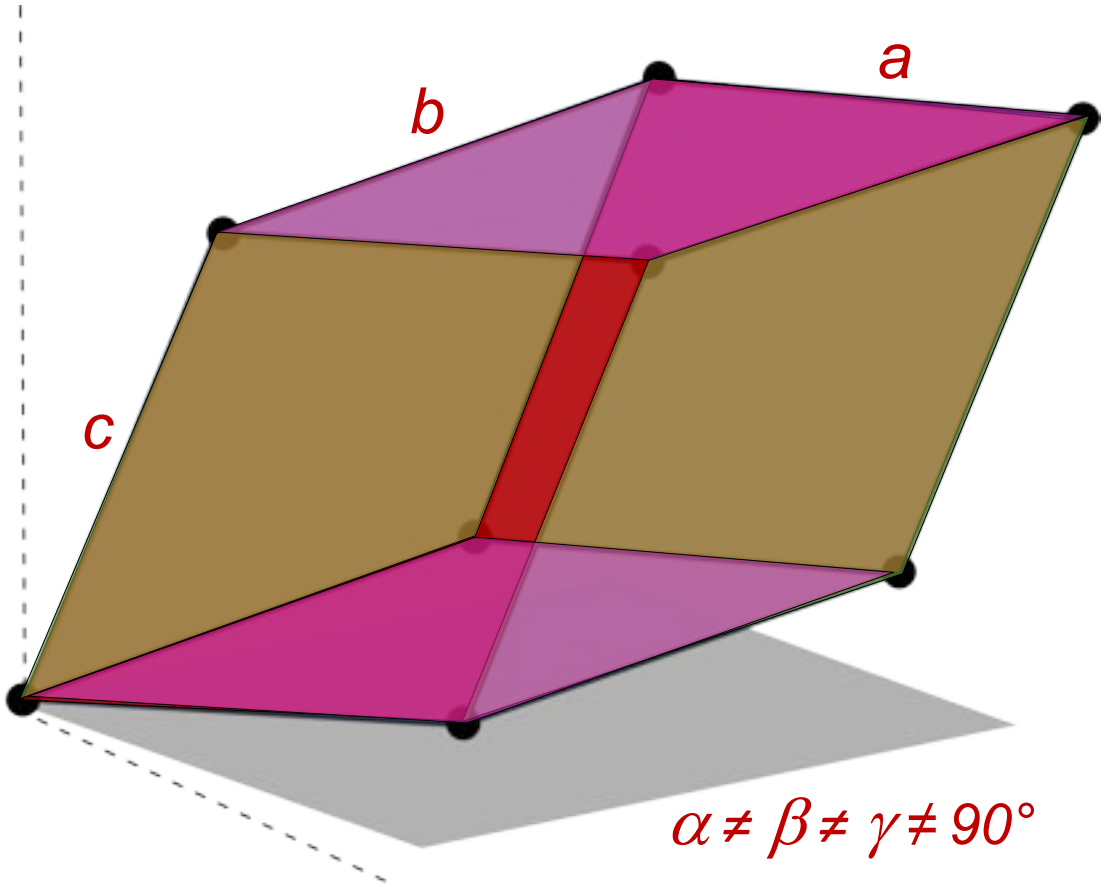
Source: Frank Hoffmann

The Concept of the Unit Cell

- Which geometrical regular bodies fill the space completely (without gaps) by joining them together only by translation along all three spatial directions?

→ parallelepipeds!

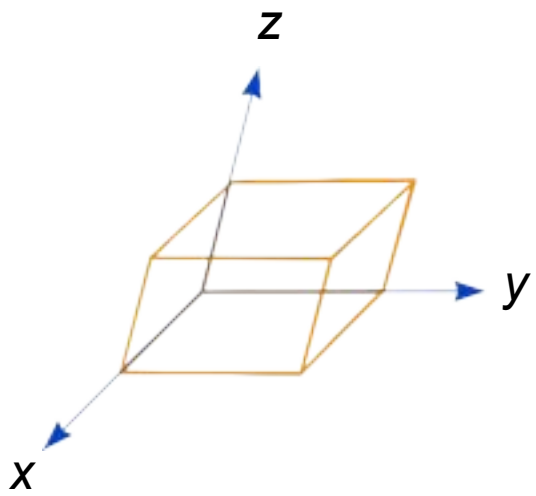
- A parallelepiped (epipedo = Greek for face) is a geometric body, which is confined by six parallelograms, of which two of each are congruent (superimposable) and lie in parallel planes.

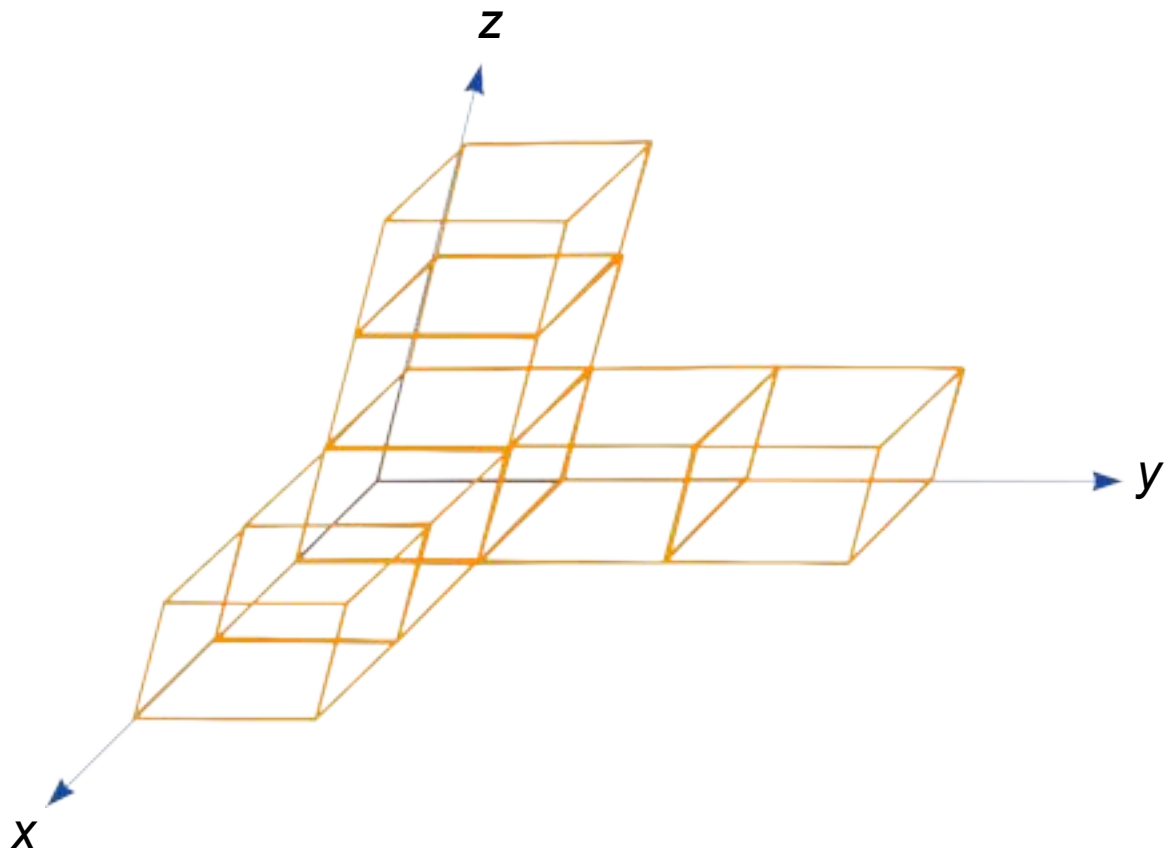


Source: Frank Hoffmann

The Unit Cell Definition

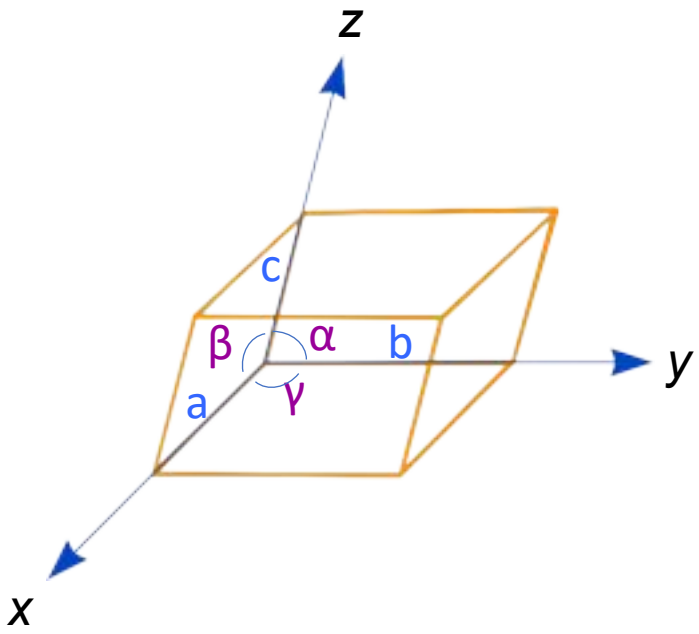
- The unit cell is the unit, which builds up the whole crystal structure by repeated translations along all three spatial directions.





Source: Frank Hoffmann

Unit Cell Attributes



Metric

- it is defined by six cell/lattice parameters
  - the three cell/lattice constants, the lengths of the edges (a, b, and c)
  - and three angles between these edges (α, β, and γ)

Symmetry

- it contains all present symmetry elements
- defines the minimum size of the unit cell

Chemical Composition (Stoichiometry)

- the chemical content of an unit cell corresponds to the chemical composition of the considered compound (!)

H_2O

2H:1O

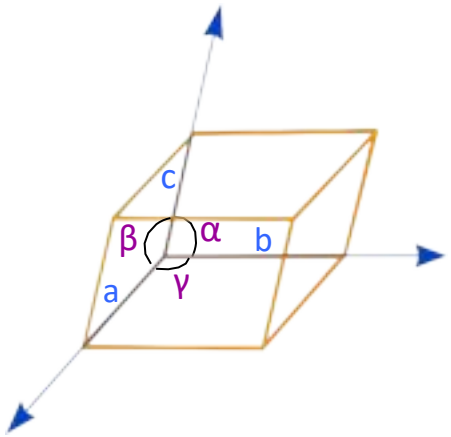
HO HO HO

HO HO HO

H_2O H_2O	H_2O H_2O	H_2O H_2O
H_2O H_2O	H_2O H_2O	H_2O H_2O

Source: Frank Hoffmann

7 – Crystal System



Classification of unit cells

Every imaginable crystal of the world belongs to one of altogether 7 possible crystal systems

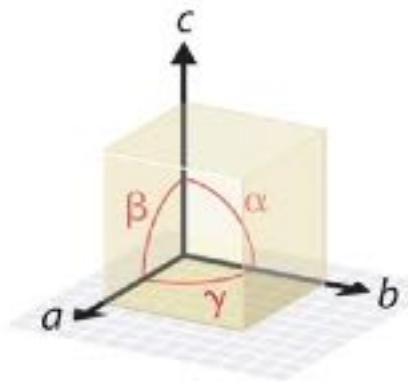
restrictions for	*cell constants*	*angles*	*maximum symmetry*
triclinic	a ≠ b ≠ c	$\alpha \neq \beta \neq \gamma \neq 90°$	$\bar{1}$
monoclinic	a ≠ b ≠ c	$\alpha = \gamma = 90°, \beta \neq 90°$	2/m
orthorhombic	a ≠ b ≠ c	$\alpha = \beta = \gamma = 90°$	mmm
tetragonal	a = b ≠ c	$\alpha = \beta = \gamma = 90°$	4/mmm
trigonal	a = b ≠ c	$\alpha = \beta = 90°; \gamma = 120°$	$\bar{3}$m
hexagonal	a = b ≠ c	$\alpha = \beta = 90°; \gamma = 120°$	6/mmm
cubic	a = b = c	$\alpha = \beta = \gamma = 90°$	m$\bar{3}$m

symmetry

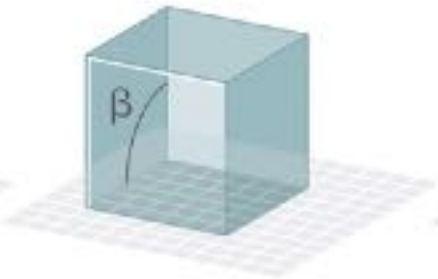
hexagonal crystal *family*

Source: Frank Hoffmann

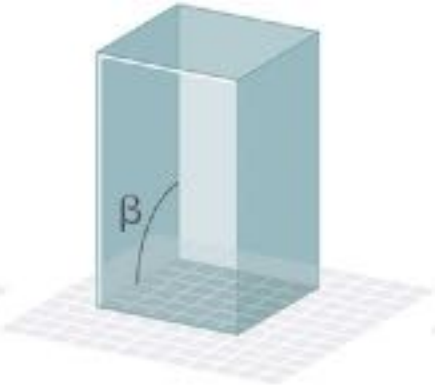
7 – Crystal System



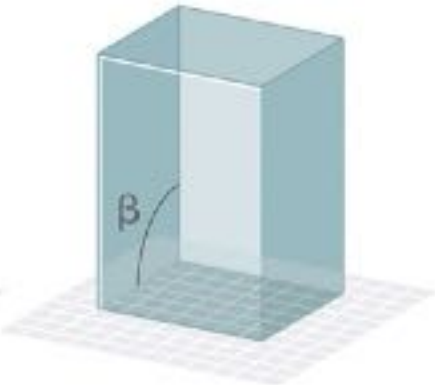
Edges and angles



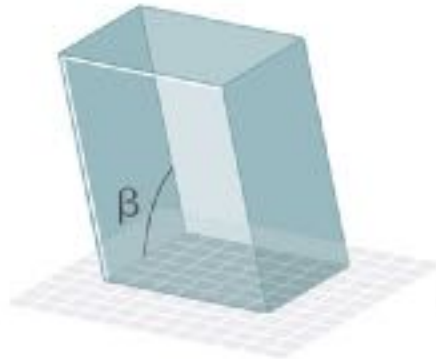
Cubic
$a = b = c$
$\alpha = \beta = \gamma = 90°$



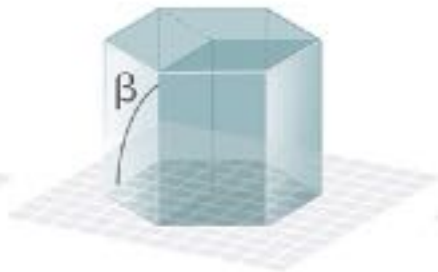
Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$



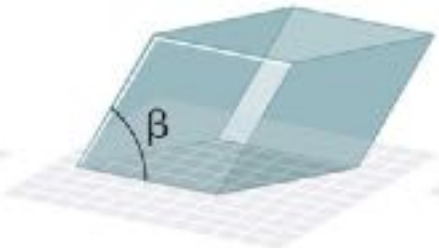
Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



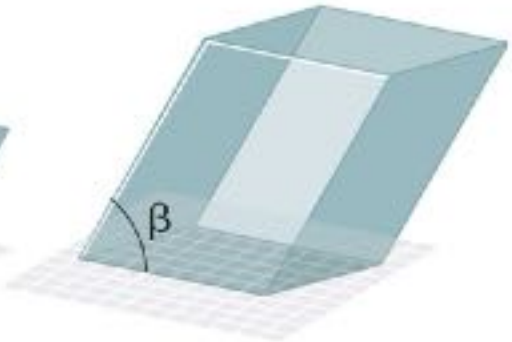
Monoclinic
$a \neq b \neq c$
$\alpha = \gamma = 90° \neq \beta$



Hexagonal
$a = b \neq c$
$\alpha = \beta = 90°, \gamma = 120°$



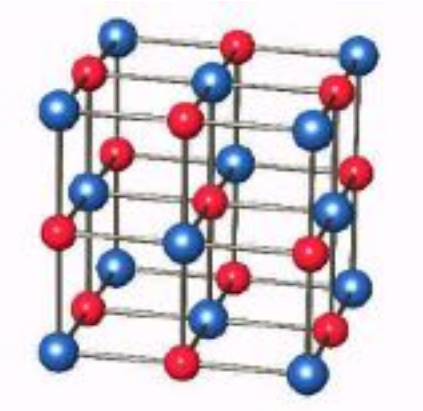
Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$



Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

Source: Frank Hoffmann

Crystal Structure = Lattice + Motif/Base



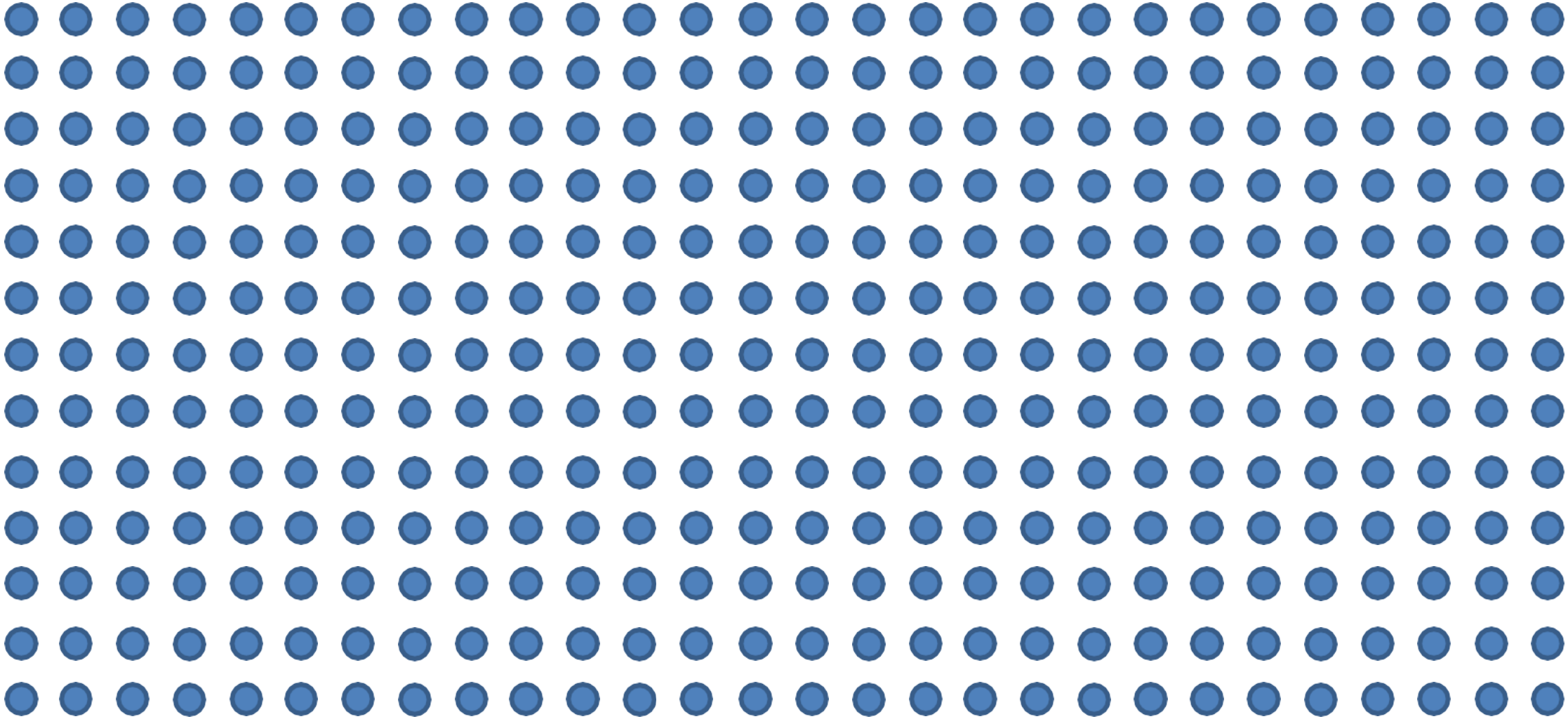
crystals have a

crystal structure

crystal structure = lattice + motif

Lattice

- Lattice = infinite arrangement of points in space (3D) / in the plane (2D) / on a line (1D),
  in which all points have the same surroundings



Lattice - Surroundings

- Lattice = infinite arrangement of points in space (3D) / in the plane (2D) / on a line (1D),
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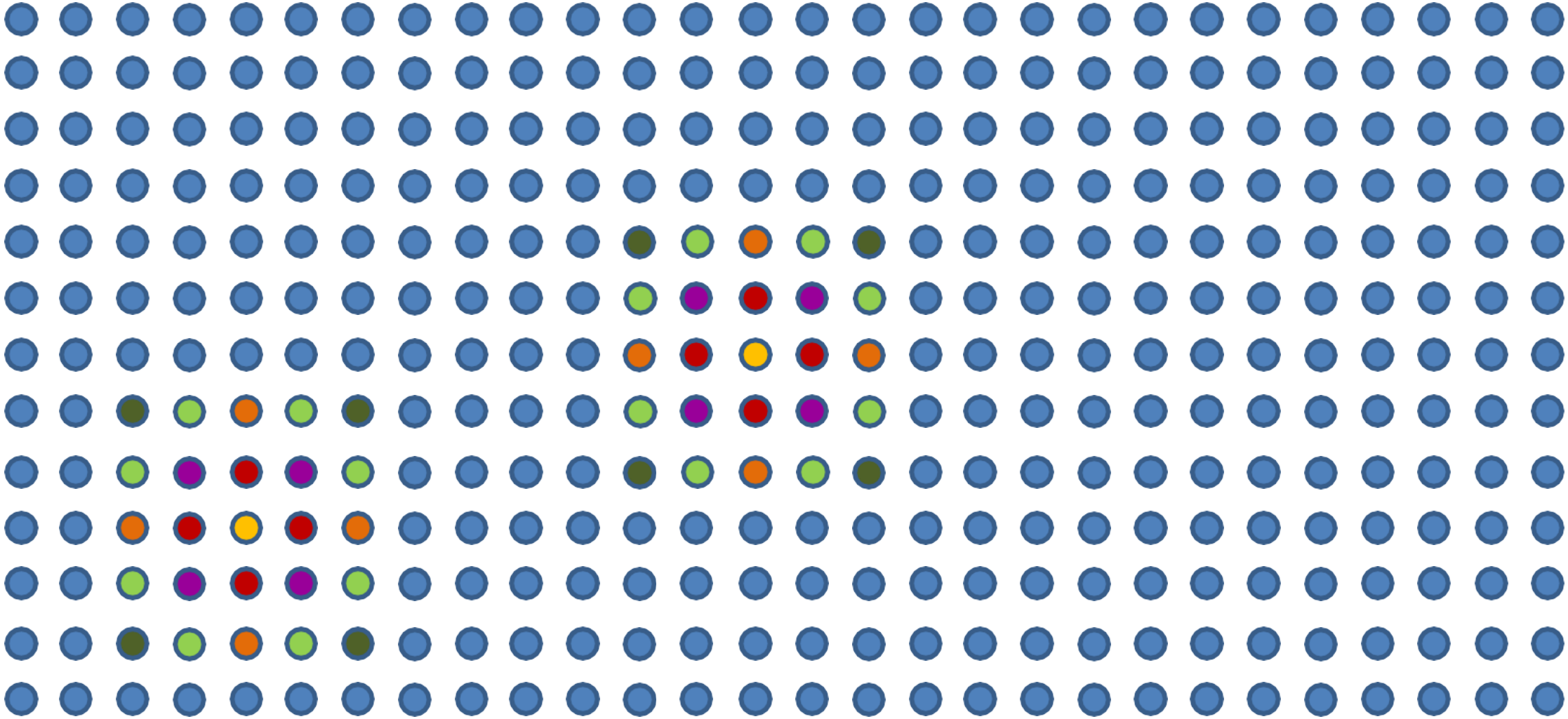

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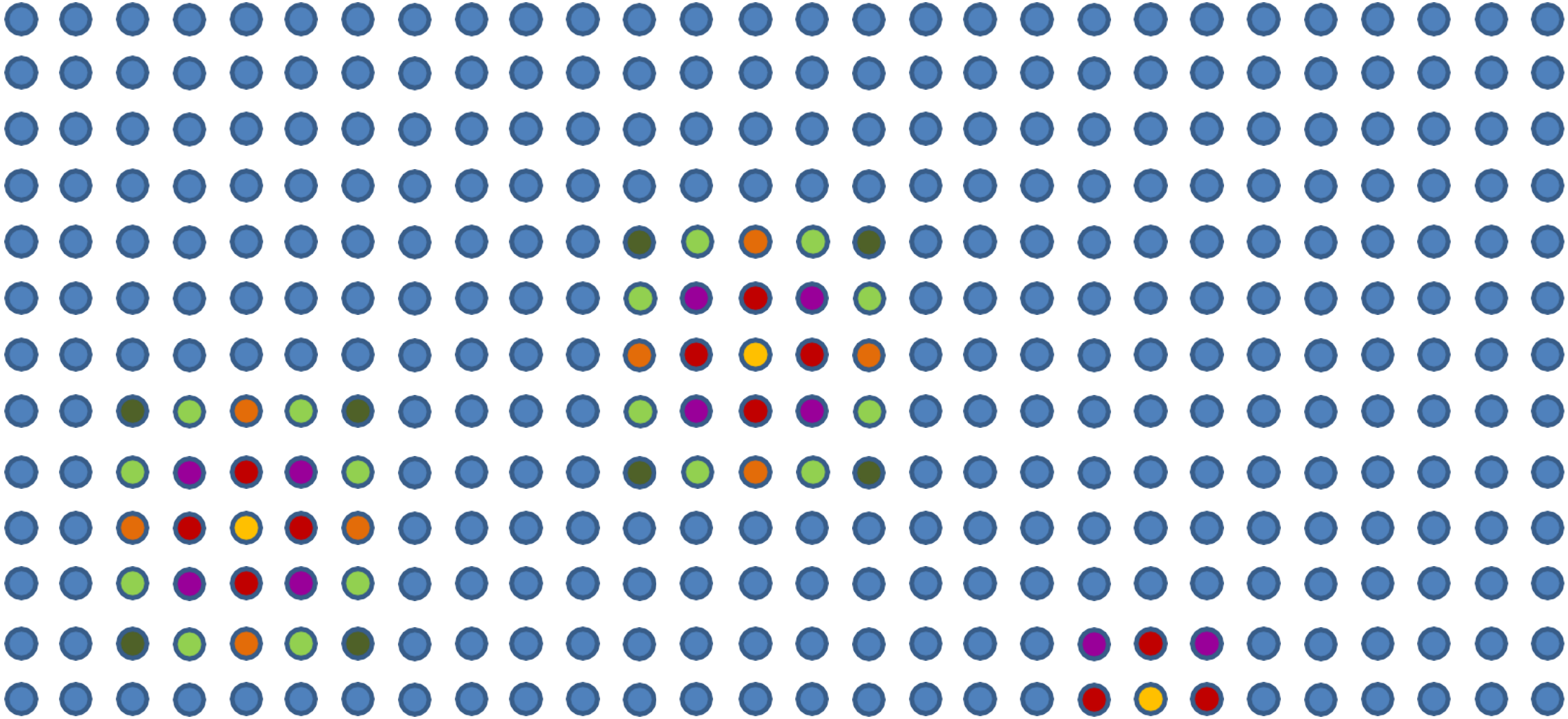
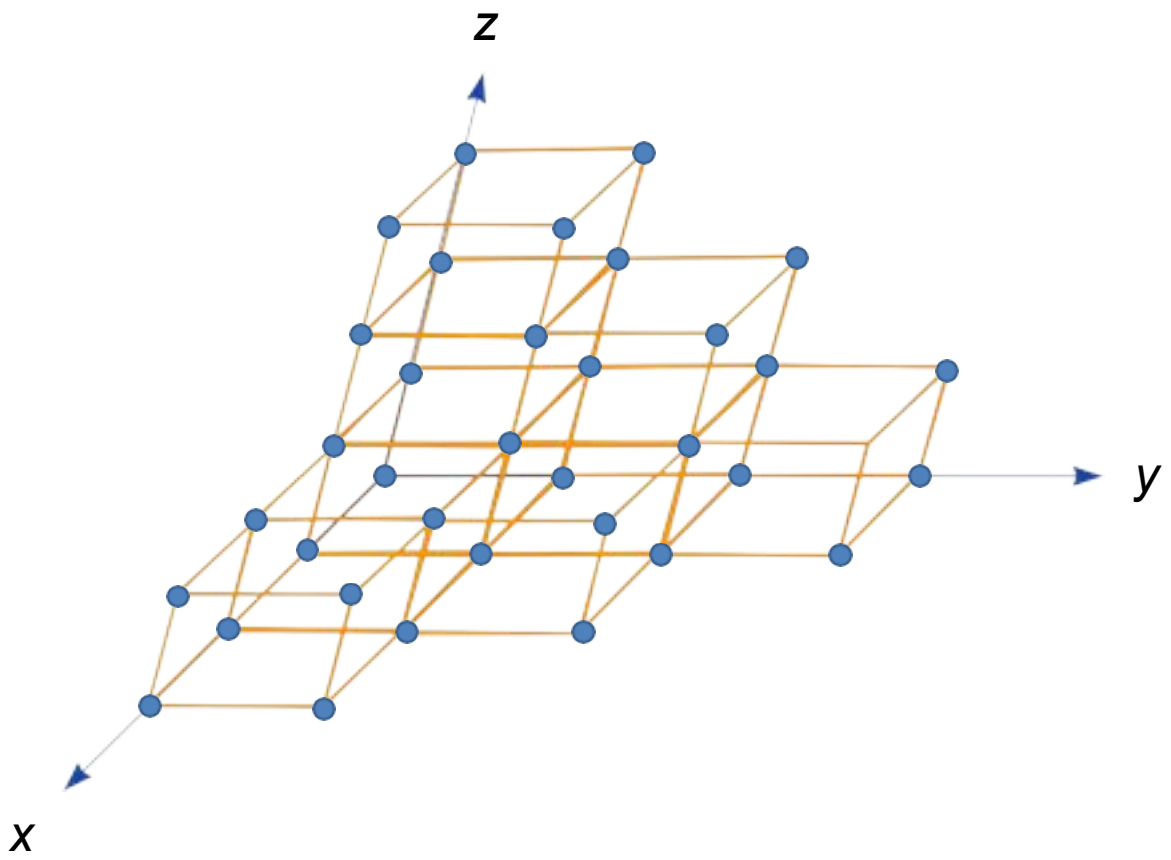


Lattice Points

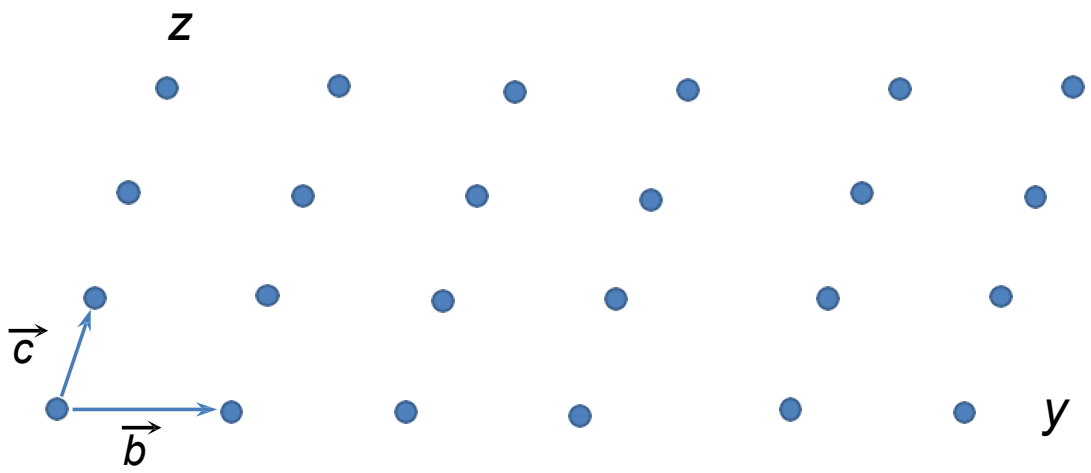
- the lattice points are the connection points between the unit cells



Source: Frank Hoffmann

Crystal Structure = Lattice + Base/Motif

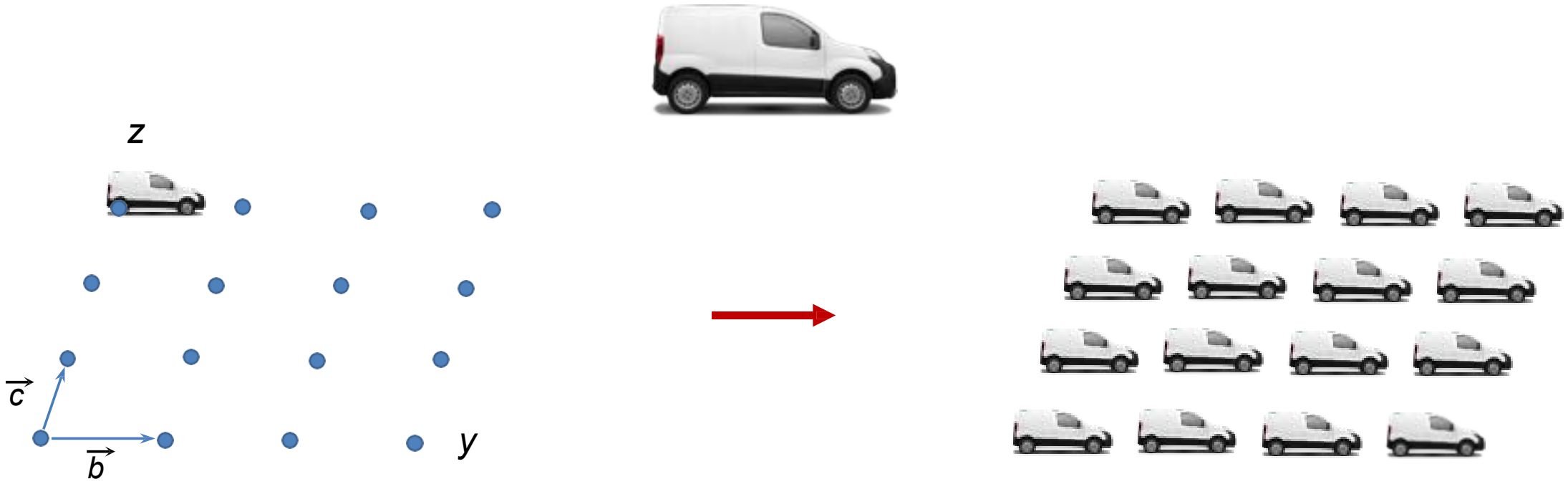
- every corner of all unit cells builds a lattice point
- a lattice is characterized by its lattice vectors (translation vectors) = they *span* the unit cell
- the lattice points can be transferred into each other by these vectors



Source: Frank Hoffmann

Crystal Structure = Lattice + Base/Motif

- the motif consists of the arrangement of the building blocks (atoms, molecules) of a unit cell
- the motif is *represented* by a lattice point



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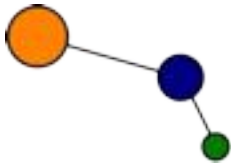
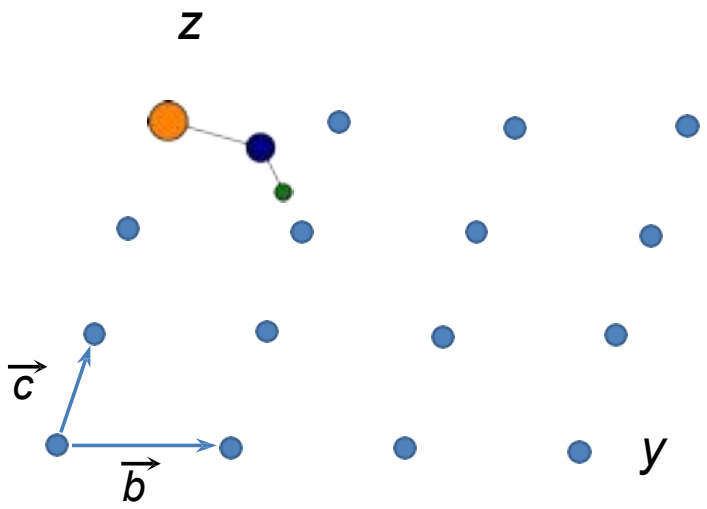
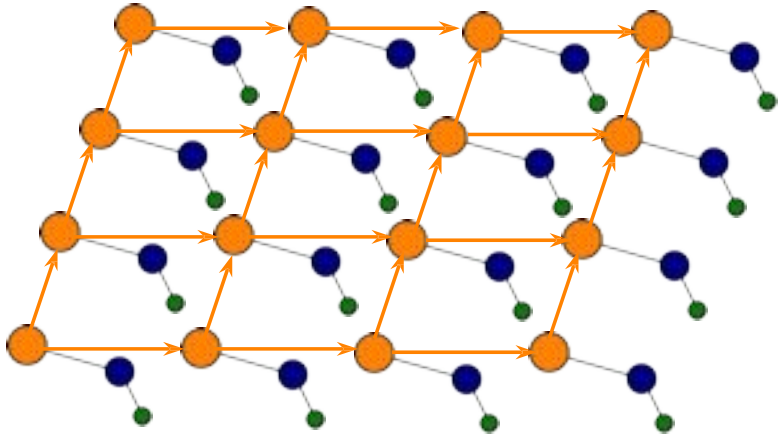


three atomic molecule





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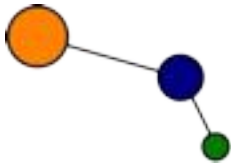

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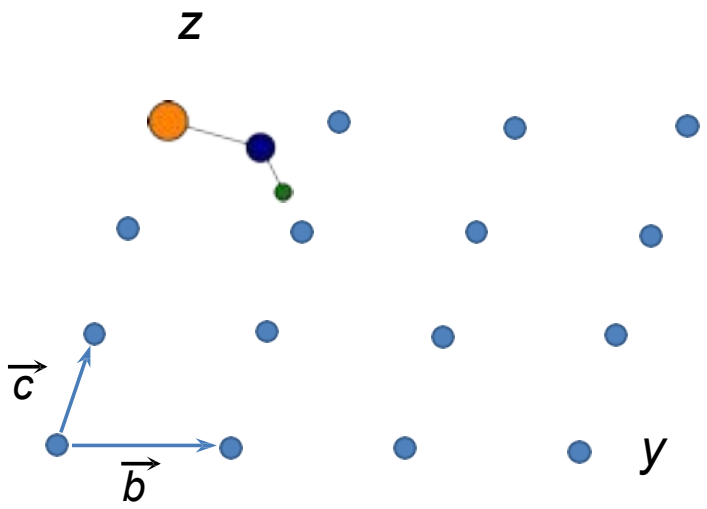

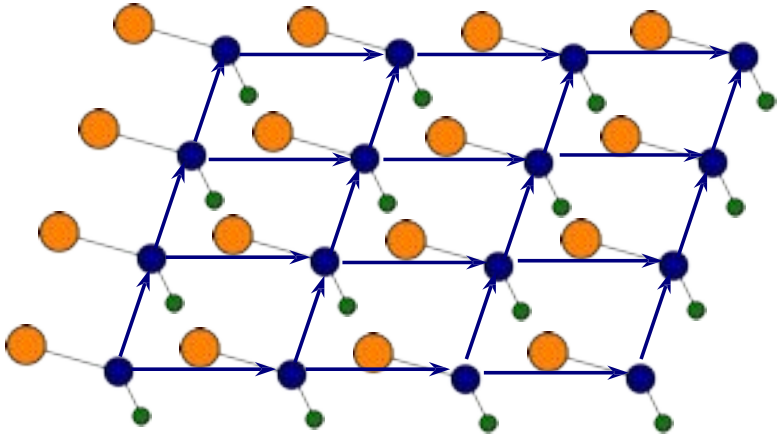

⟶ All building blocks of a crystal structure are subject to the same translation principle!

Source: Frank Hoffmann

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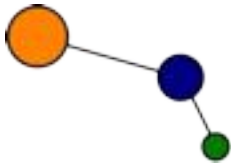
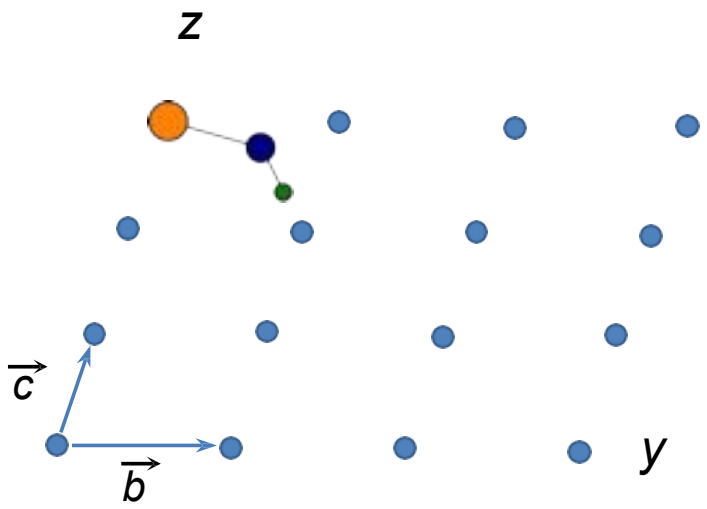
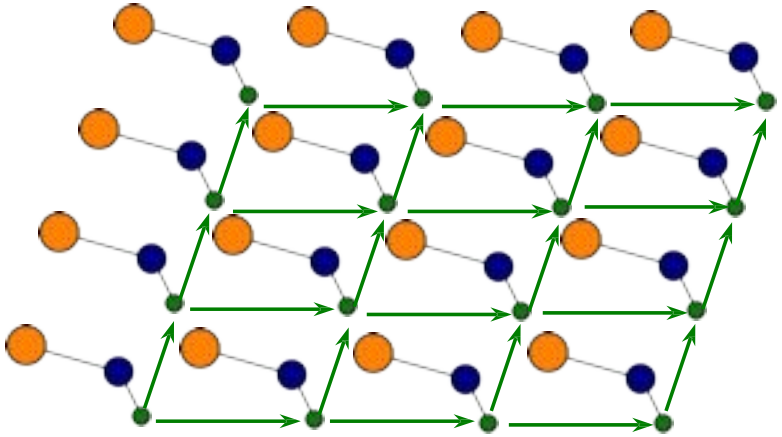


three atomic molecule





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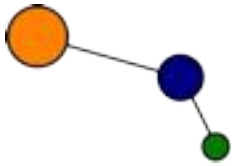

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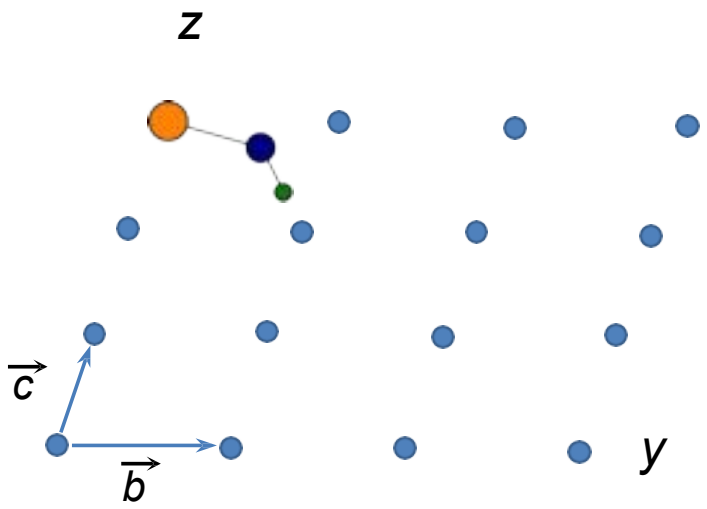
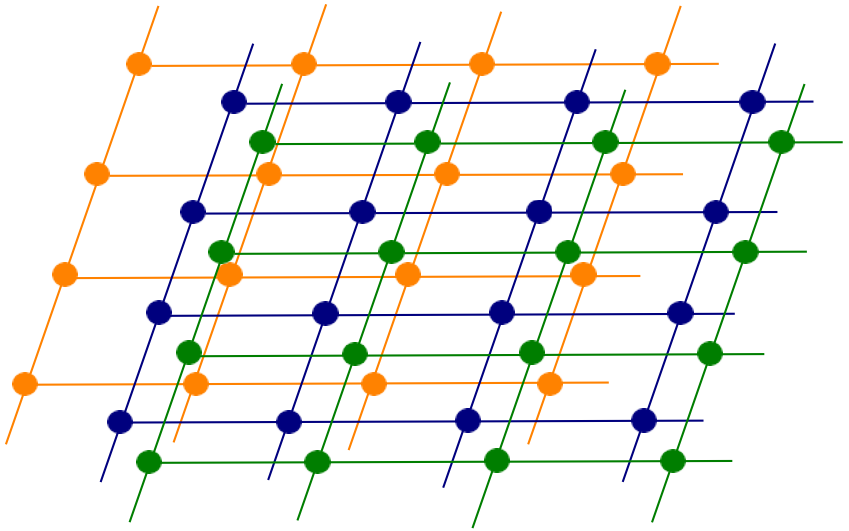




→ All building blocks of a crystal structure are subject to the same translation principle!

→ All atoms of a crystal build *congruent* crystal lattices!

Source: Frank Hoffmann

Morphology of Crystals

7 crystal systems

triclinic

monoclinic

orthorhombic

tetragonal

trigonal

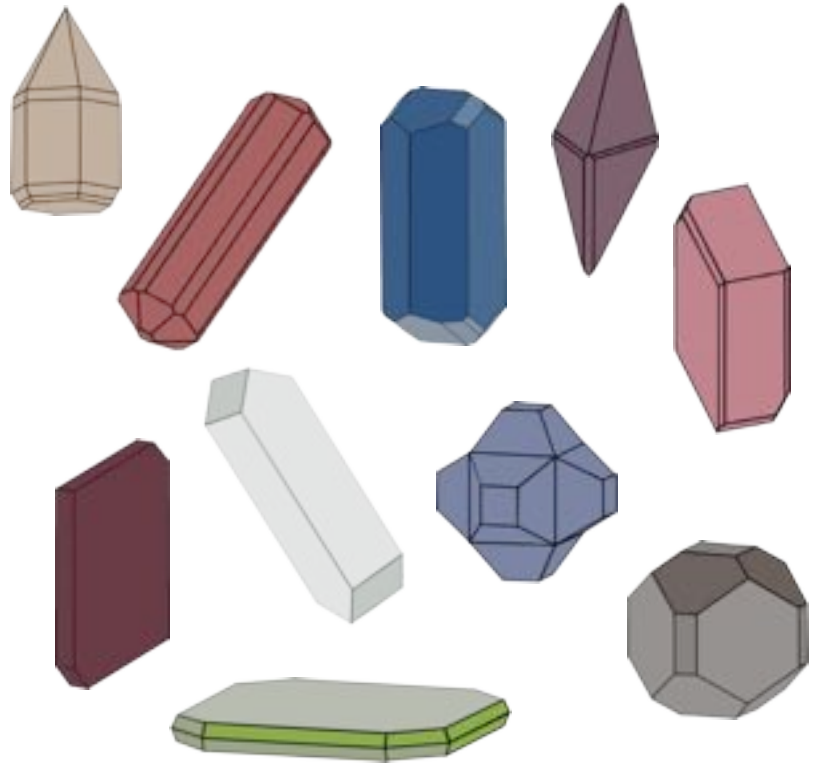
hexagonal

cubic

?

Rock Crystal (Quartz, SiO_2)

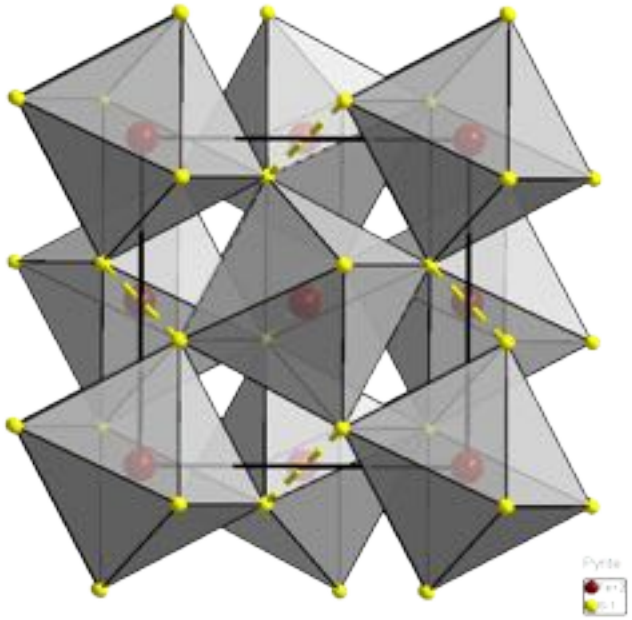
countless forms of appearance

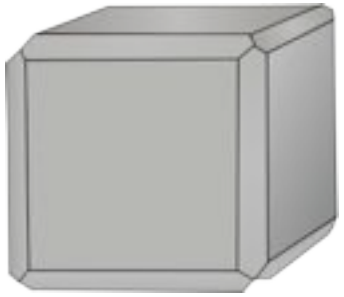


Source: Frank Hoffmann

Morphology of Pyrite

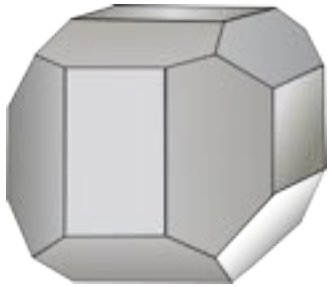
- FeS_2
- cubic crystal system
- space group *P*a3
- a = 5.14 Å
- FeS_6 octahedra
- S-SFe_3 tetrahedra



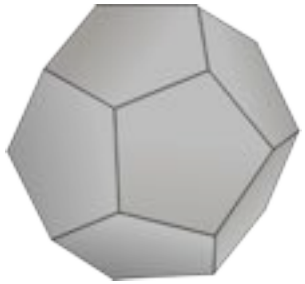


cube

octahedron



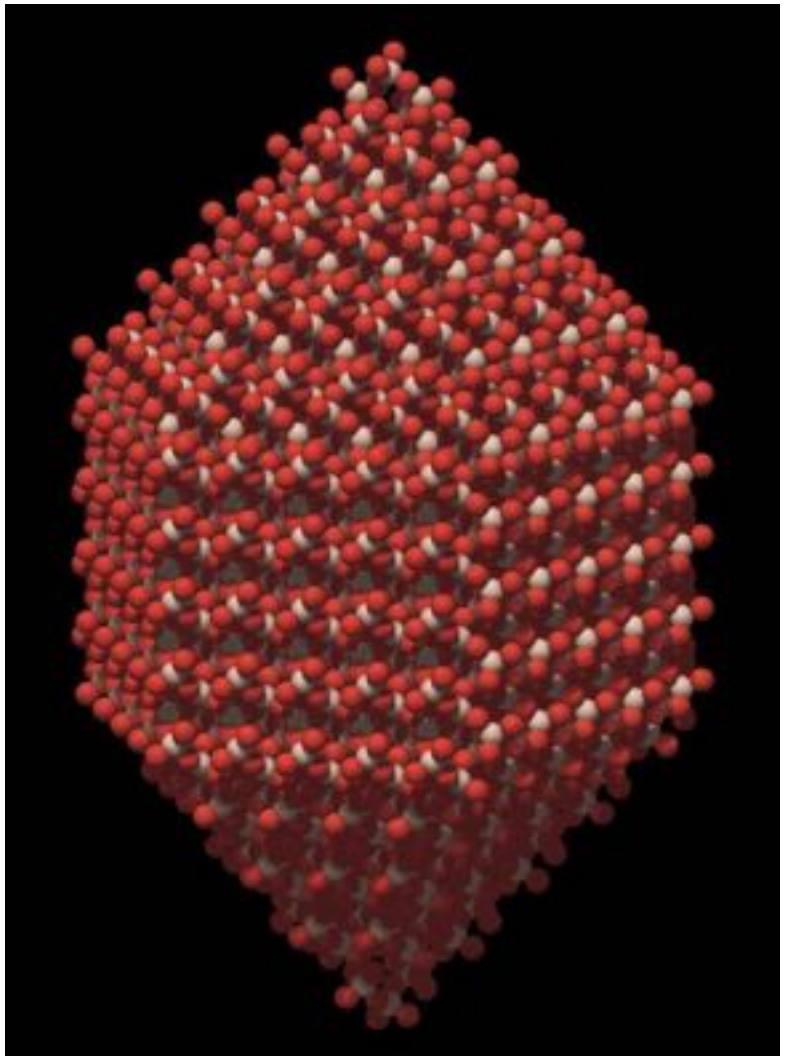
rhombic dodecahedron

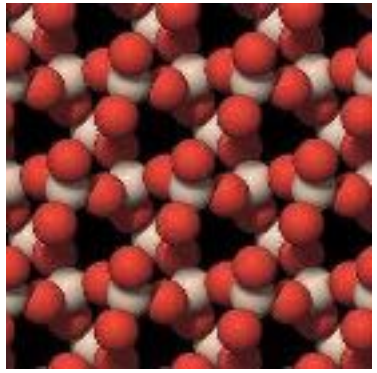


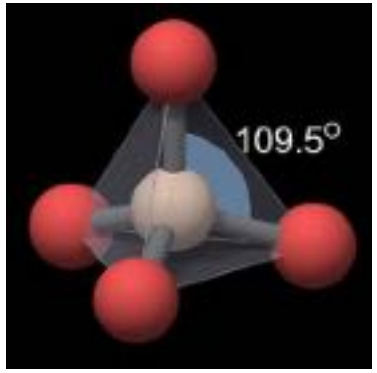
pentagon dodecahedron

Correspondence Principle

- Quartz (SiO_2)







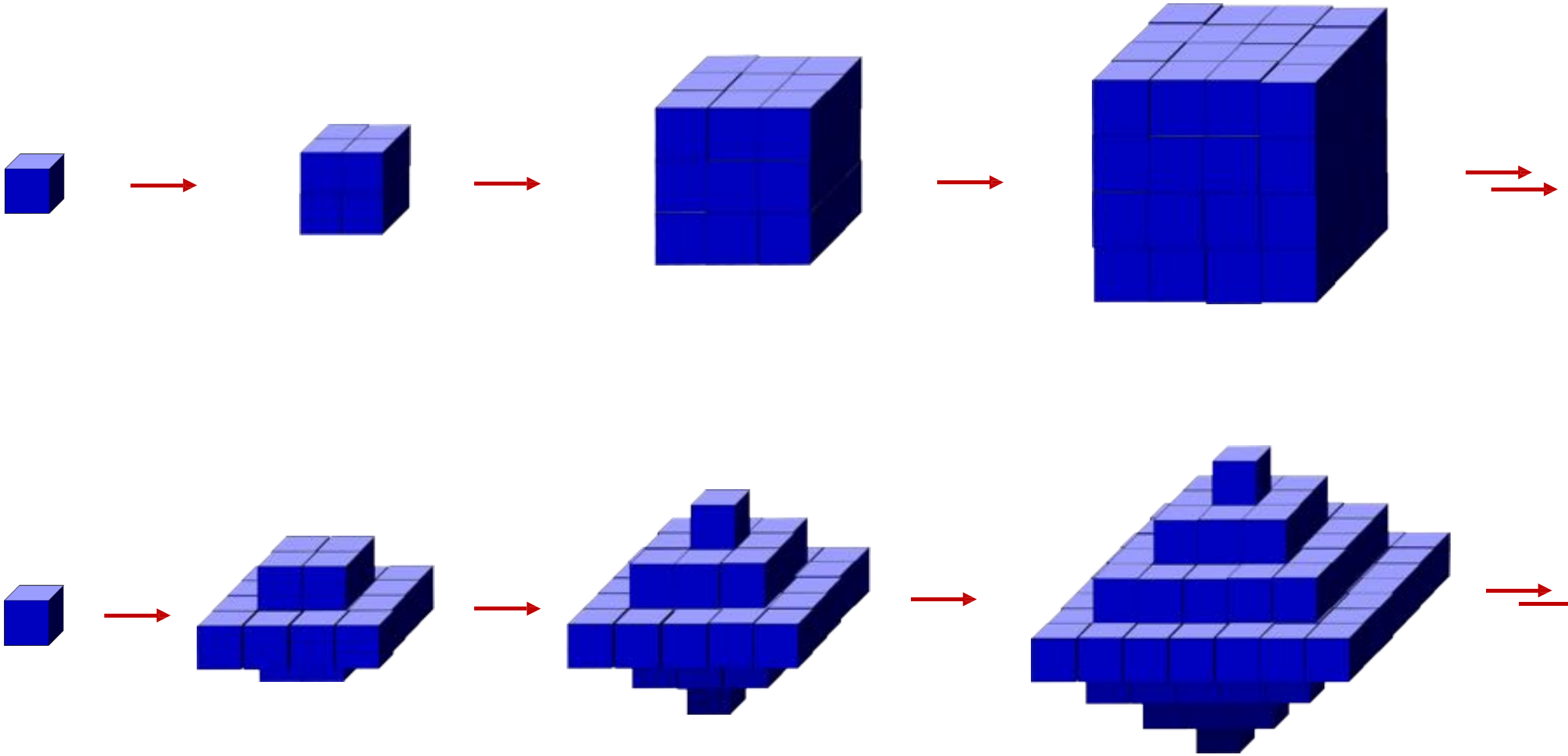
SiO_4 tetrahedra

macroscopically

?

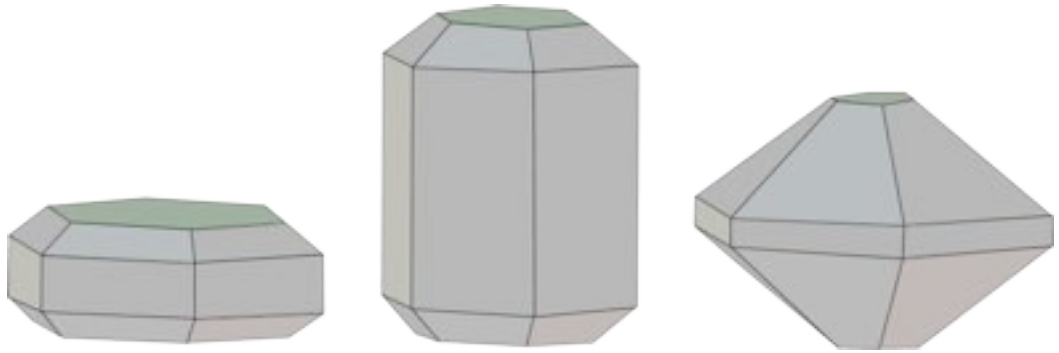
microscopically

Stacking Cubes – Face Development



Source: Frank Hoffmann

Facet and Habitus



same facet – different habitus

same habitus (isometric) – different facet

- the total set of faces developed on a crystal is called *Facet ('costume')*

  → number and composition of faces of the outer limiting planes of a crystal

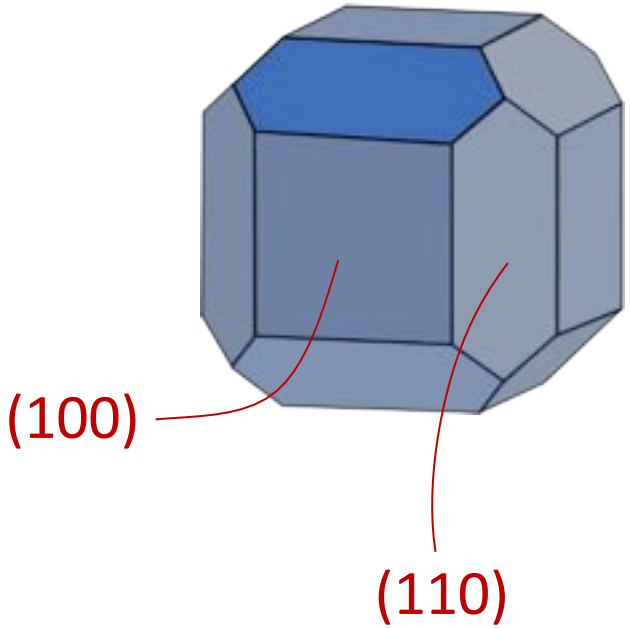
- the relative face development, i.e. their relative sizes gives rise to the *habitus*

- two crystals can have the same facet but different habitus, and they can have the same habitus but different trachts

- habitus: isometric, needle-like, plate-like, cubically, column…

Source: Frank Hoffmann

Miller Indices



combination of a hexahedron (cube)
and a rhombic dodecahedron

→ Miller indices are used to name the crystal faces in a systematic manner, and are also used to denominate lattice planes.

Source: Frank Hoffmann

Miller Indices

William Hallowes Miller

(1801 – 1880)

René Just Haüy

(1743 – 1822)

Source: Frank Hoffmann

Hauyenite

hauyne / hauynite

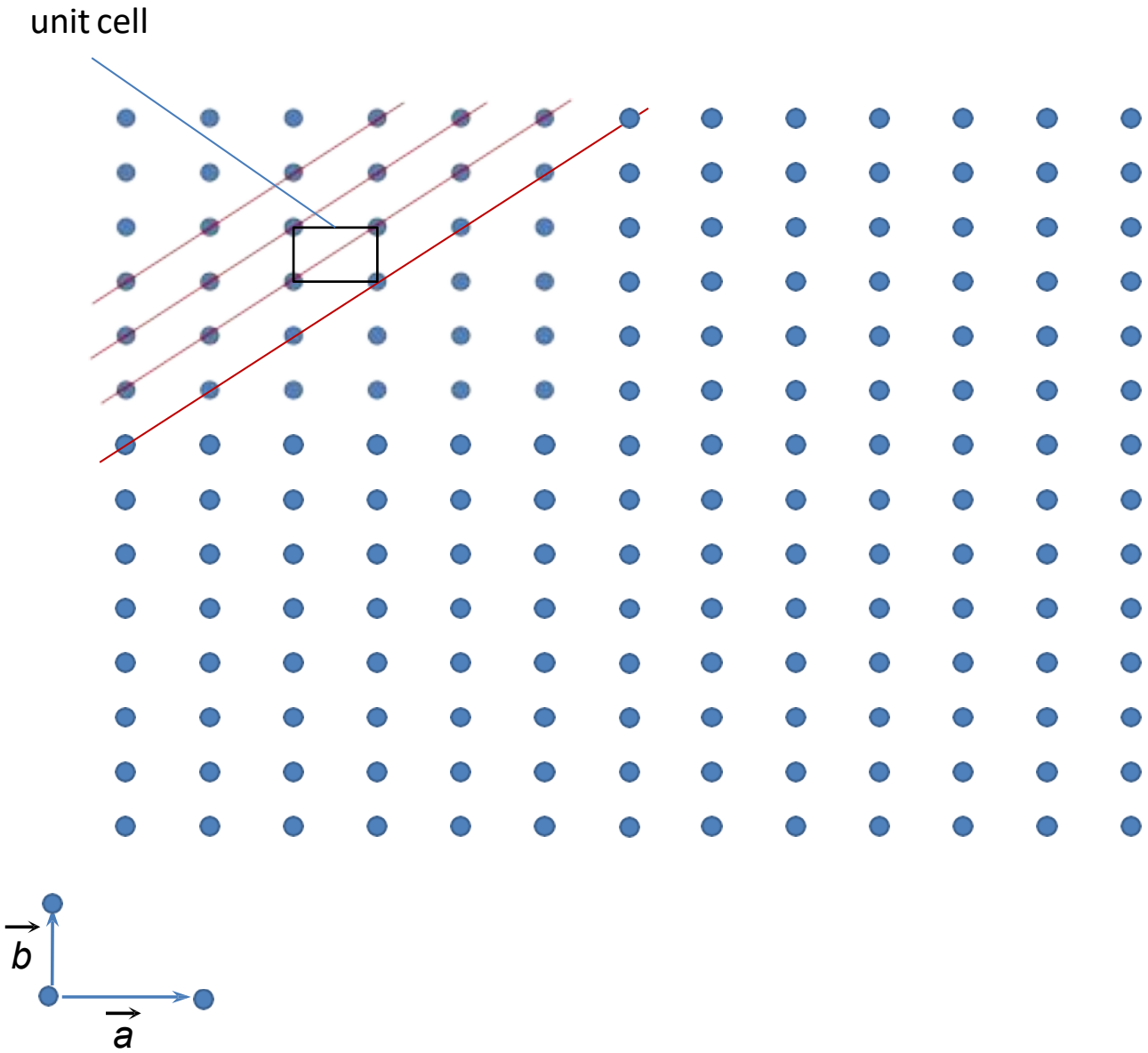
tecto(alumo)silicate

$Na_3Ca(Si_3Al_3)O_{12}(SO_4)$

René Just Haüy

(1743 – 1822)

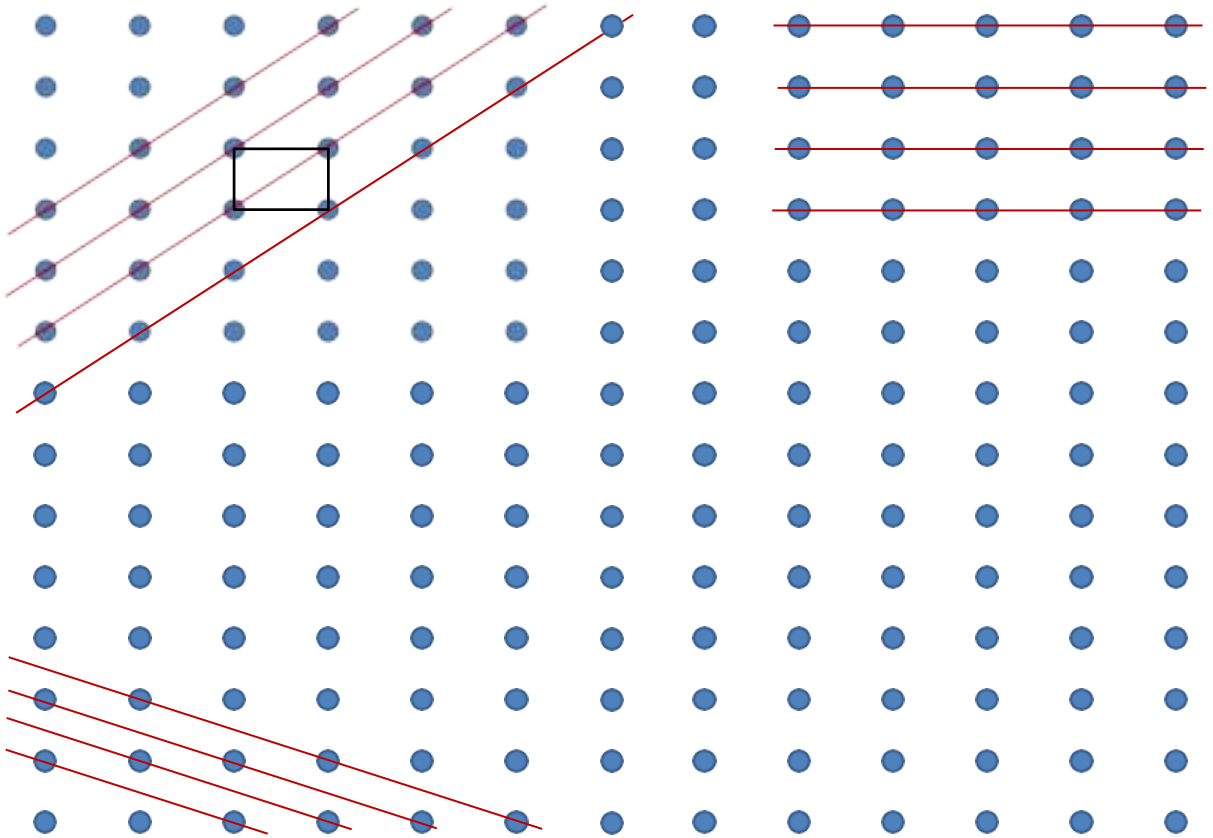
Lattice Planes

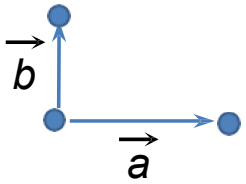


- lattice planes are a family of *parallel* planes which intersects the Bravais lattice and are *periodic*
- these crystallographic planes are *fictitious* planes linking nodes, i.e. lattice points

Source: Frank Hoffmann

Lattice Planes



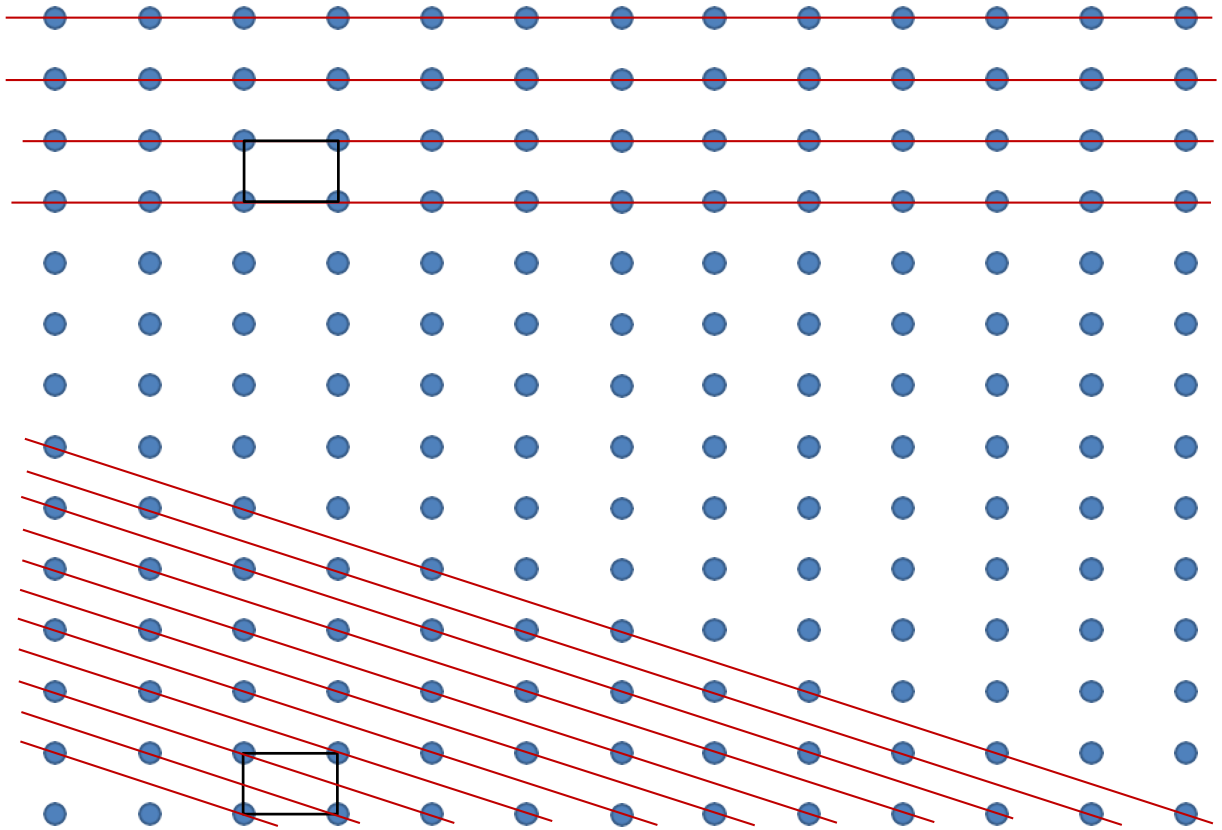


- lattice planes are a family of *parallel* planes which intersects the Bravais lattice and are *periodic*
- these crystallographic planes are *fictitious* planes linking nodes, i.e. lattice points
- in principle there is an infinite number of plane families (all parallel planes of a particular type)
- *Miller indices* form a notation system for such planes and are expressed by three integers: (h k l)

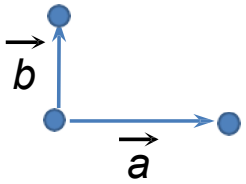
Source: Frank Hoffmann

Determining Miller Indices

(010)



(120)

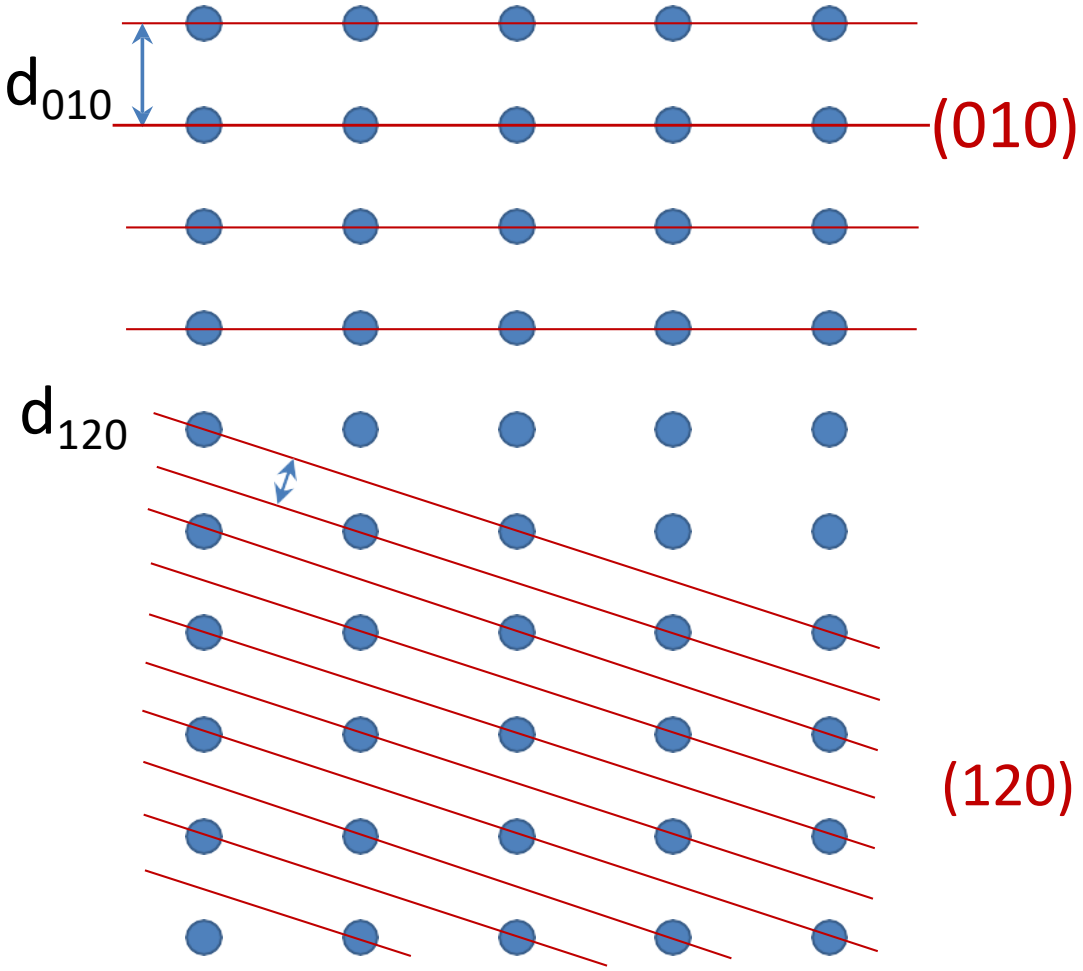


- In how many fractions do the planes intersect the respective lattice constants a, b, (and c)?

→ If one of the indices is zero, it means that the planes do not intersect that axis (the intercept is "at infinity")

Source: Frank Hoffmann

d - Spacings

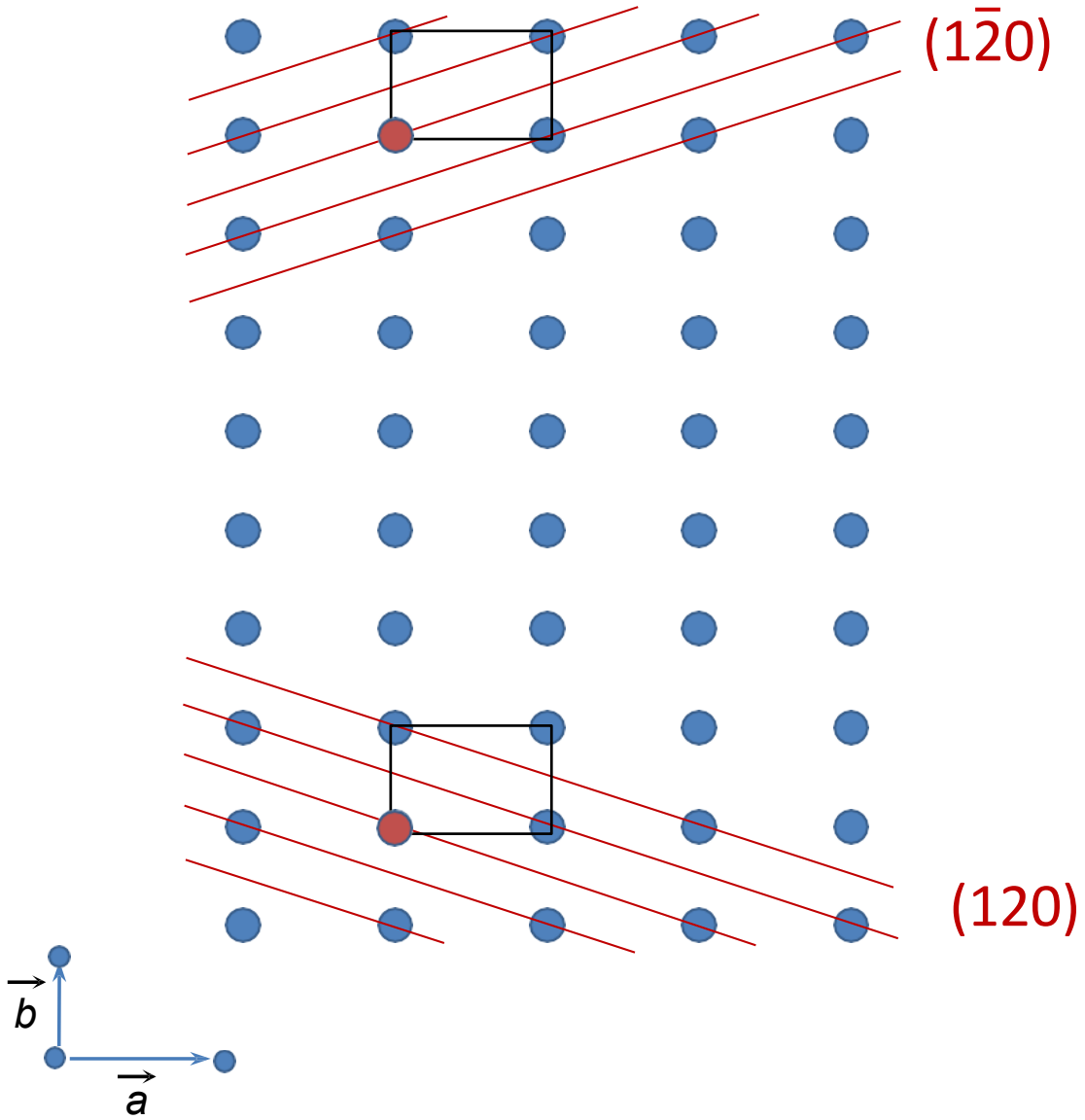


→ the lower the indices the higher the density of lattice points onto this plane

→ the lower the indices the larger the distance *d* between two adjacent planes of a plane family

Source: Frank Hoffmann

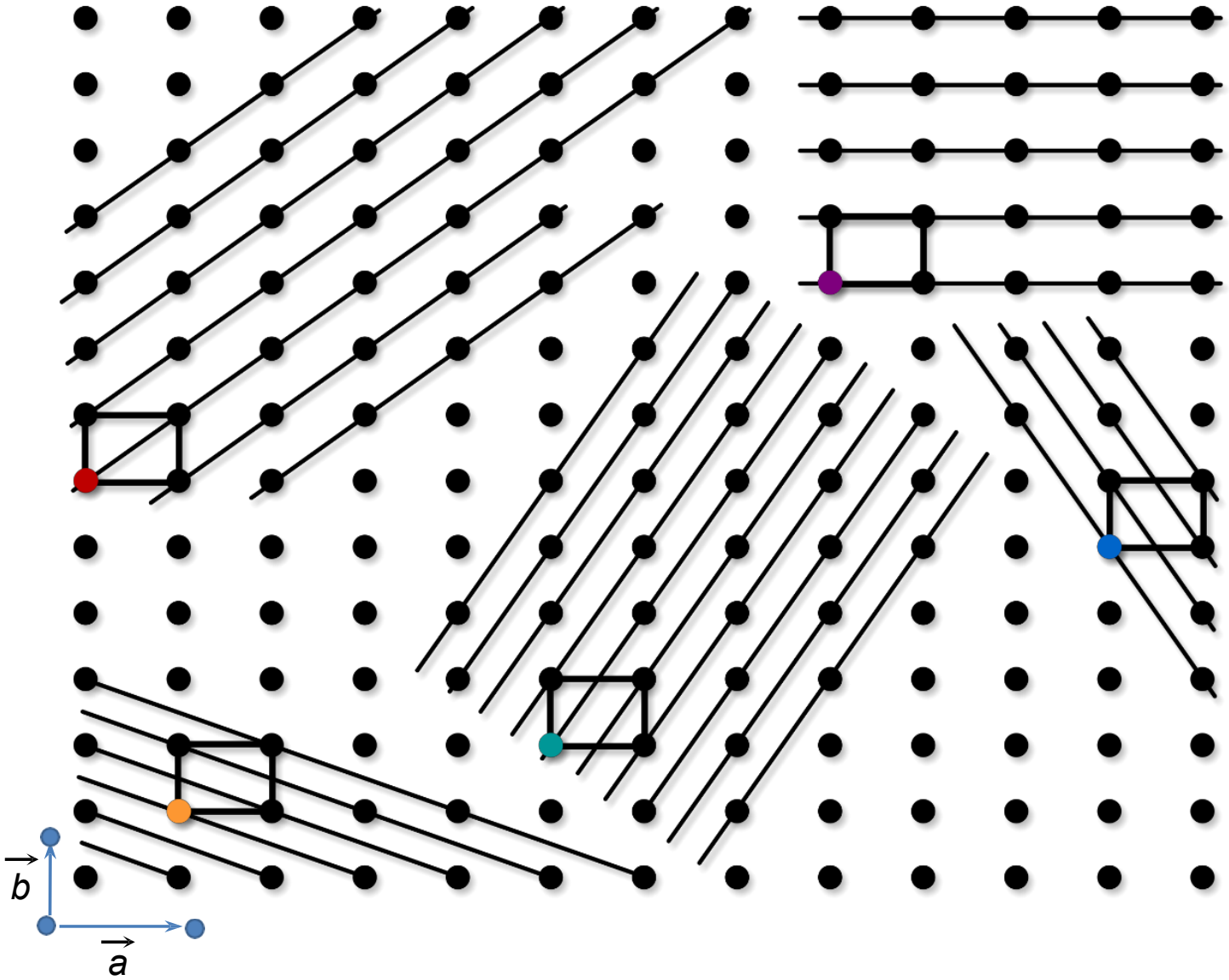
Negative Miller Indices



- if the intercepts are on the negative side of the coordinate system the indices get a bar above the number (= minus)

Source: Frank Hoffmann

Exercise - Miller Indices



A: ?

B: ?

C: ?

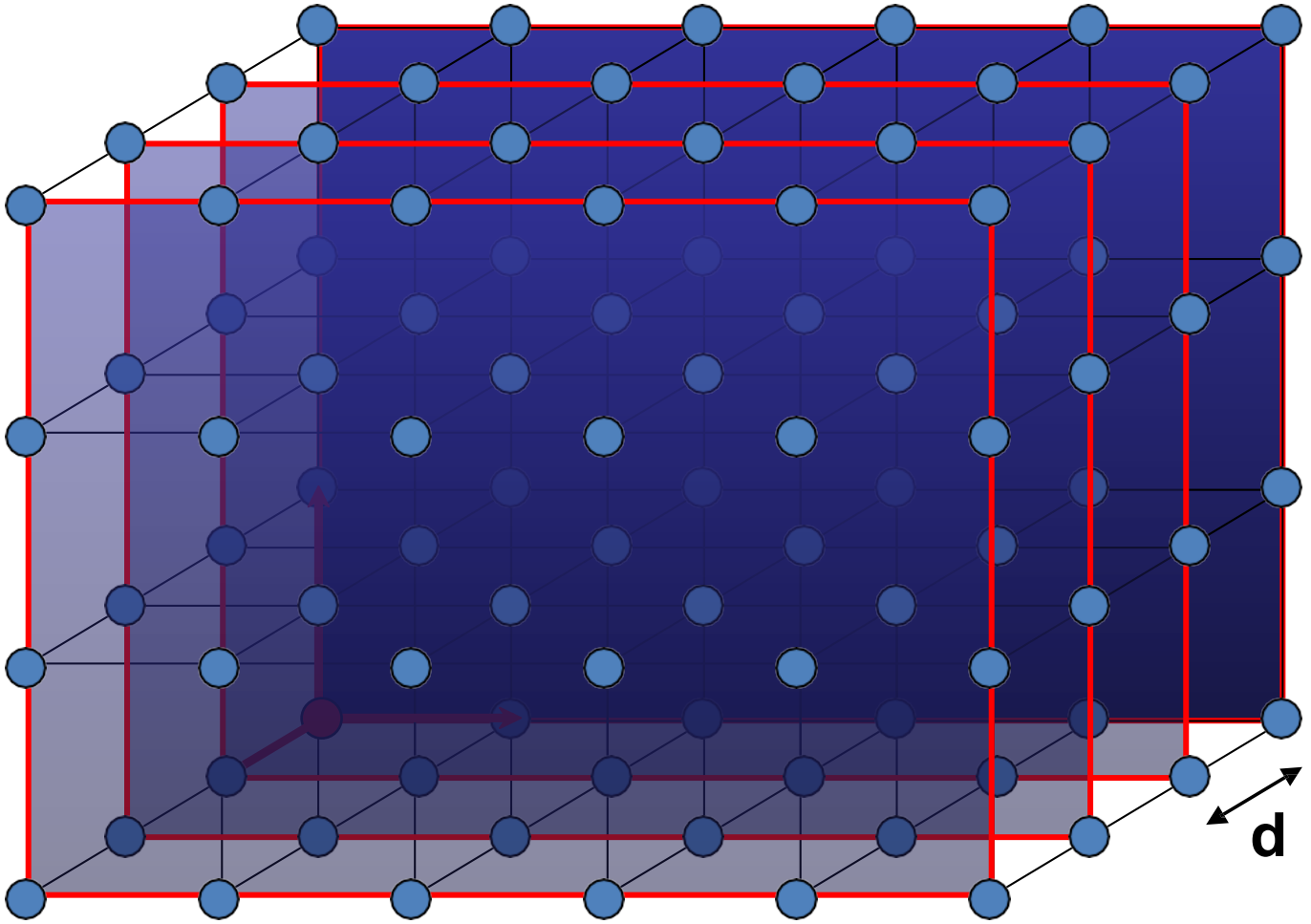
D: ?

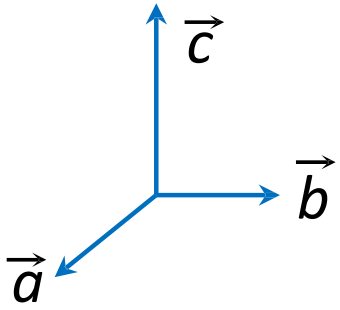
E: ?

Source: Frank Hoffmann

Miller Indices in 3D

(1 0 0)

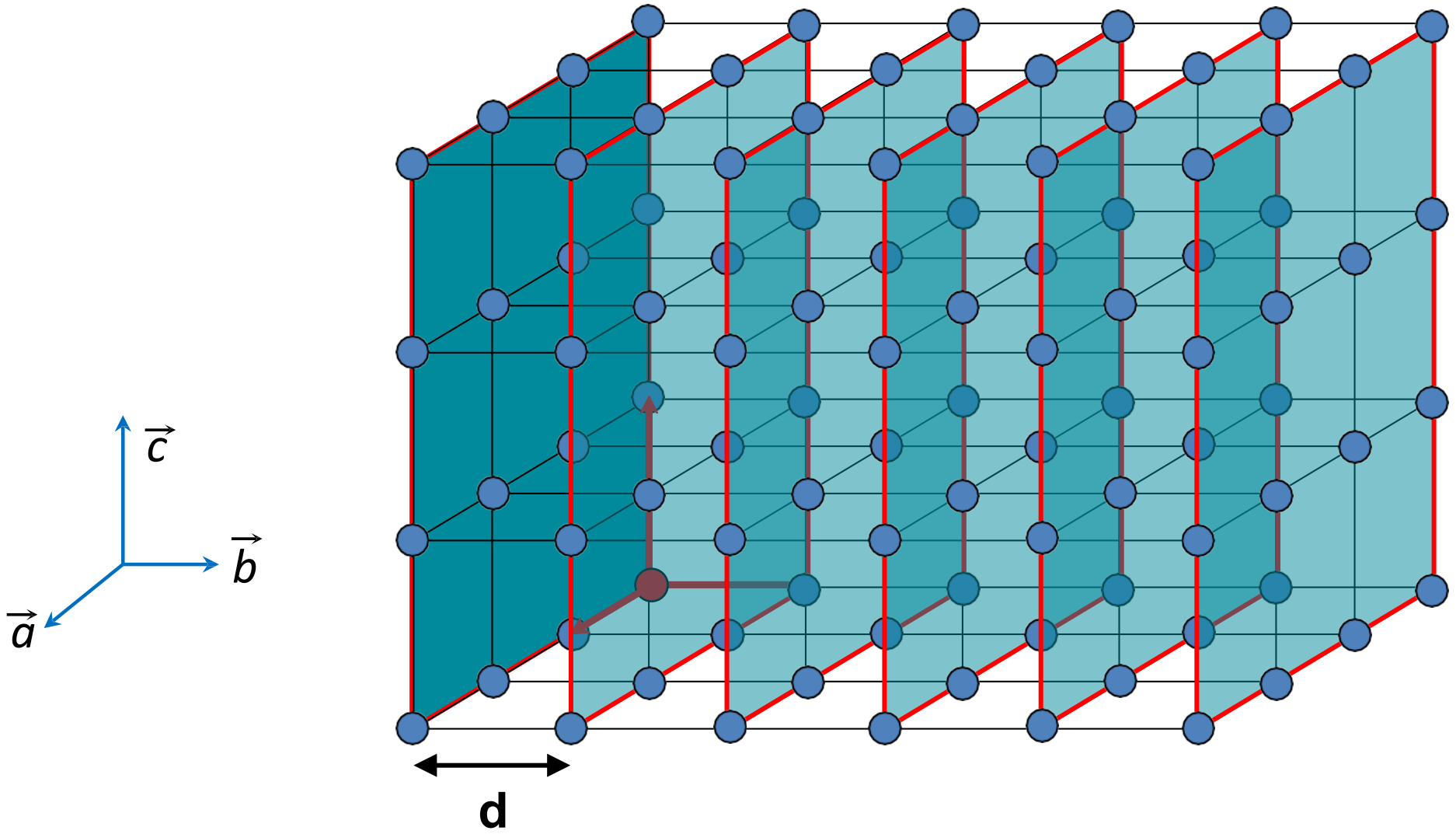




Source: Frank Hoffmann

Miller Indices in 3D

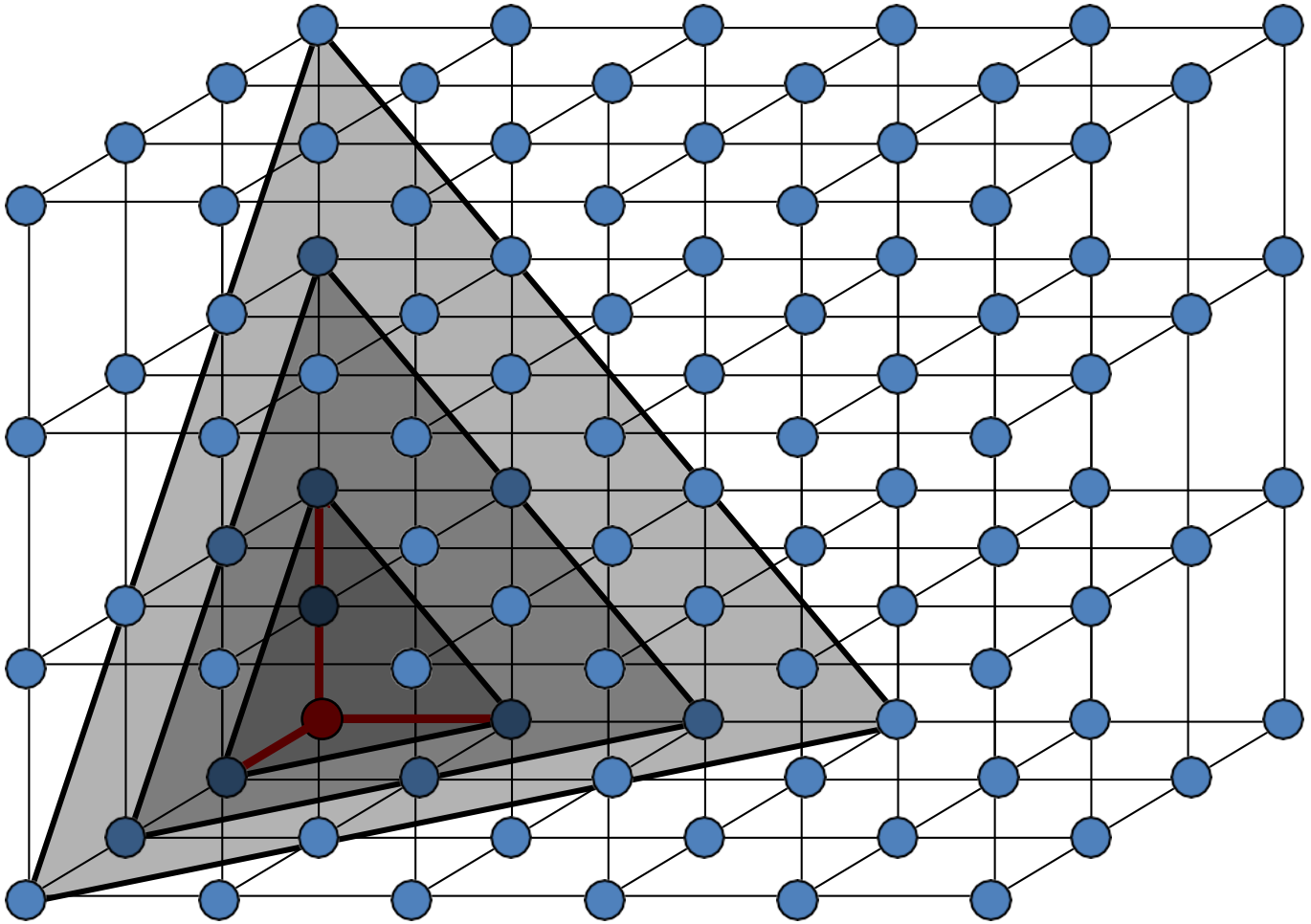
(0 1 0)

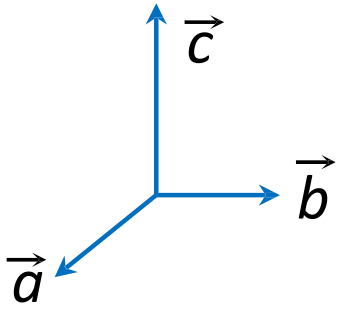


Source: Frank Hoffmann

Miller Indices in 3D

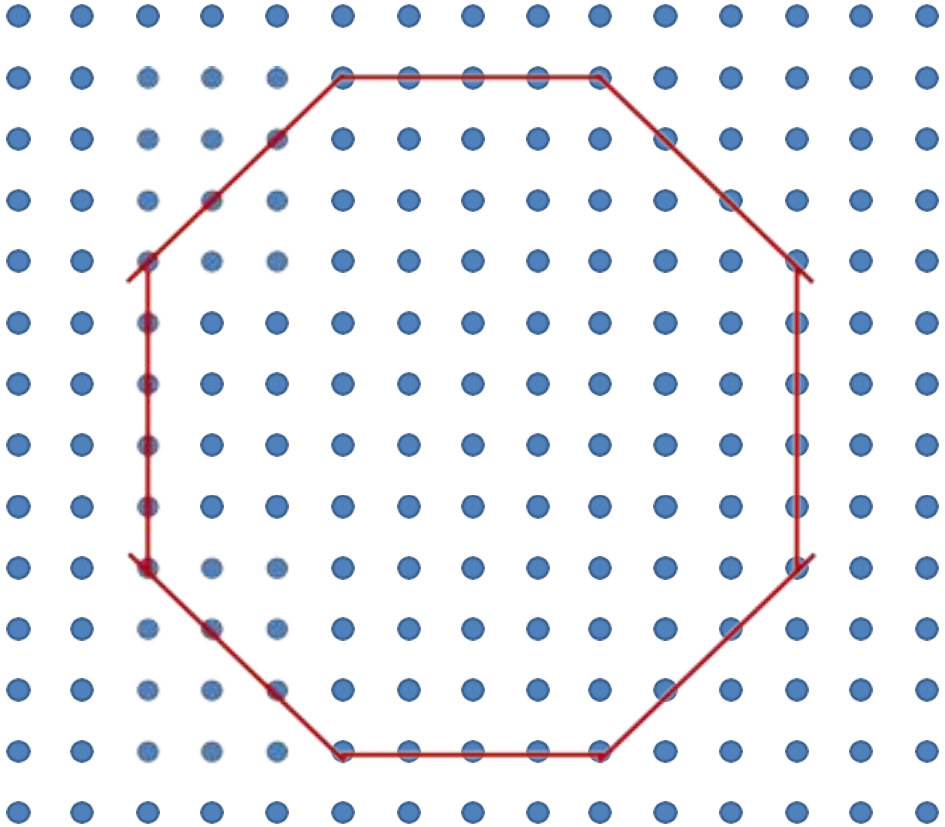
(1 1 1)

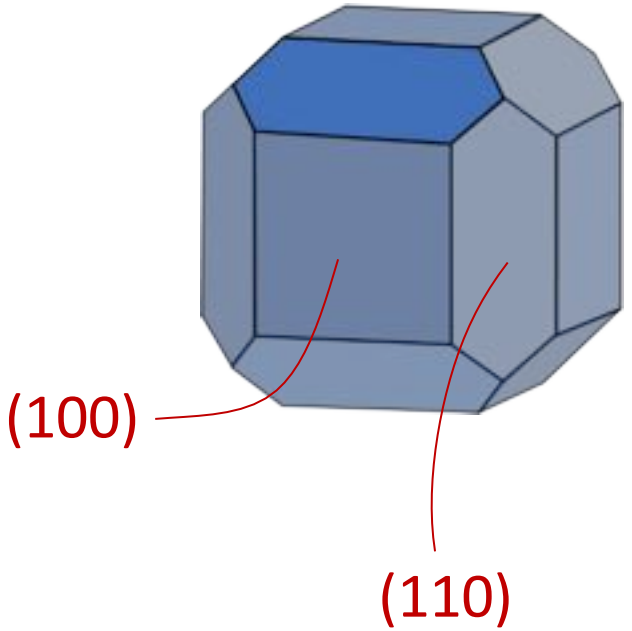




Source: Frank Hoffmann

Miller Indices of Faces



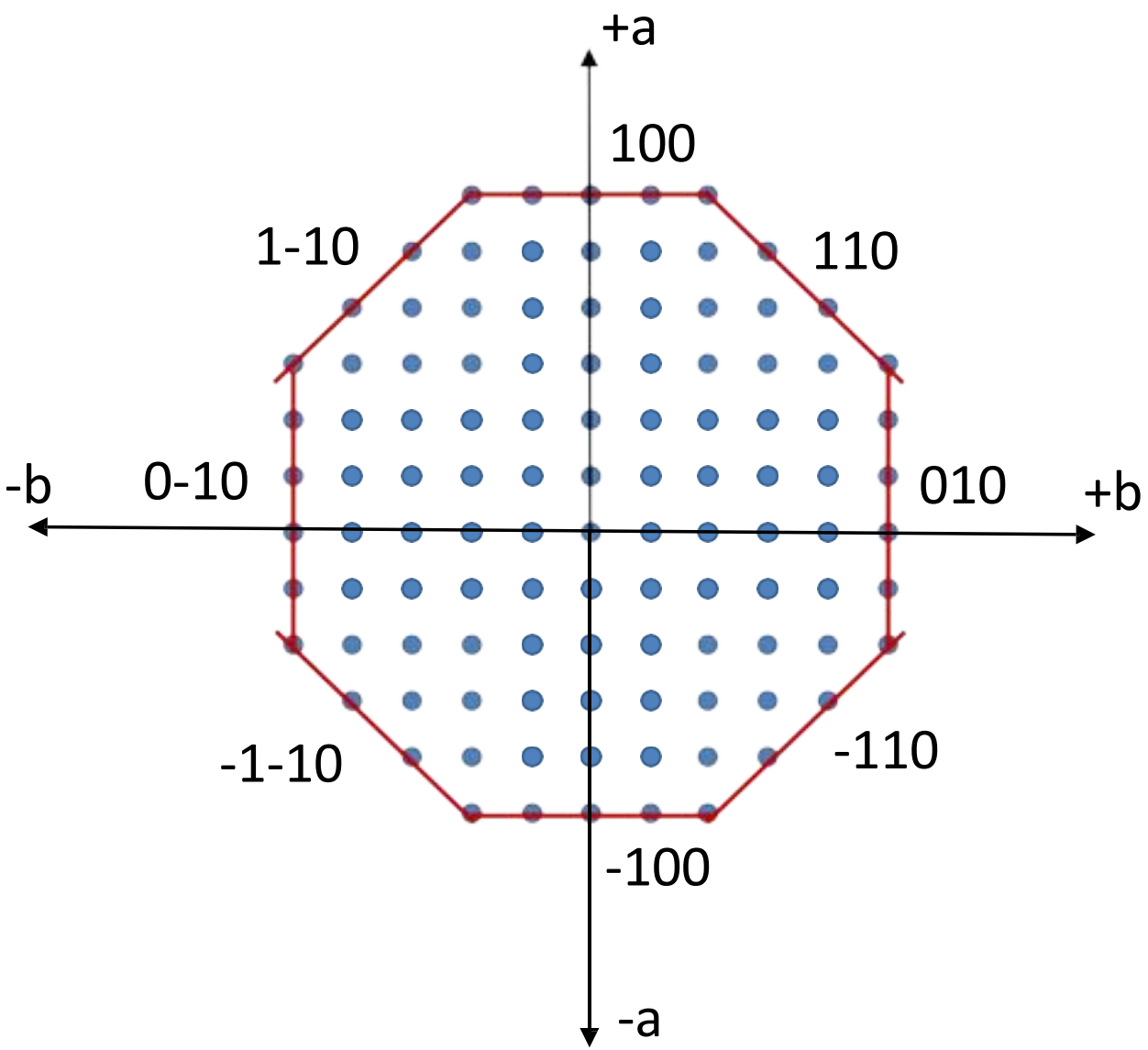


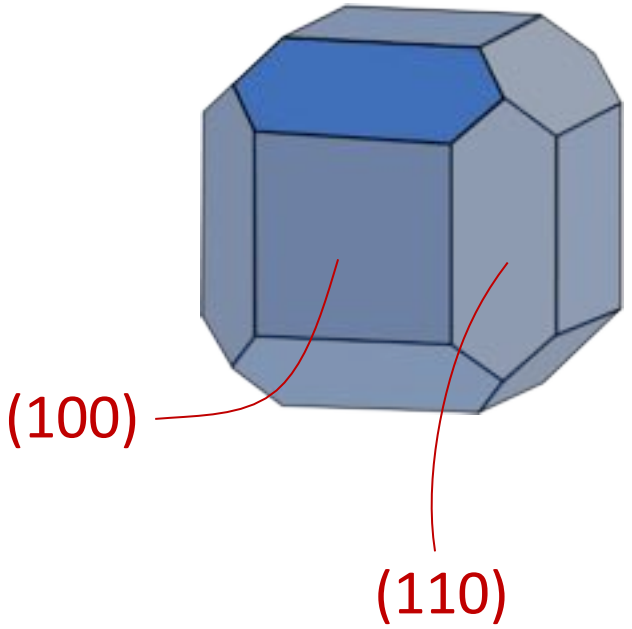
combination of a hexahedron (cube) and
a rhombic dodecahedron

→ the outermost planes of a crystal build the faces!

Source: Frank Hoffmann

Miller Indices of Faces



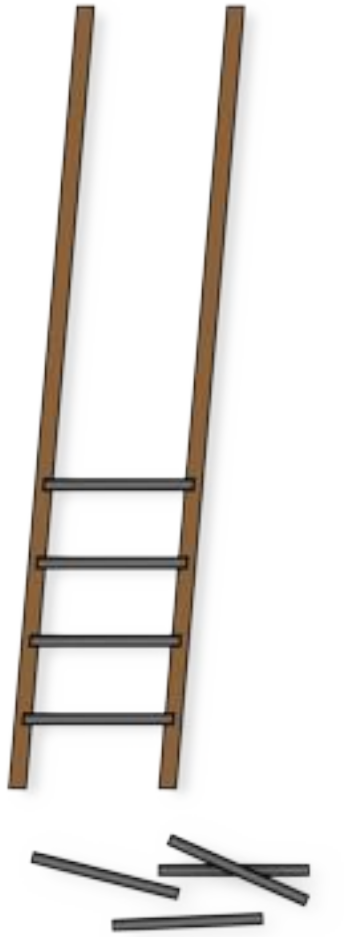


combination of a hexahedron (cube) and a rhombic dodecahedron

→ the outermost planes of a crystal build the faces!

Source: Frank Hoffmann

Systematization of Crystal Structures



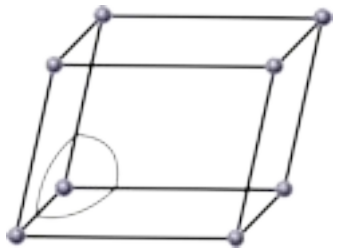
2. Step: Bravais lattices
primitive + centered

14

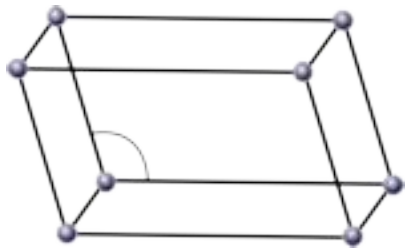
1. Step: Crystal Systems
metric + symmetry of the UC

7

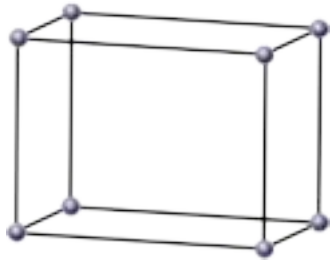
7 Primitive Lattices



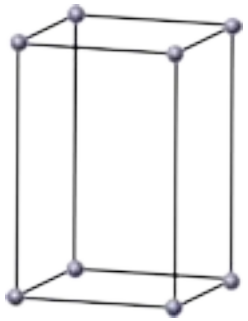
triclinic



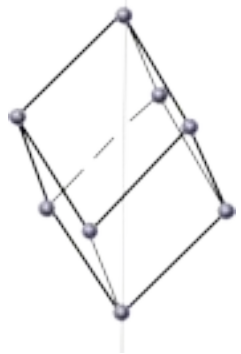
monoclinic



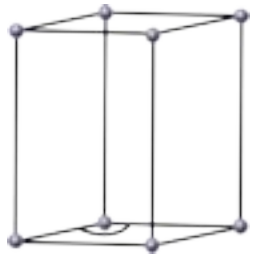
ortho-rhombic



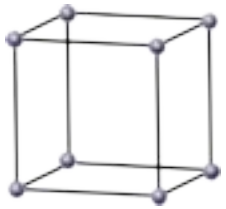
tetragonal



trigonal



trigonal/ hexagonal



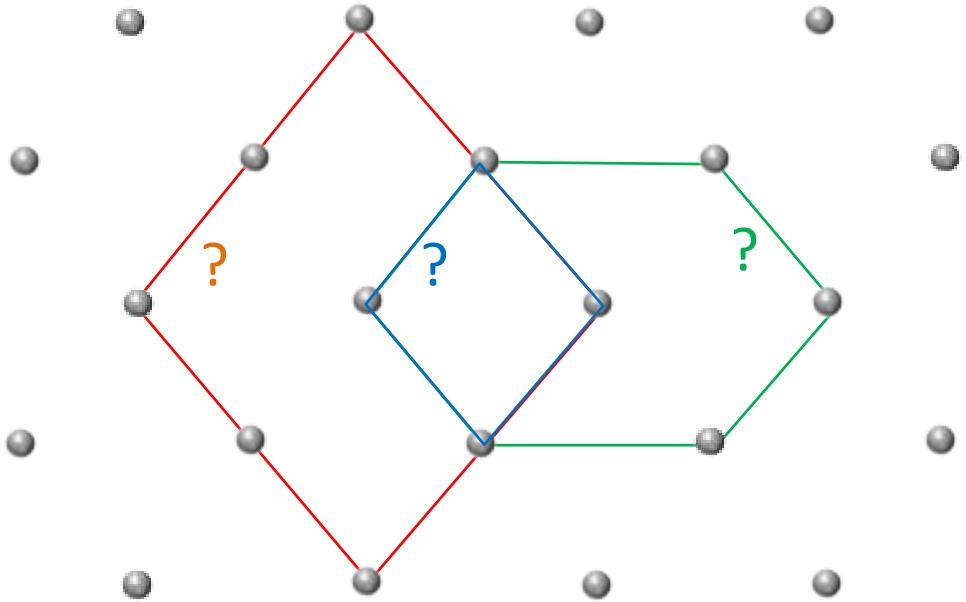
cubic

- primitive = simple
- there are lattice points only at every corner of the unit cell, but not inside the cell or at the faces or edges
- a primitive unit cell comprises exactly 1 motif (1/8 * 8 = 1)
- the primitive unit cell is the *smallest* possible unit cell
- it is always possible to find such a primitive unit cell

Source: Frank Hoffmann

Choice of the Unit Cell

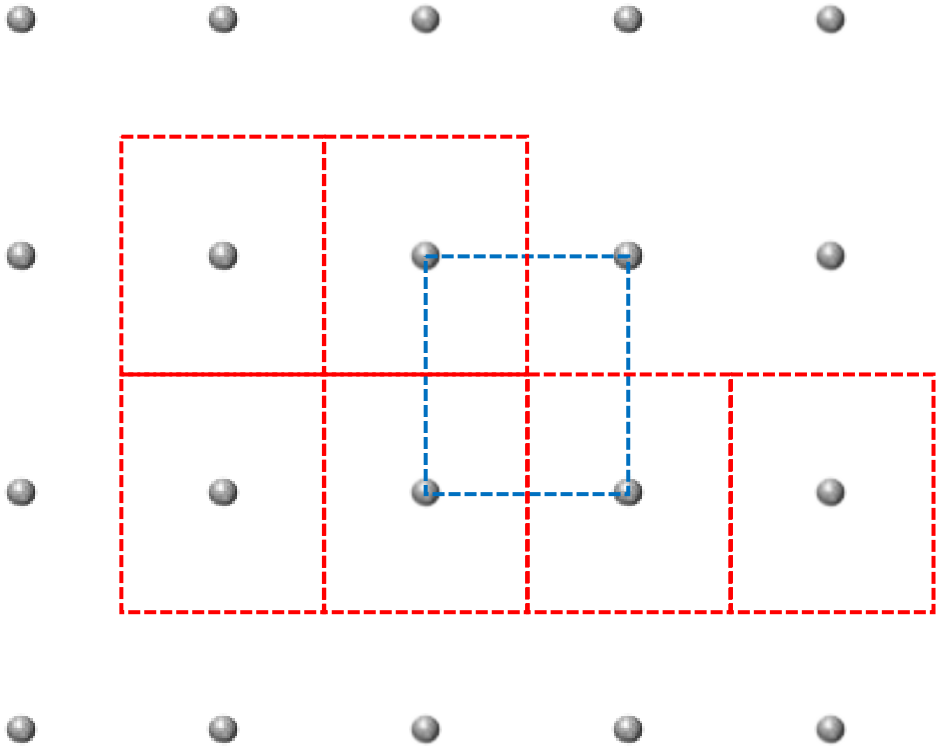
Is the smallest possible unit cell always the best cell?



→ centering of cells / 14 Bravais lattices

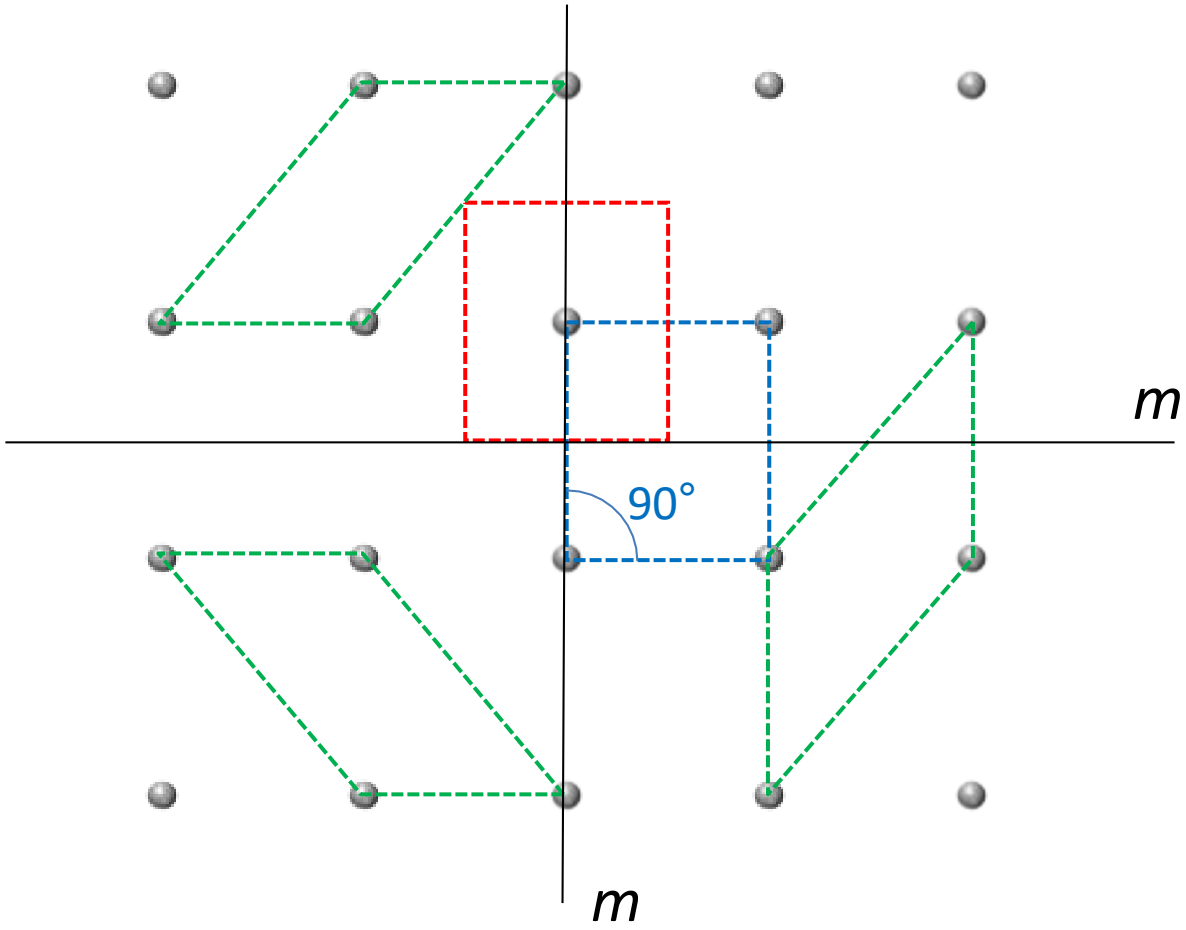
Source: Frank Hoffmann

Choice of the Unit Cell



Source: Frank Hoffmann

Choice of the Unit Cell

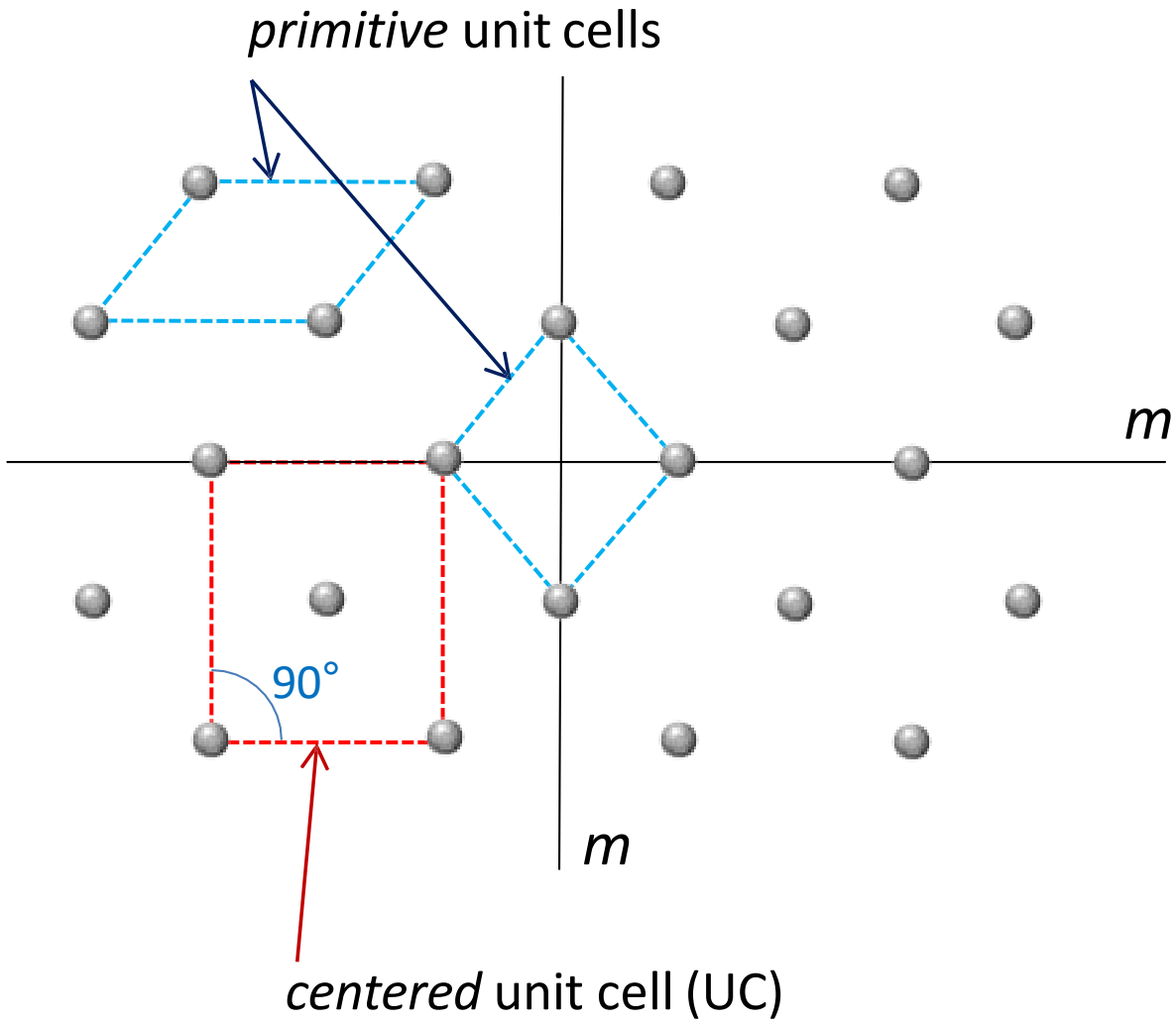


5 *possible* primitive unit cells,
all with the same 'volume'

- The unit cell should be as small as possible; short lattice vectors!
- At the same time it should represent the symmetry of the crystal; this means that the lattice vectors should run parallel to symmetry axes or perpendicular to symmetry planes.
- **The axes should be**, if possible, orthogonal **(or hexagonal)**!

Source: Frank Hoffmann

Choice of the Unit Cell

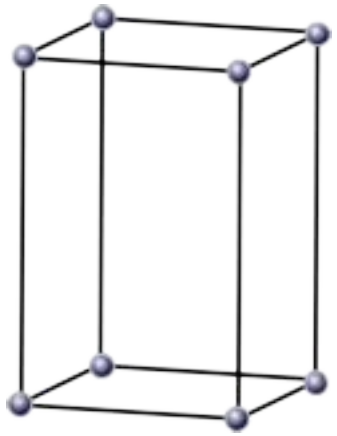


- Due to symmetry reasons it is sometimes advantageous to choose not the smallest possible unit cell!
- *Centered* cells contain additional lattice points.
- The purpose is to describe the crystal in a *higher symmetric system of coordinates*!
- But note: The crystal system does not change!
- The centered unit cell possess the *same symmetry* as the primitive one, but the symmetry becomes more evident!

Source: Frank Hoffmann

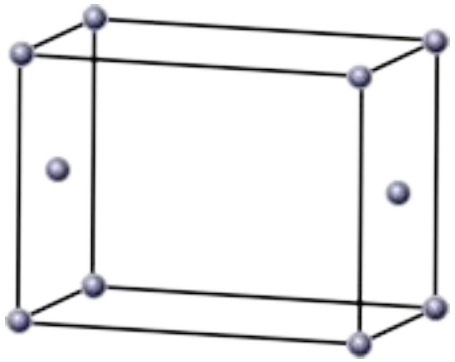
Centered Cells

- If lattice points are only at the corners of the unit cell, it is a primitive lattice; there are 7 different primitive lattices.
- Addition of further lattice points – under retention of the symmetry – give rise to 7 more lattices, 7 centered lattices. This leads to the 14 Bravais lattices.



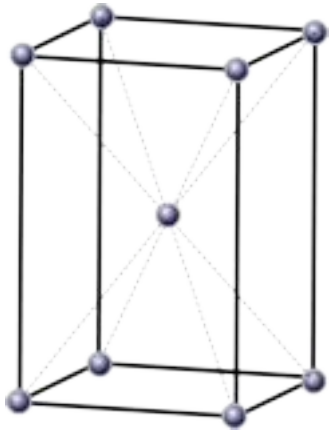
primitive unit cell

P



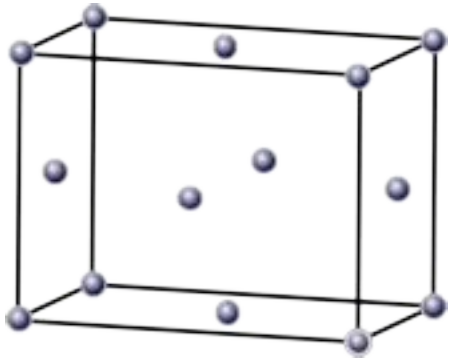
single-side face-centered unit cell

C(AB)



body-centered unit cell

I



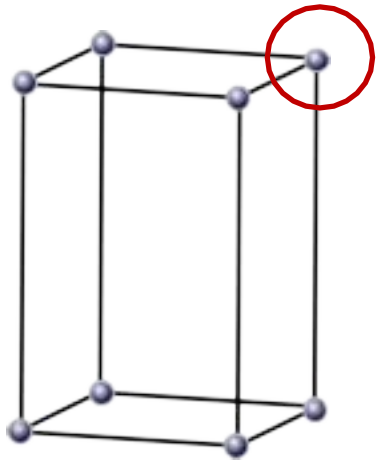
all-side face-centered unit cell

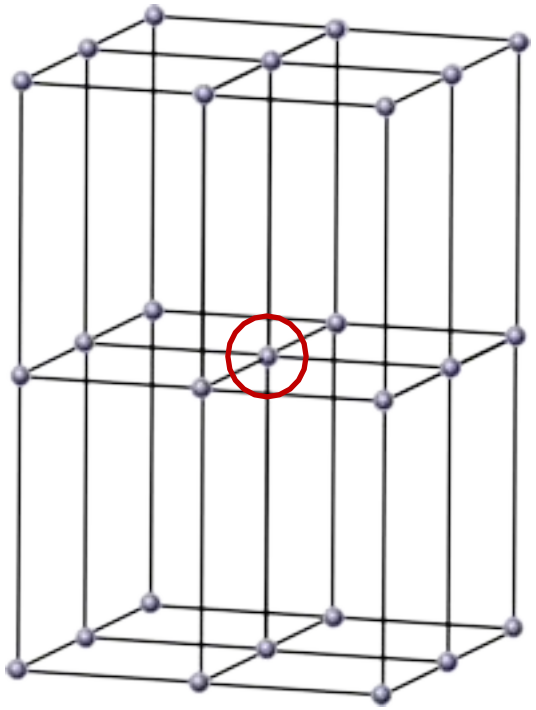
F

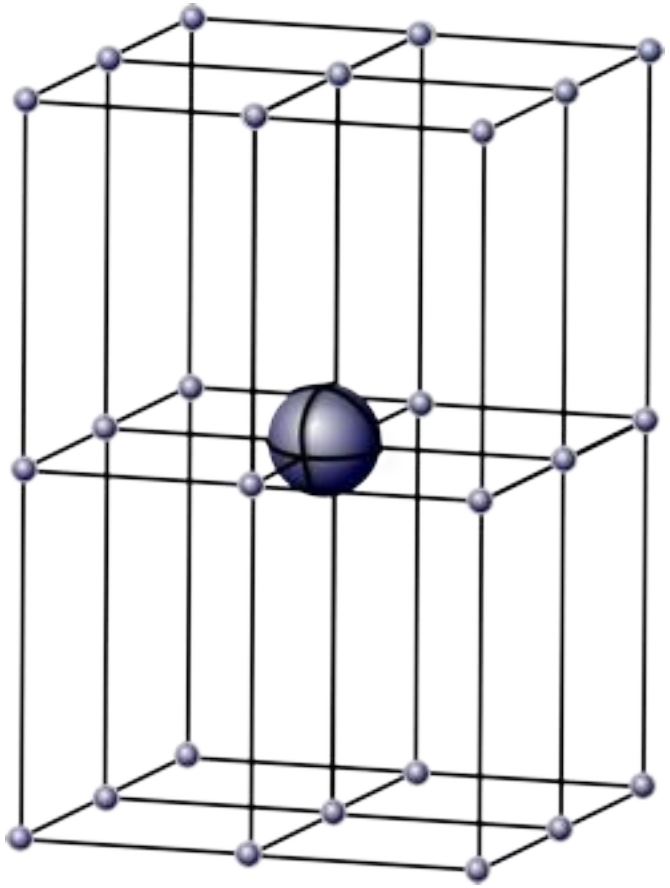
Source: Frank Hoffmann

Centered Cells – Formula Units

P





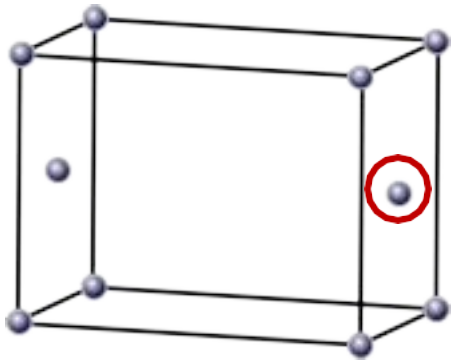


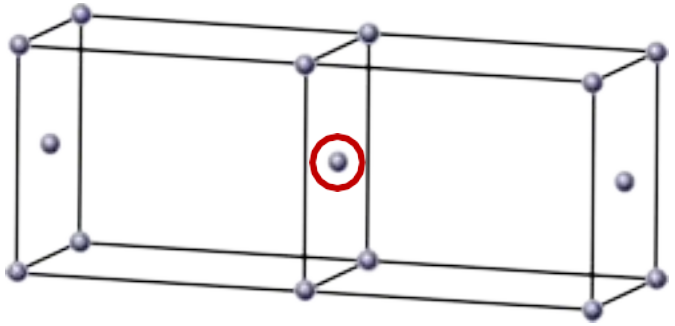
8 corners x 1/8 = 1 lattice point/unit cell

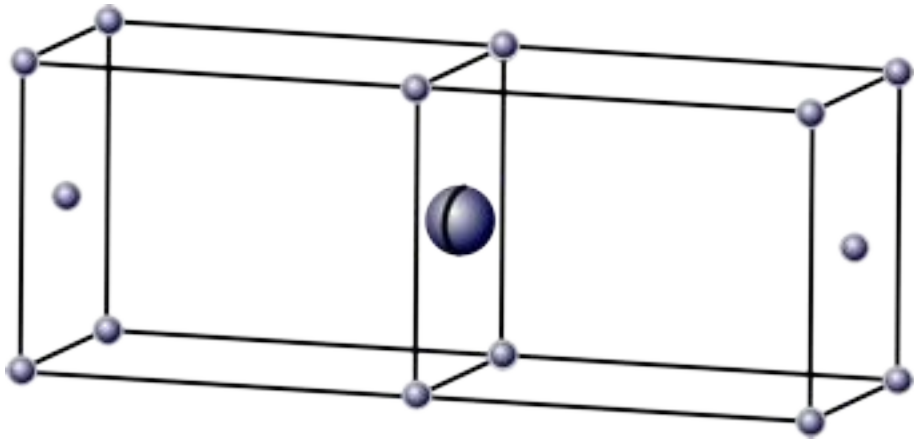
Source: Frank Hoffmann

Centered Cells – Formula Units

C(AB)





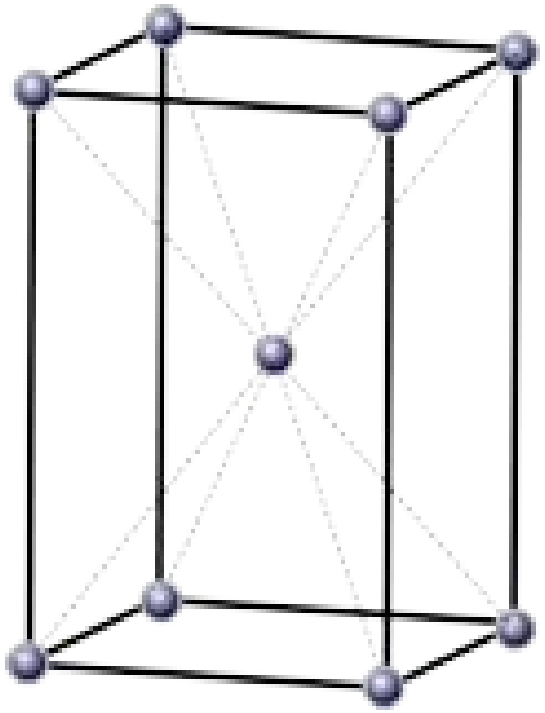


(8 corners x 1/8) + (2 faces x 1/2) = 2 lattice points/unit cell

Source: Frank Hoffmann

Centered Cells – Formula Units

I

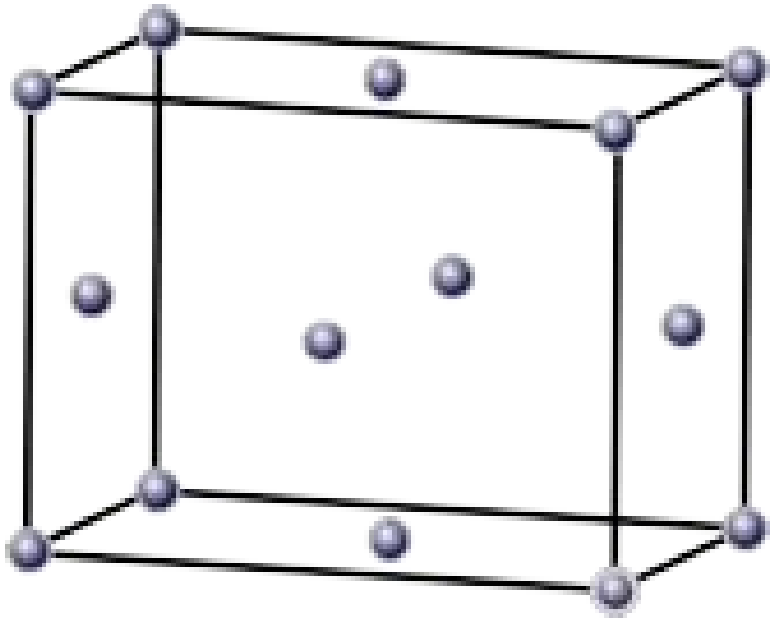


(8 corners x 1/8) + (1 inside) = 2 lattice points/unit cell

Source: Frank Hoffmann

Centered Cells – Formula Units

F

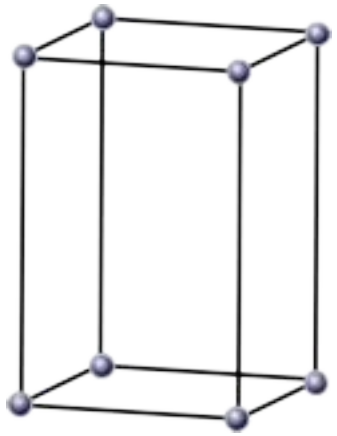


(8 corners x 1/8) + (6 faces x 1/2) = 4 lattice points/unit cell

Source: Frank Hoffmann

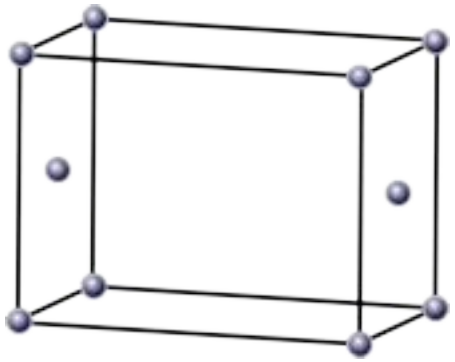
Centered Cells

- If lattice points are only at the corners of the unit cell, it is a primitive lattice; there are 7 different primitive lattices.
- Addition of further lattice points – under retention of the symmetry – give rise to 7 more lattices, 7 centered lattices. This leads to the 14 Bravais lattices.



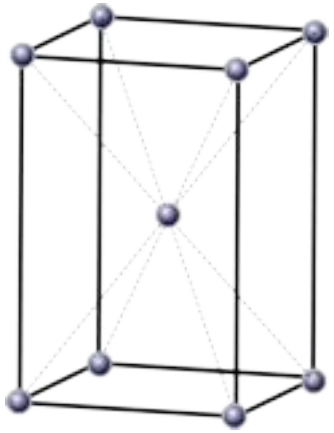
primitive unit cell

P



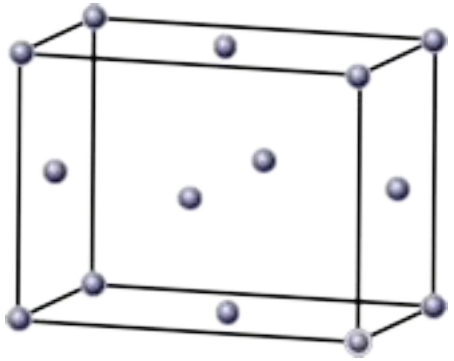
single-side face-centered unit cell

C(AB)



body-centered unit cell

I



all-side face-centered unit cell

F

Source: Frank Hoffmann

14 Bravais Lattices

Bravais lattices

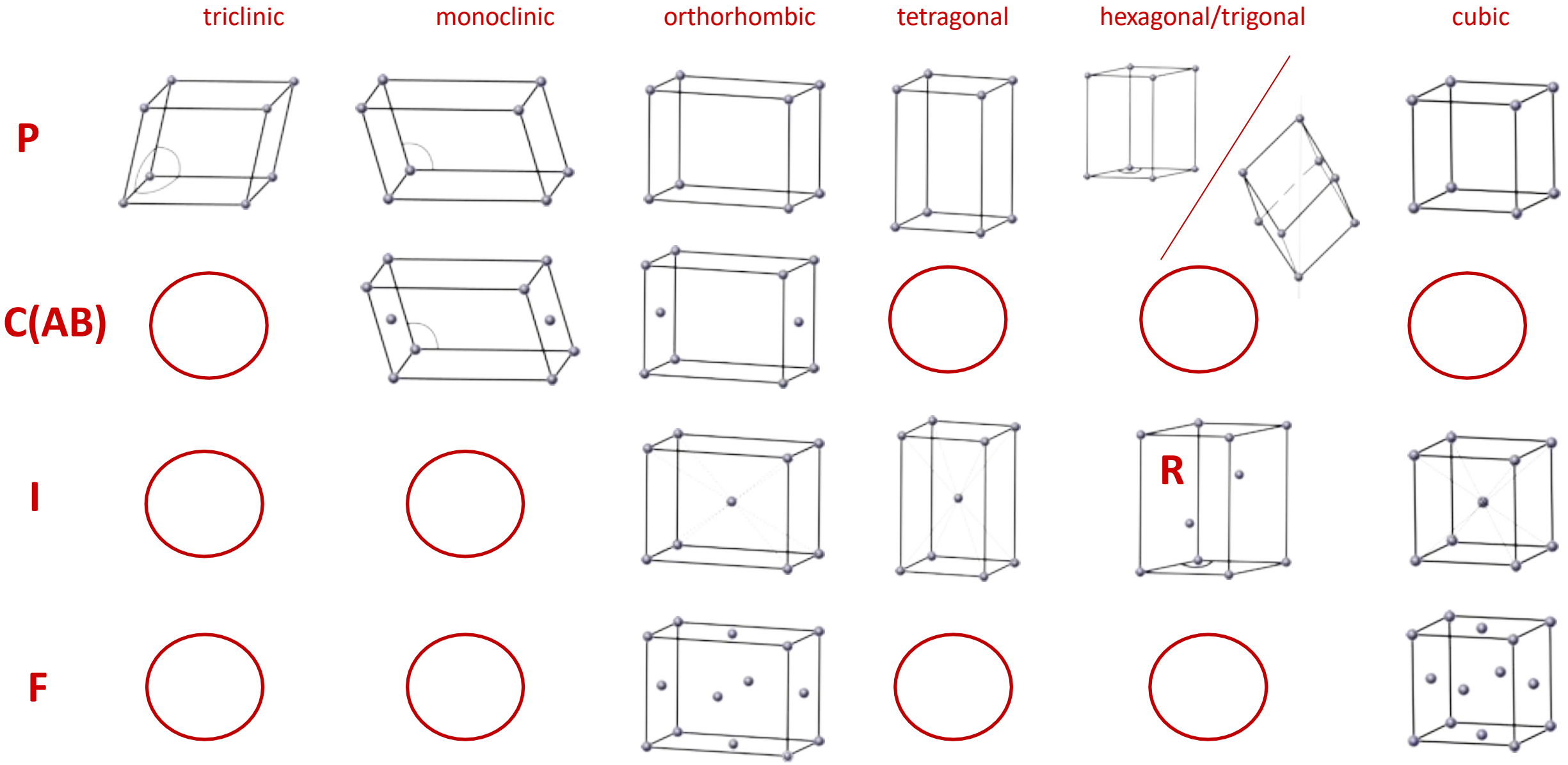
crystal systems

$7 \times 4 = 14$ (?)

kind of centerings

Source: Frank Hoffmann

14 Bravais Lattices



14 Bravais Lattices

Auguste Bravais

* 23th August 1811 in Annonay, Frankreich
† 30th March 1863 in Le Chesnay
French physicist, crystallographer, universal scholar

in 1848 he could show that there are only
14 unique different lattice types in 3D space

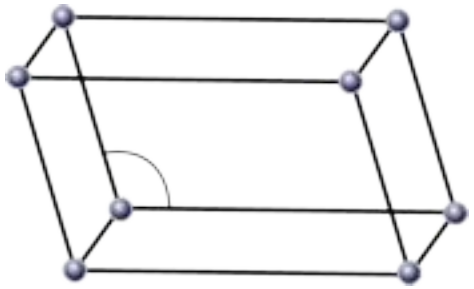
→ some of the 28 conceivable lattice types are redundant

→ some of them are not possible due to symmetry reasons

Source: Frank Hoffmann

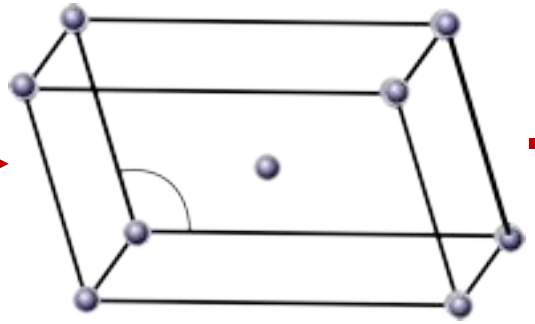
14 Bravais Lattices - Redundancy

monoclinic



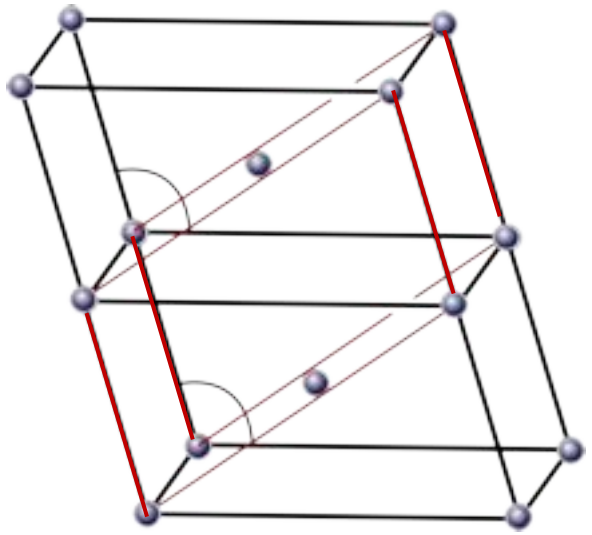
P

?



I

!

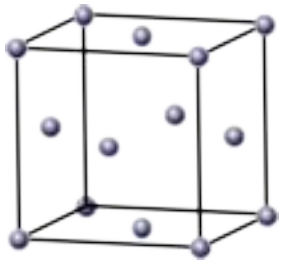


monoclinic **C**

Source: Frank Hoffmann

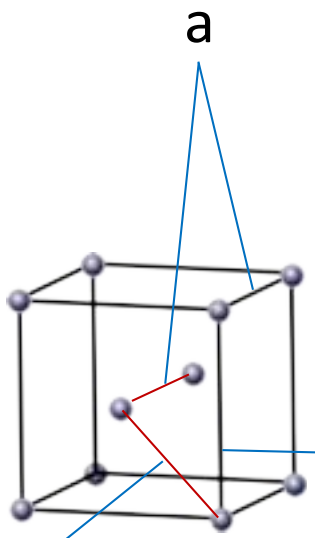
14 Bravais Lattices – Incompatible Symmetry

cubic



F

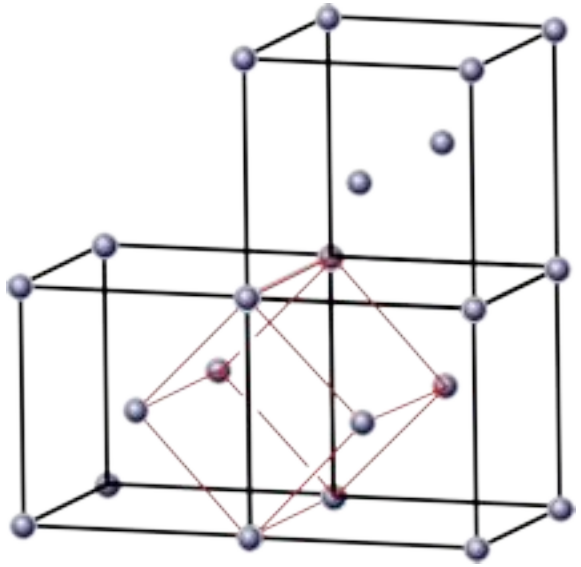
?



C

a? $\longrightarrow$ $\frac{\sqrt{2}}{2}$ a!

!

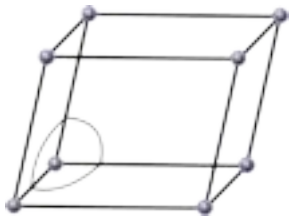


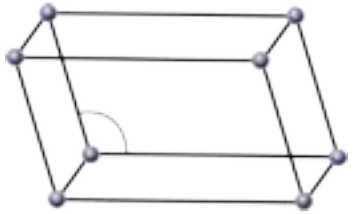
tetragonal **P**

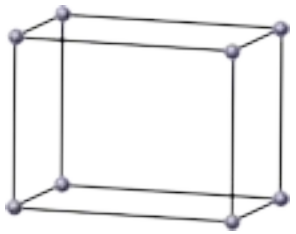
Source: Frank Hoffmann

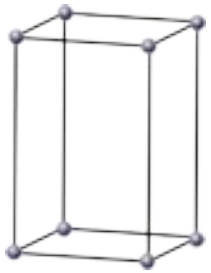
14 Bravais Lattices

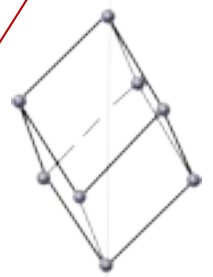
P

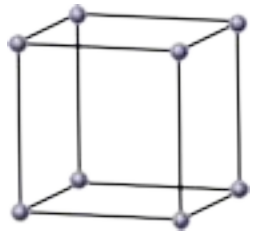




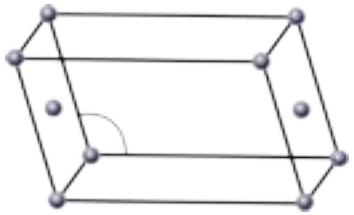


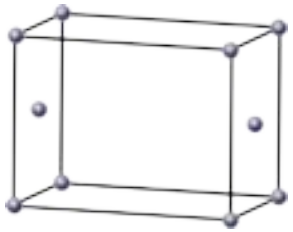




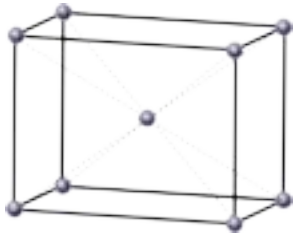


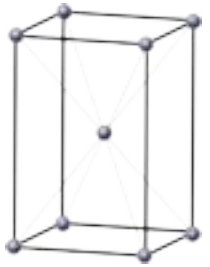
C(AB)

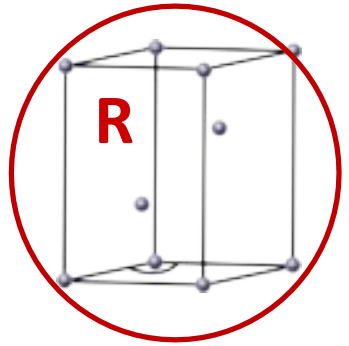




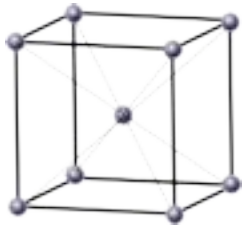
I



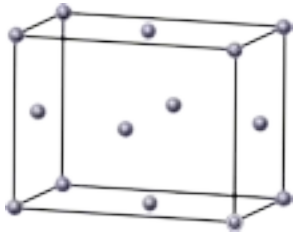


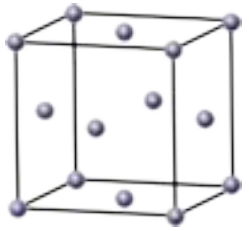


R ?

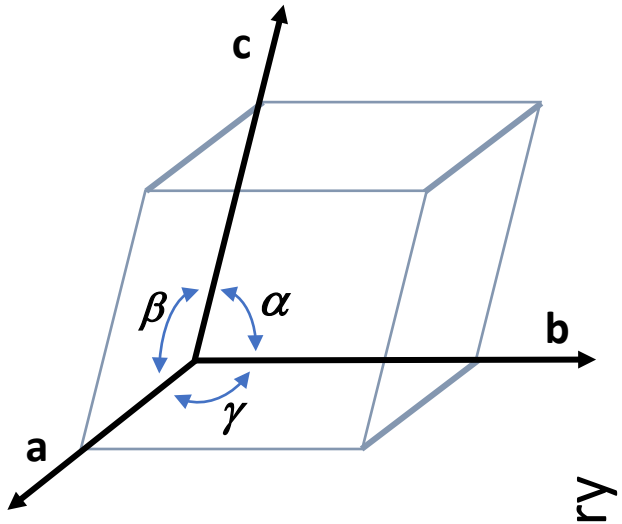


F





14 – Bravais Lattice



Higher Symmetry

Crystal Family	Bravais Lattice
CUBIC a = b = c α = β = γ = 90°	P, I, F
TETRAGONAL a = b ≠ c α = β = γ = 90°	P, I
ORTHORHOMBIC a ≠ b ≠ c α = β = γ = 90°	P, I, F, C
HEXAGONAL a = b ≠ c α = β = 90° γ = 120°	P
TRIGONAL a = b = c α = β = γ ≠ 90°	P
MONOCLINIC a ≠ b ≠ c α = γ = 90° β ≠ 120°	P, C
TRICLINIC a ≠ b ≠ c α ≠ β ≠ γ ≠ 90°	P

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

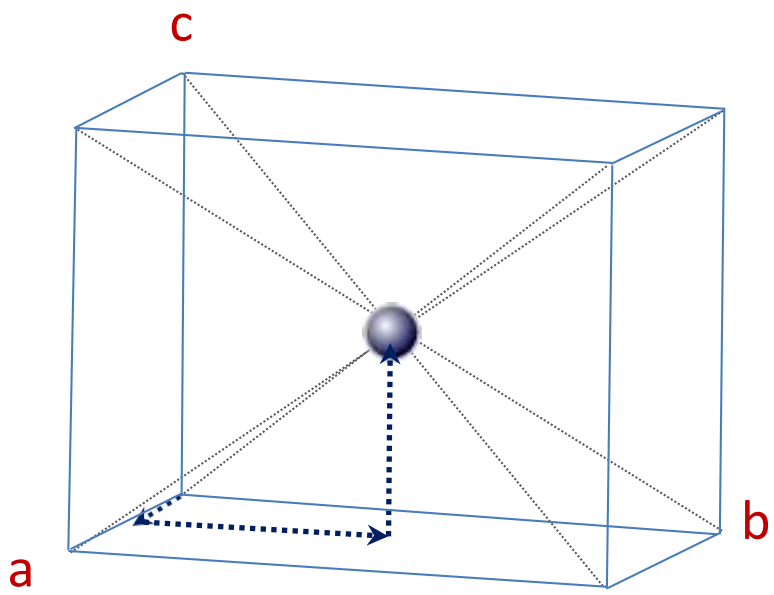
Fractional Coordinates

- Atom sites: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c)

a = 5 Å, b = 20 Å, c = 15 Å $\quad \alpha = \beta = \gamma = 90°$

Atom 1: x = 2.5 Å, y = 10 Å, z = 7.5 Å ← absolute coordinates

Atom 1: 0.5, 0.5, 0.5 ← relative or fractional coordinates



Source: Frank Hoffmann

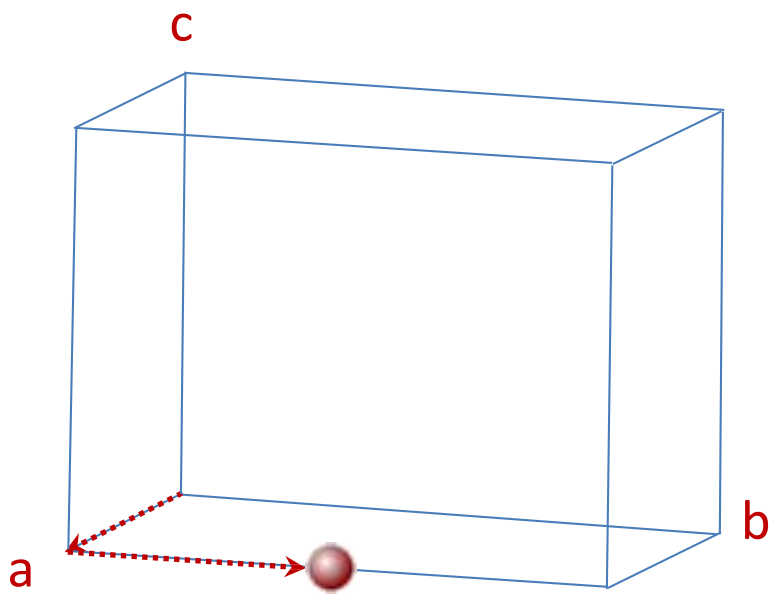
Fractional Coordinates

- Atom sites: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c)

a = 5 Å, b = 20 Å, c = 15 Å $\quad \alpha = \beta = \gamma = 90°$

Atom 2: x = 5 Å, y = 10 Å, z = 0 Å ← absolute coordinates

Atom 2: 1, 0.5, 0 ← relative or fractional coordinates



Source: Frank Hoffmann

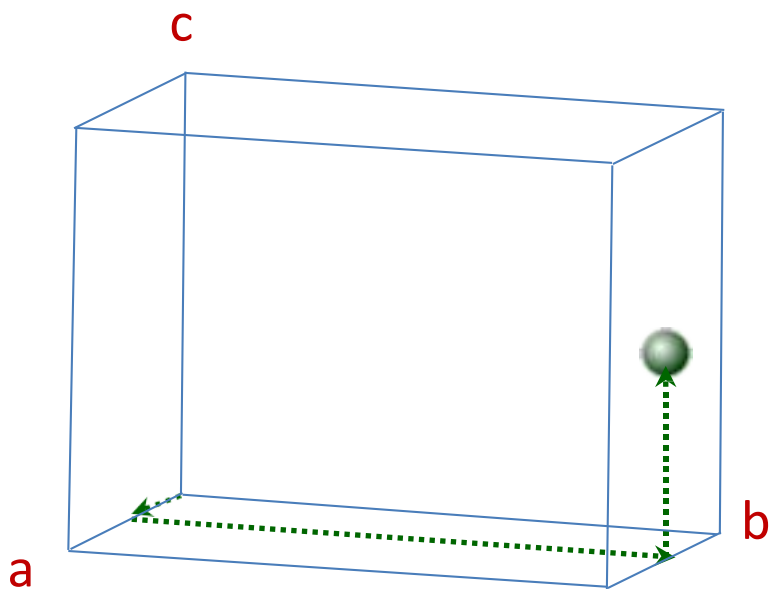
Fractional Coordinates

- Atom sites: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c)

a = 5 Å, b = 20 Å, c = 15 Å $\quad \alpha = \beta = \gamma = 90°$

Atom 3: x = 2.5 Å, y = 20 Å, z = 7.5 Å ← absolute coordinates

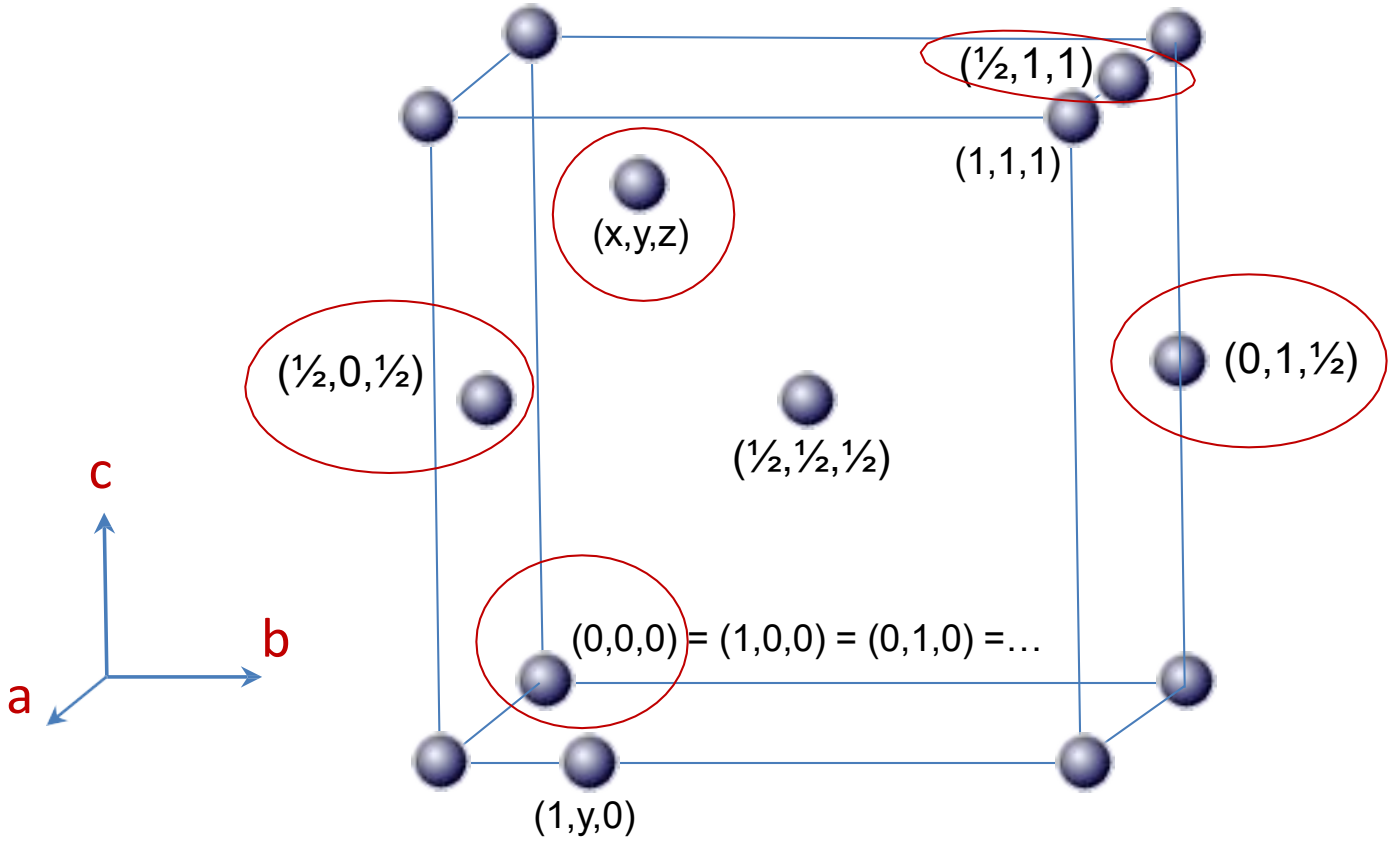
Atom 3: 0.5, 1, 0.5 ← relative or fractional coordinates



Source: Frank Hoffmann

Fractional Coordinates

- Atom sites: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c)



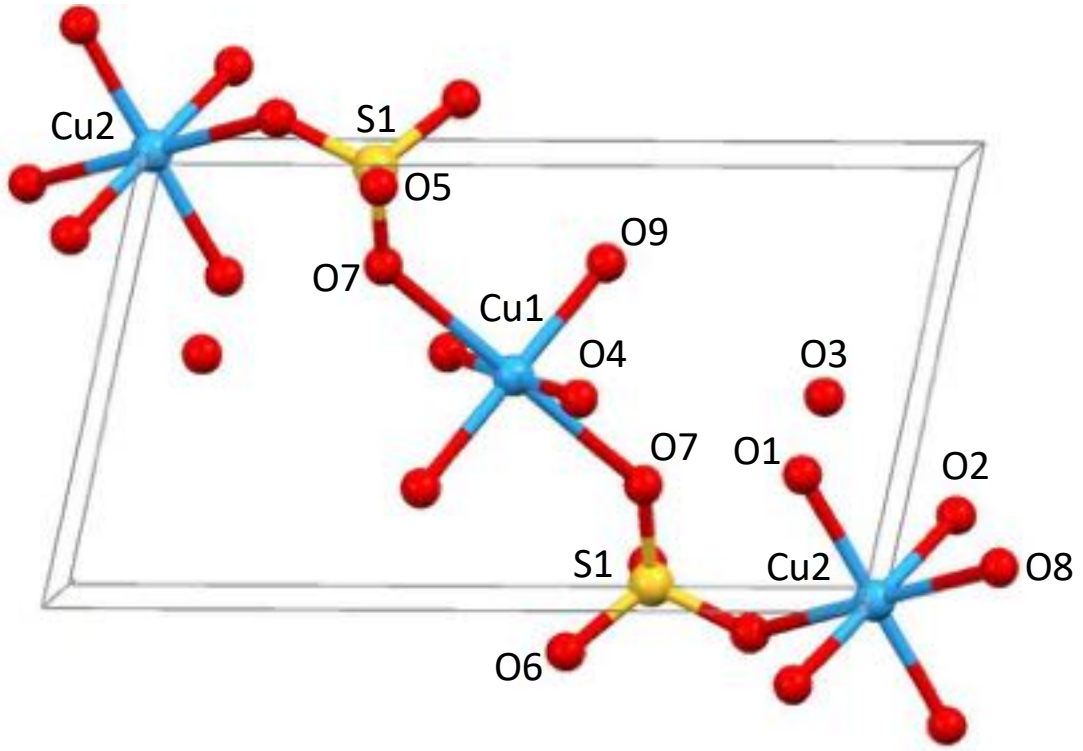
Source: Frank Hoffmann

Fractional Coordinates - $CuSO_4.5H_2O$

Chalcanthite

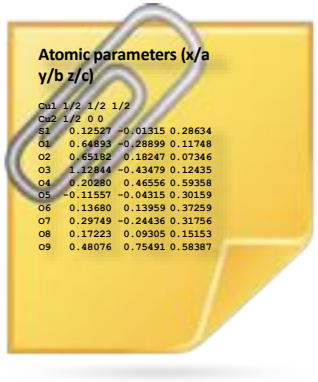
Atomic parameters (x/a y/b z/c)

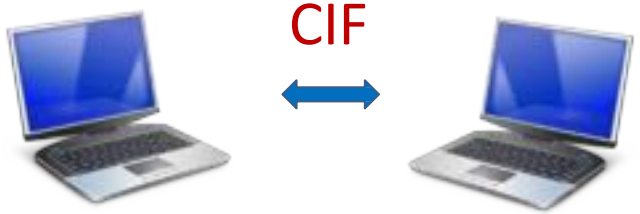
Cu1	1/2	1/2	1/2
Cu2	1/2	0	0
S1	0.12527	-0.01315	0.28634
O1	0.64893	-0.28899	0.11748
O2	0.65182	0.18247	0.07346
O3	1.12844	-0.43479	0.12435
O4	0.20280	0.46556	0.59358
O5	-0.11557	-0.04315	0.30159
O6	0.13680	0.13959	0.37259
O7	0.29749	-0.24436	0.31756
O8	0.17223	0.09305	0.15153
O9	0.48076	0.75491	0.58387



Space-group $P\bar{1}$
triclinic
a = 5.9553 Å
b = 6.1084 Å
c = 10.7048 Å

α = 77.4090°
β = 82.3720°
γ = 72.6740°

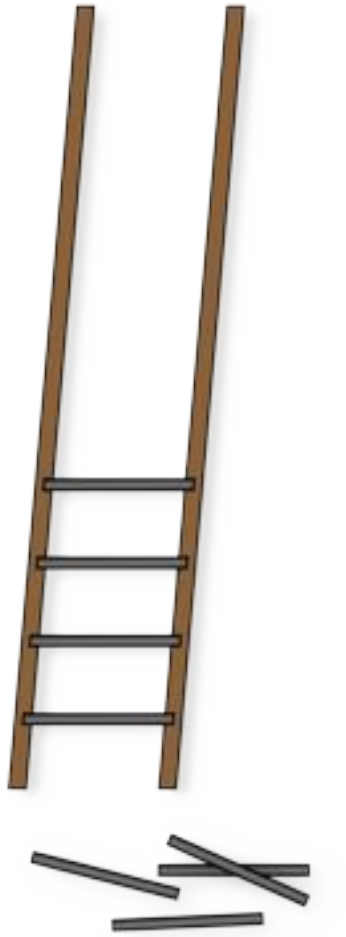




Crystallographic Information File

Source: Frank Hoffmann

Systematization of Crystal Structures



3. Step: Crystal classes
crystallographic PG — 32

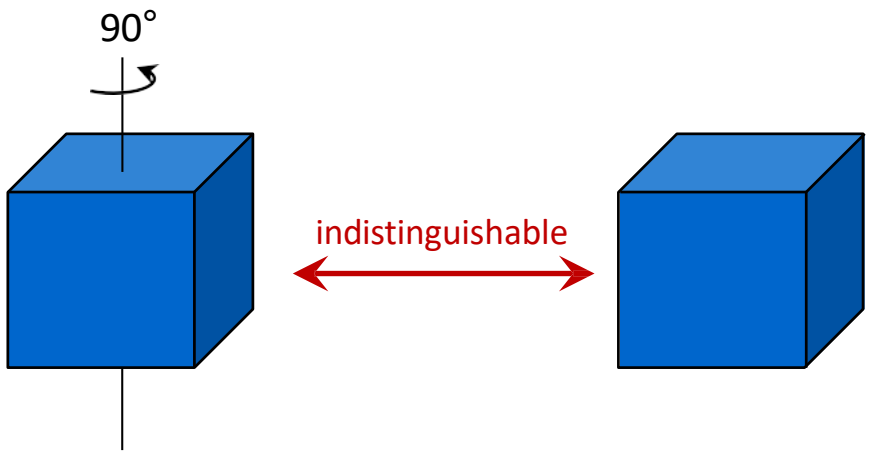
2. Step: Bravais lattices
primitive + centered — 14

1. Step: Crystal Systems
metric + symmetry of the UC — 7

Symmetry Operation and Symmetry Element

Symmetry operation (SO)

- is a (geometrical) reorganization/transformation, which maps an object onto itself
- by this operation a congruent image of the motif is generated, i.e. an image which is indistinguishable of the starting point

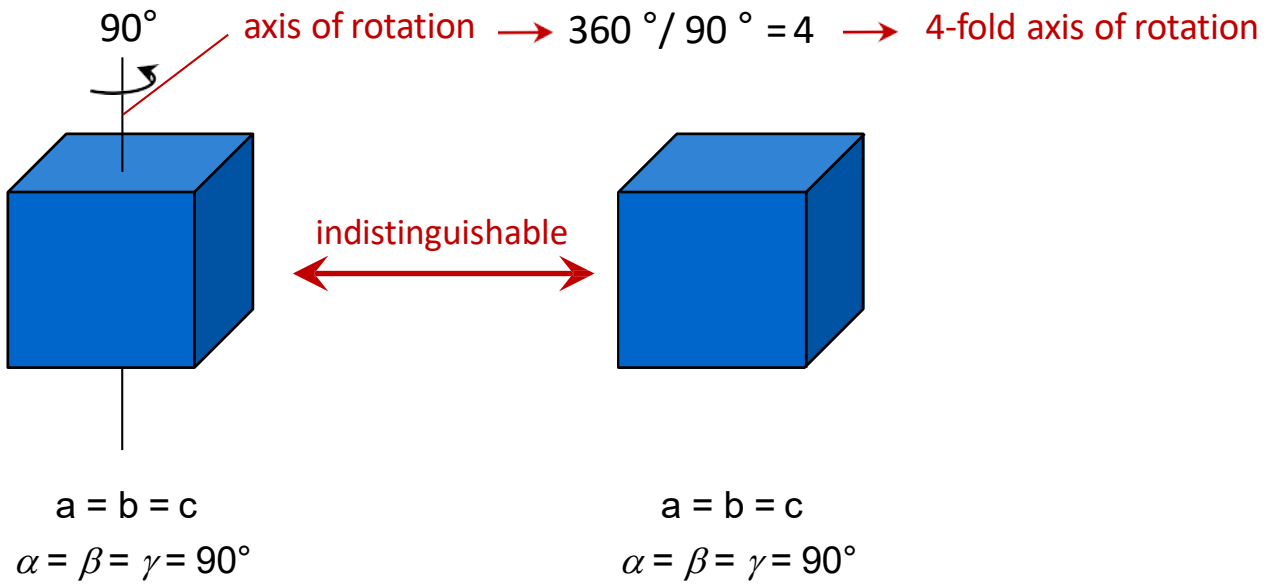


Source: Frank Hoffmann

Symmetry Operation and Symmetry Element

Symmetry element (SE)

- is the geometrical object (point, line, plane) on which the SO is carried out

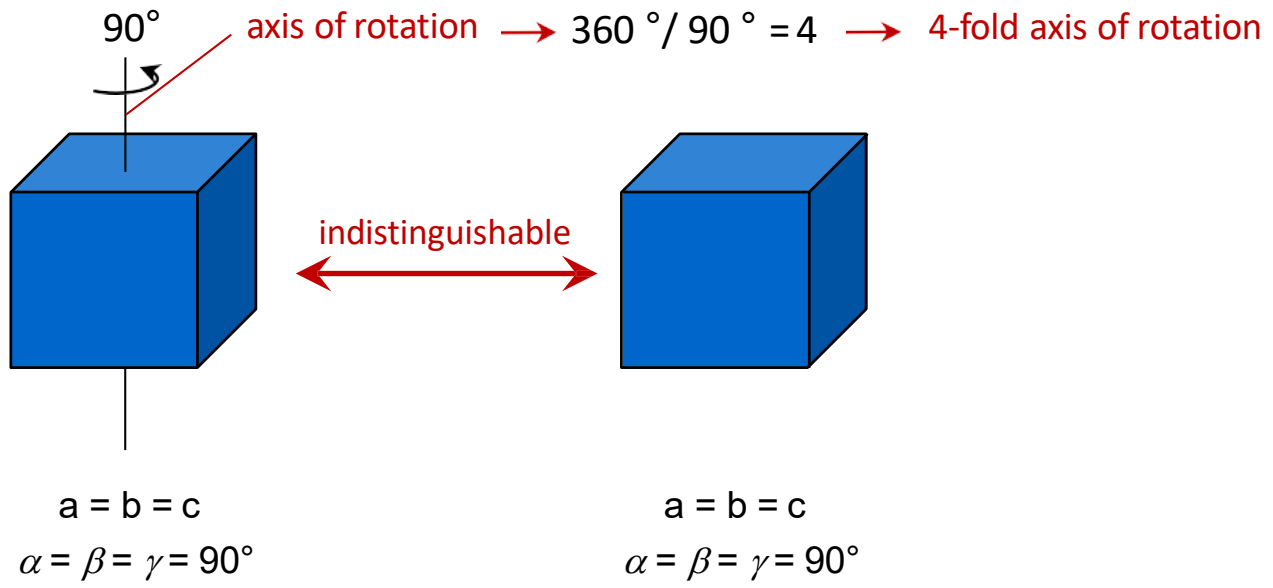


Source: Frank Hoffmann

Symmetry Operation and Symmetry Element

Symmetry element (SE)

- is the geometrical object (point, line, plane) on which the SO is carried out
- it comprises at least all invariant spatial points (fixed points) of the operation

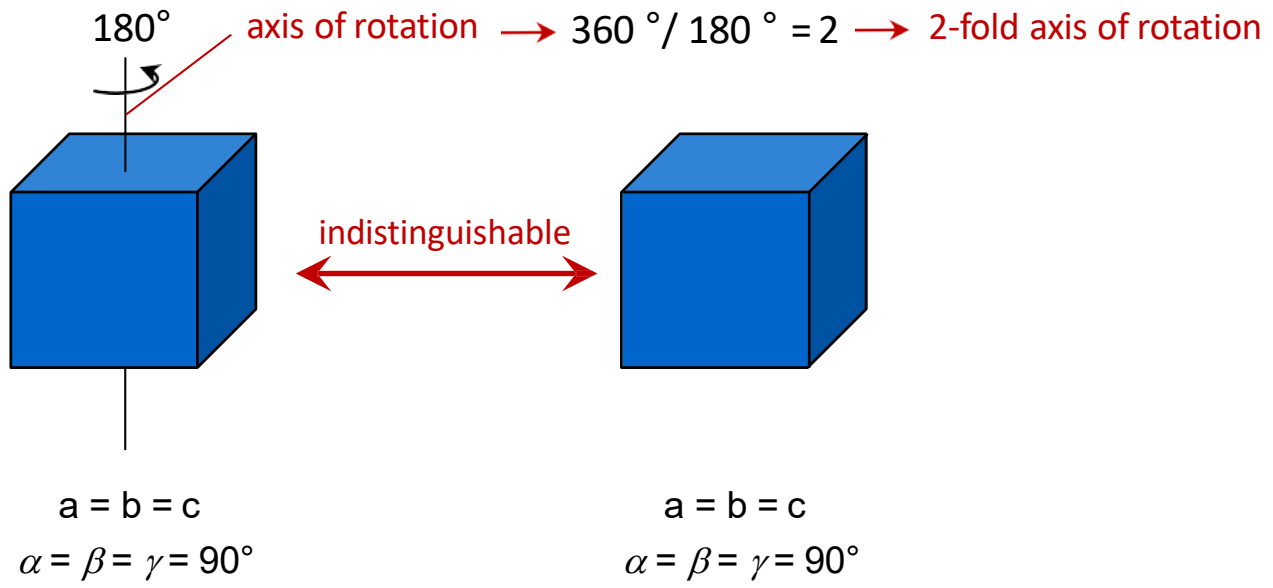


Source: Frank Hoffmann

Symmetry Operation and Symmetry Element

Symmetry element (SE)

- is the geometrical object (point, line, plane) on which the SO is carried out
- it comprises at least all invariant spatial points (fixed points) of the operation
- usually on one SE several different SO can be carried out



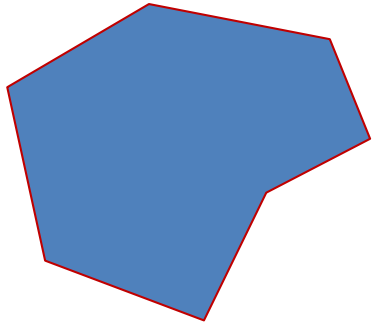
Source: Frank Hoffmann

Symmetry concerning macroscopic object

Symmetry elements of macroscopic objects

1. Identity
2. Mirror plane
3. Axis of rotation
4. Center of inversion
5. Rotoinversion axis

even the most asymmetric objects have at least one SE



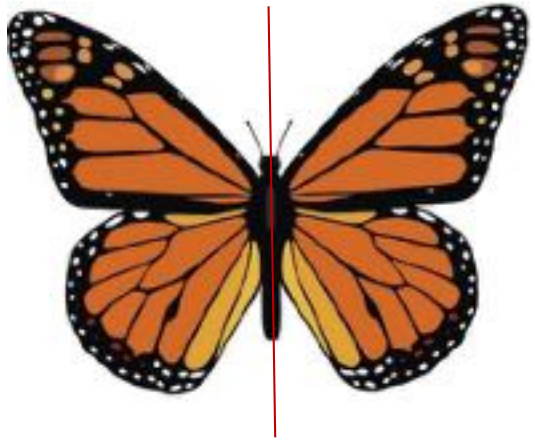
identity
1-fold axis of rotation
(rotation by 360°)

symbol *E*

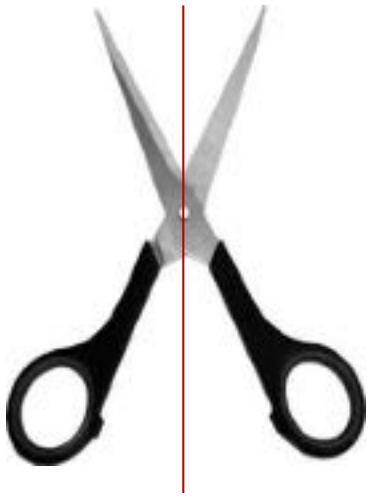
Source: Frank Hoffmann

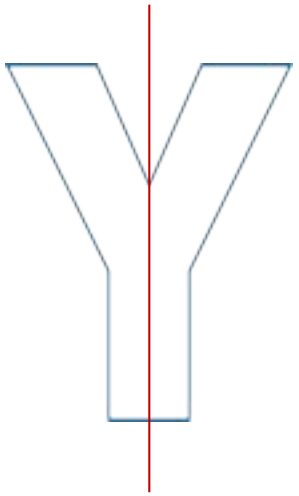
Mirror Symmetry

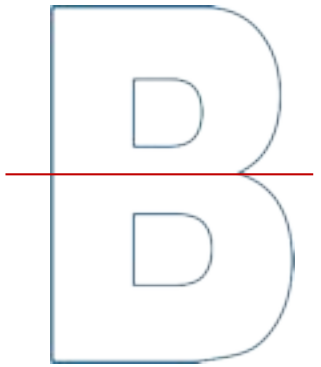
- also called ‘line symmetry’ or ‘reflection symmetry’ or ‘bilateral symmetry’
- an object which does not change upon undergoing a reflection has mirror symmetry, it is mirror symmetric
- In 2D there is a line of symmetry or mirror line, in 3D a plane of symmetry or mirror plane

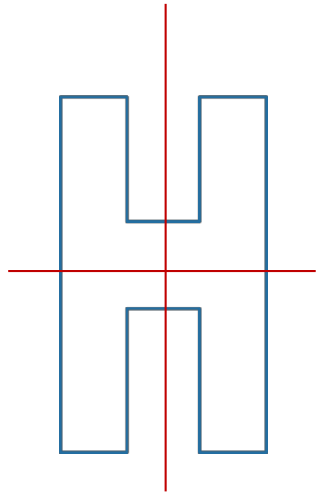


mirror plane









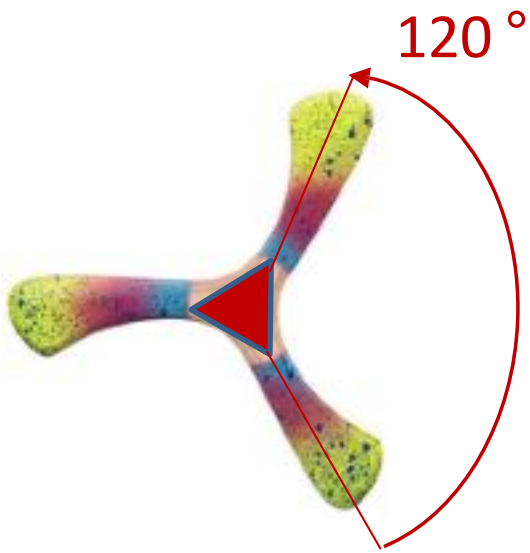
mm

symbol *m*

Source: Frank Hoffmann

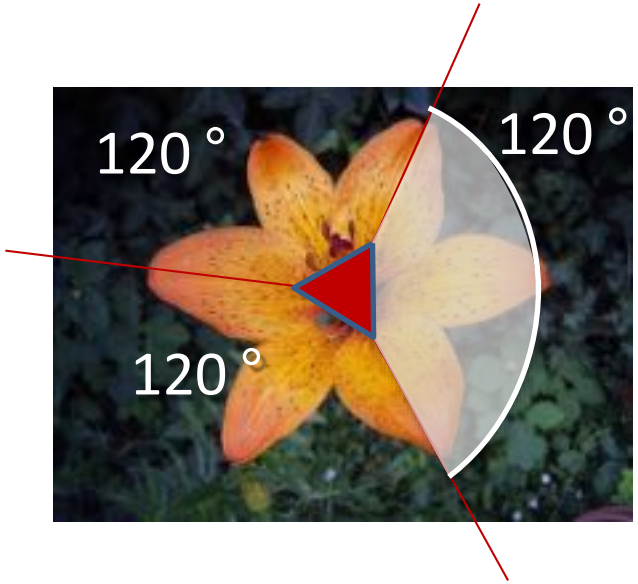
Rotational Symmetry

- single objects can have rotational symmetry of any order
- rotational symmetry may or may not be combined with mirror symmetry



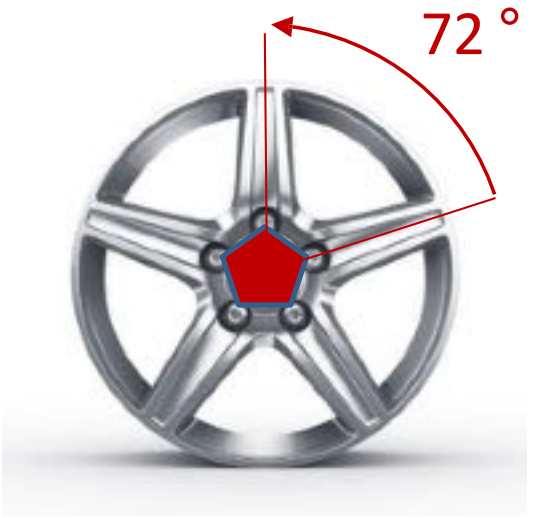
3-fold axis of rotation

3



3-fold axis of rotation

3



5-fold axis of rotation

5

∞-fold axis of rotation

SO = Rotation by 360° / n ⟶ SE = n-fold axis of rotation

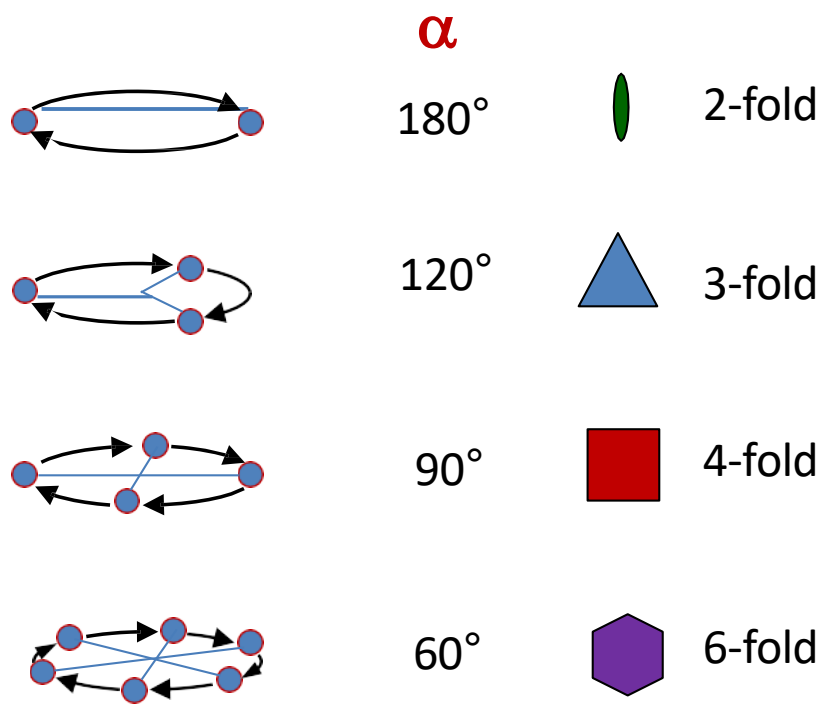
symbol n (1, 2, 3…)

Axis of Rotation

Axis of Rotation…

- rotation around a axis (= fixed points of the rotation) with an angle of rotation **α**
- after **n** rotations by **α** the starting position is reached
- **n** = order of the axis
- the number of crystal classes is limited to 32 because of the restrictions of rotational symmetry in crystals

… in crystallography

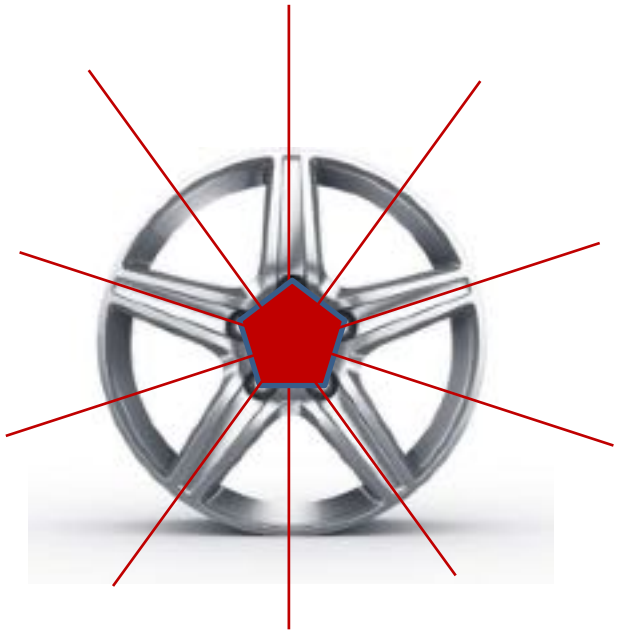


n = 2, 3, 4, 6

Source: Frank Hoffmann

Mirror + Rotational Symmetry

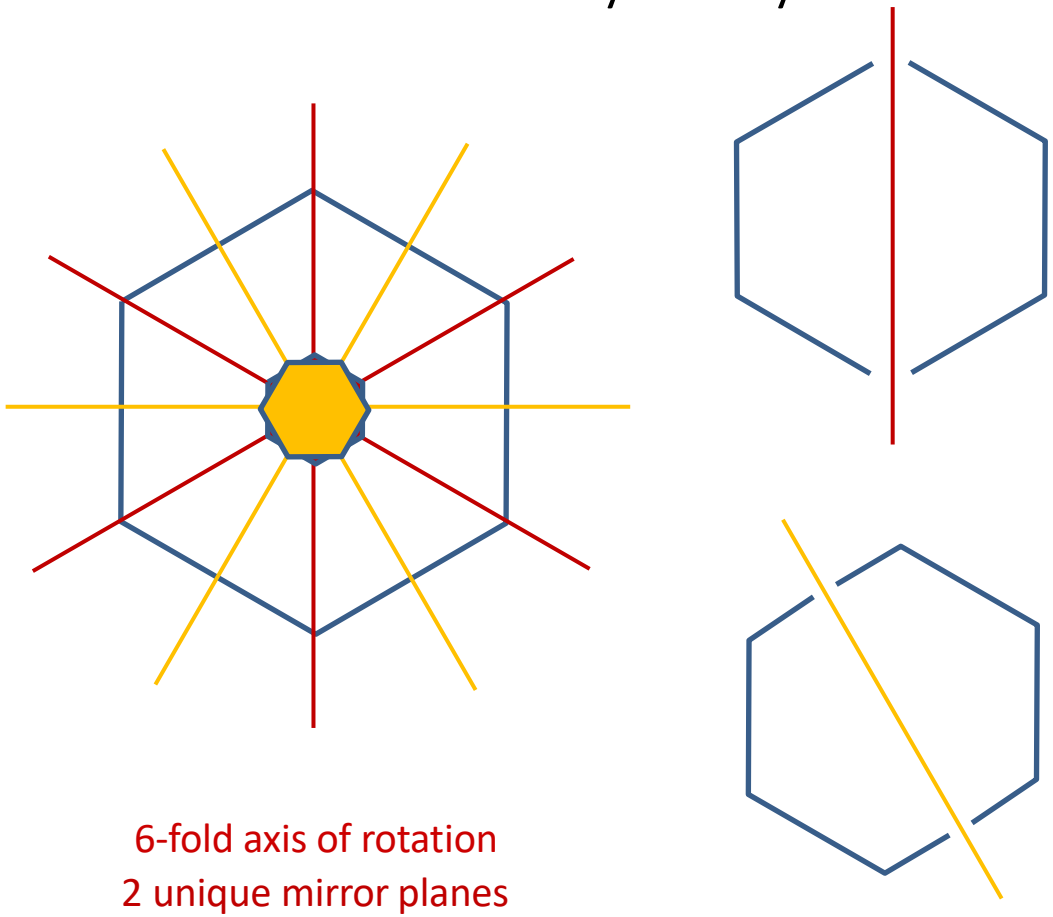
- single objects can have rotational symmetry of any order
- rotational symmetry may or may not be combined with mirror symmetry



5-fold axis of rotation

1 unique mirror plane

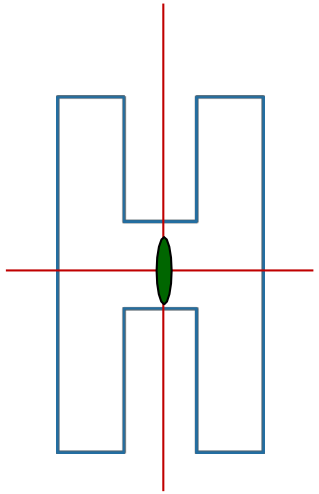
5*m*



6-fold axis of rotation

2 unique mirror planes

6*mm*

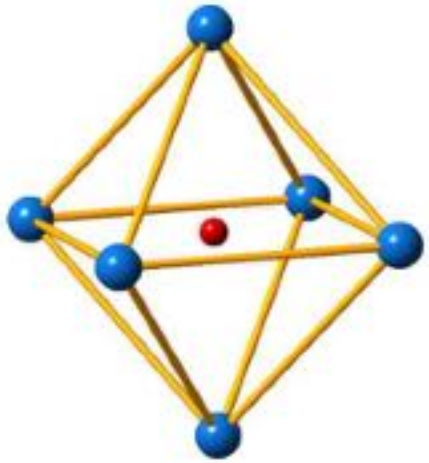


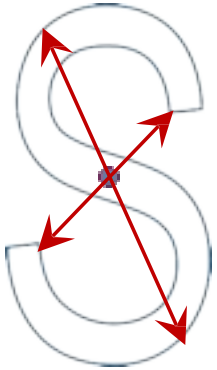
mm

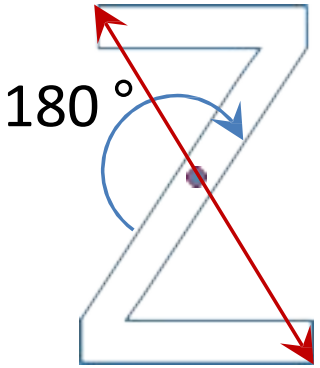
Source: Frank Hoffmann

Inversion symmetry

- also called ‘origin symmetry’ or ‘center of symmetry’
- there is always a matching part, which has the same distance from a central point but in the opposite direction
- in the plane it is identical with rotational symmetry of order 2 (2-fold axis of rotation)







symbol *i* or $\bar{1}$ (“one-bar”)

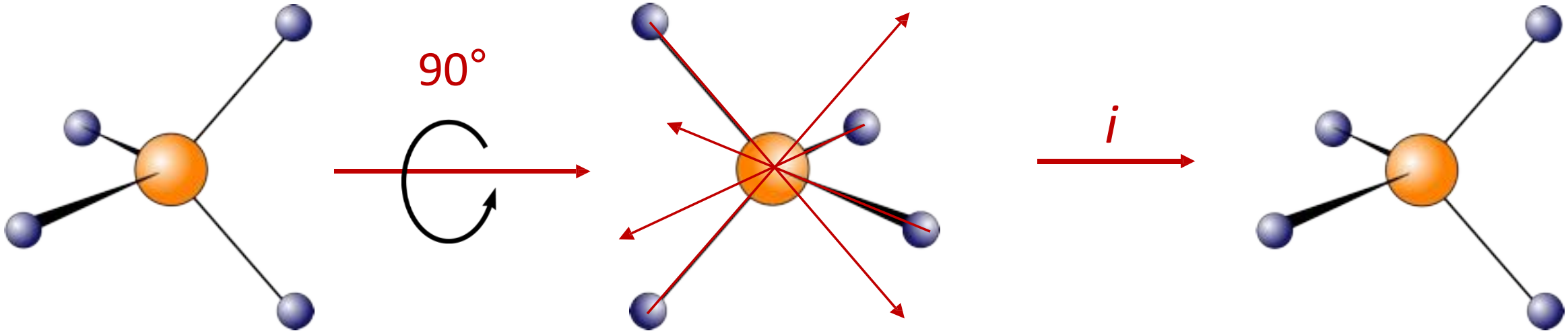
x, y, z → -x, -y, -z

Source: Frank Hoffmann

Rotation + Inversions Symmetry

- a **rotoinversion** is a combined SO, where two transformations have to be carried out
  - (1) rotation around 360°/n
  - (2) immediately followed by an inversion at a center of symmetry, which lies on the rotoinversion axis

Tetrahedron

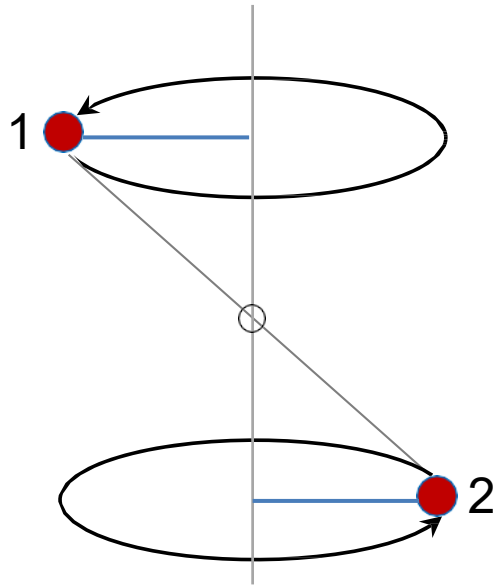


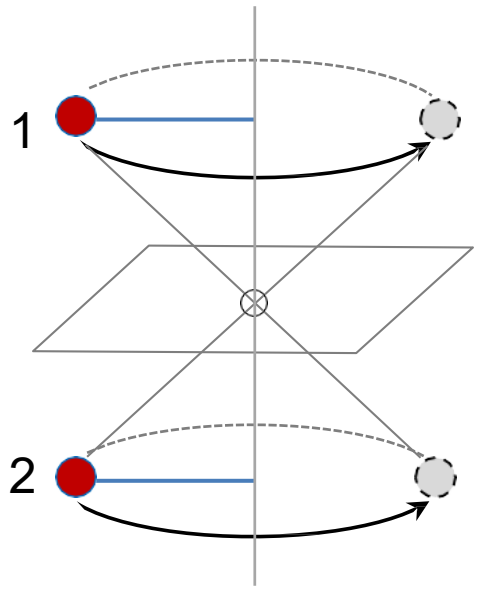
→ 4-fold rotoinversion axis

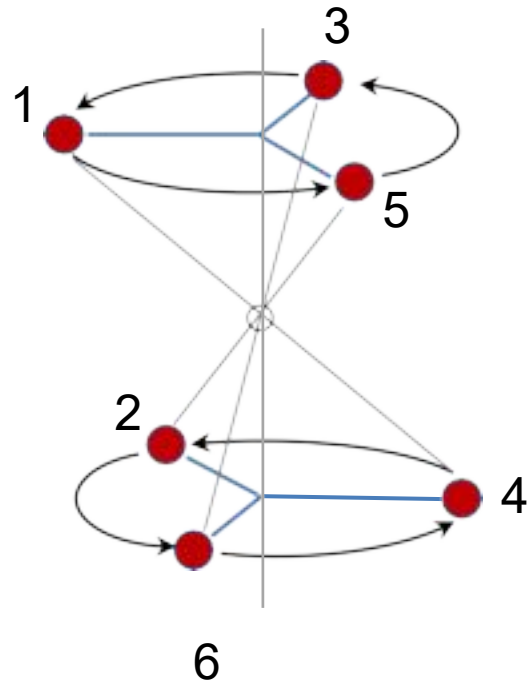
symbol $\bar{4} = 4 + \bar{1}$

Roto-inversion axes of order 1, 2, and 3

- **odd rotoinversions** possess automatically a center of inversion







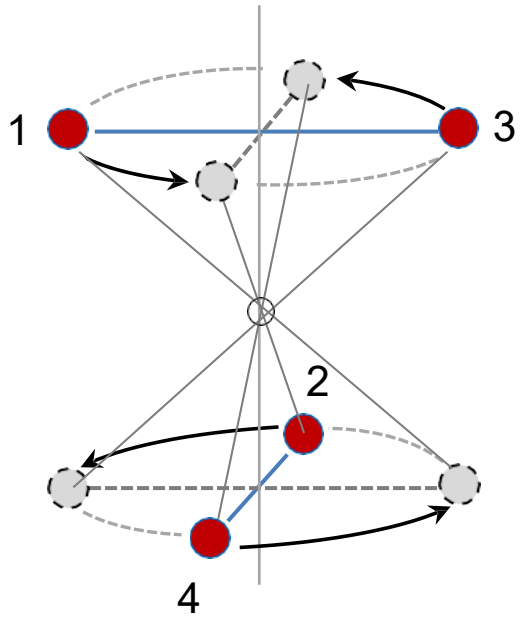
$\overline{1} = i$

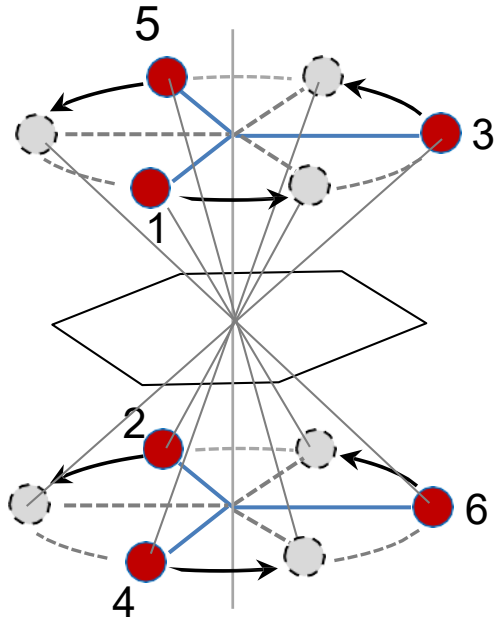
$\overline{2} = m$

$\overline{3} = 3 + \overline{1}$

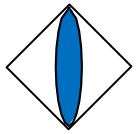
Roto-inversion axes of order 4 and 6

- **even rotoinversions** contain automatically an axis of rotation of the half order (4-bar contains a 2-fold, and 6-bar contains a 3-fold axis of rotation)
- if the order n is even, but not divisible by 4, then there is automatically a mirror plane perpendicular to the rotoinversion axis (holds for 2-bar and 6-bar)

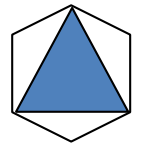




$\overline{4} = 4 + \overline{1}$



$\overline{6} = 6 + \overline{1} = 3 \perp m$

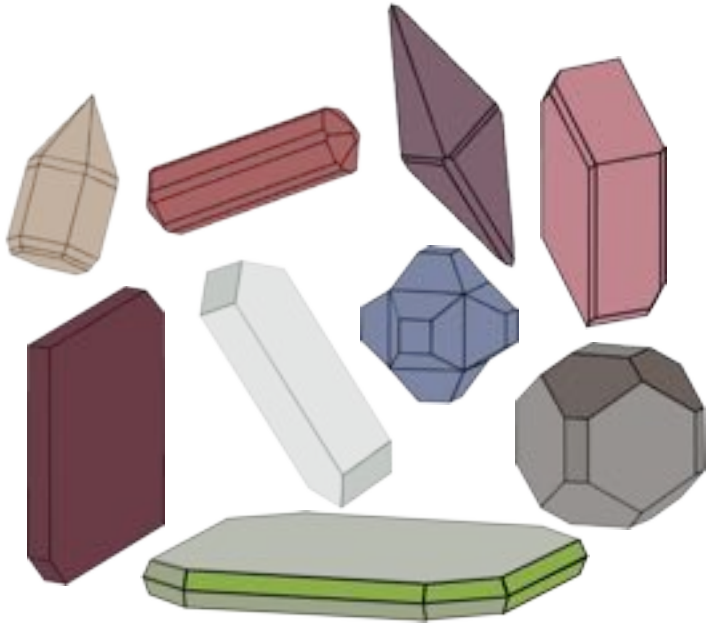


Crystal Classes

- everyday objects can have any symmetry, and symmetry elements can be combined, in principle, arbitrarily

‘infinite’ number of symmetry classes

- the symmetry of crystals – i.e. the symmetry of the external shape of crystals – is limited
- they can be classified into 32 classes only
- the symmetry has to be compatible with the repeating pattern of the crystal lattice



32 symmetry classes (point groups)

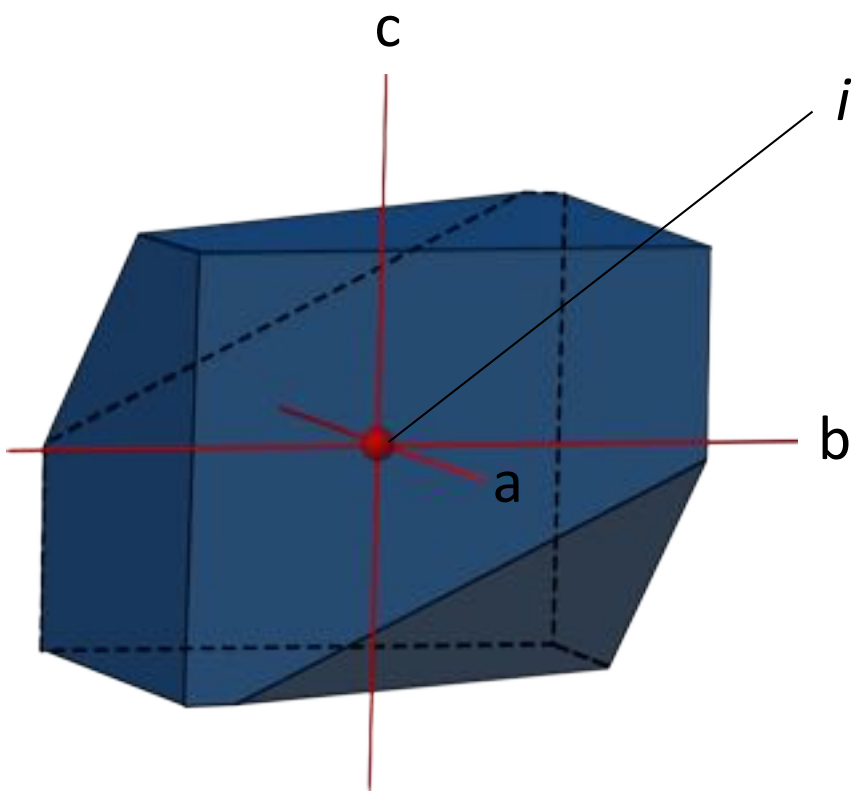
see later

Classify Crystal into Classes

1st Example

→ *no* m
→ *no* n

crystal class $\overline{1}$



pinacoidal

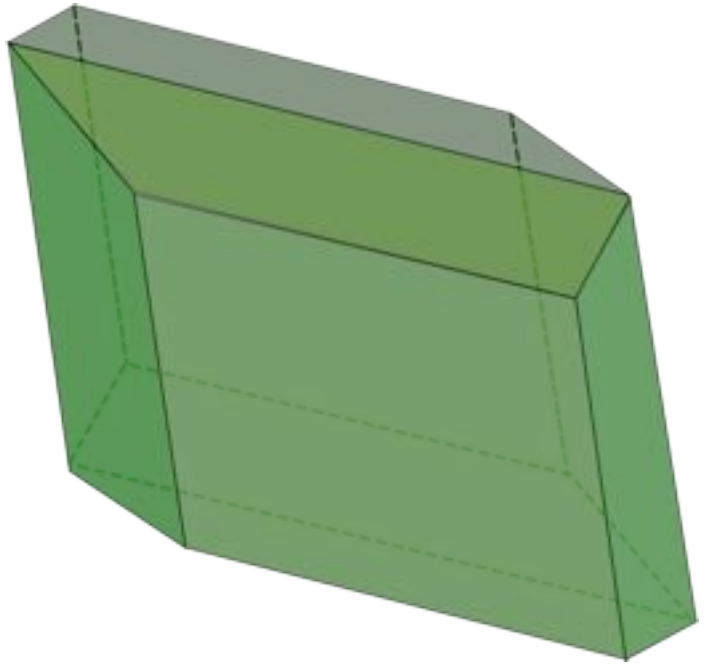
plagioclase

microcline (potassium feldspar),
turquoise, and wollastonite

Source: Frank Hoffmann

Classify Crystal into Classes

2nd Example



Source: Frank Hoffmann

Classify Crystal into Classes

2nd Example

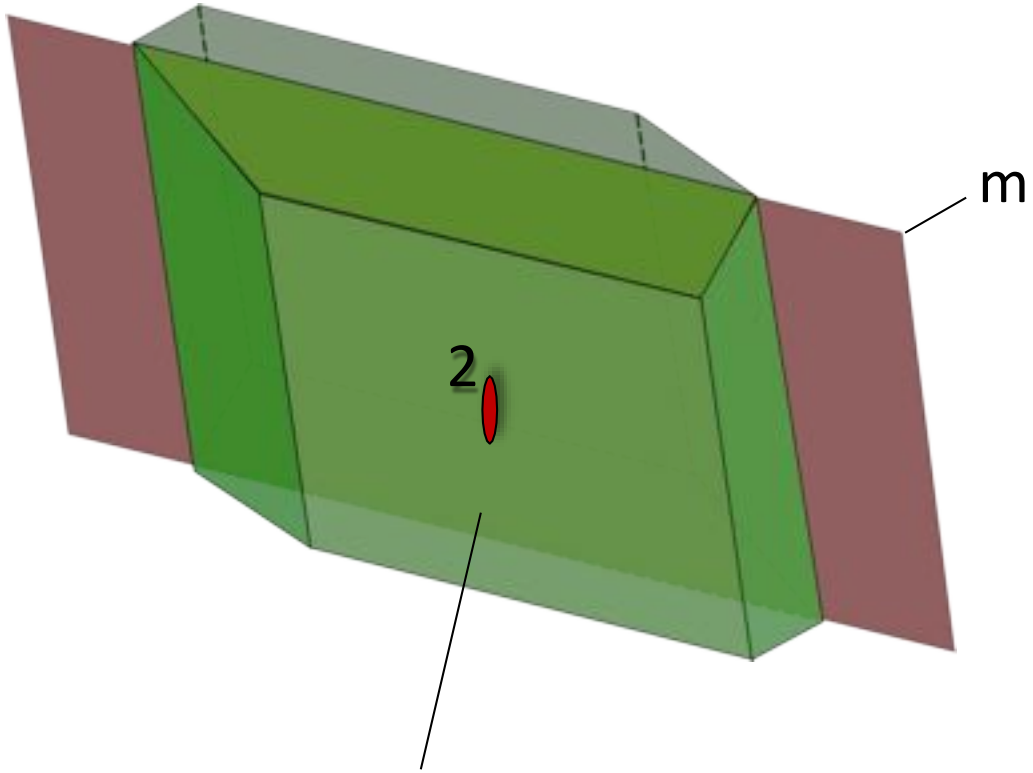
→ one m

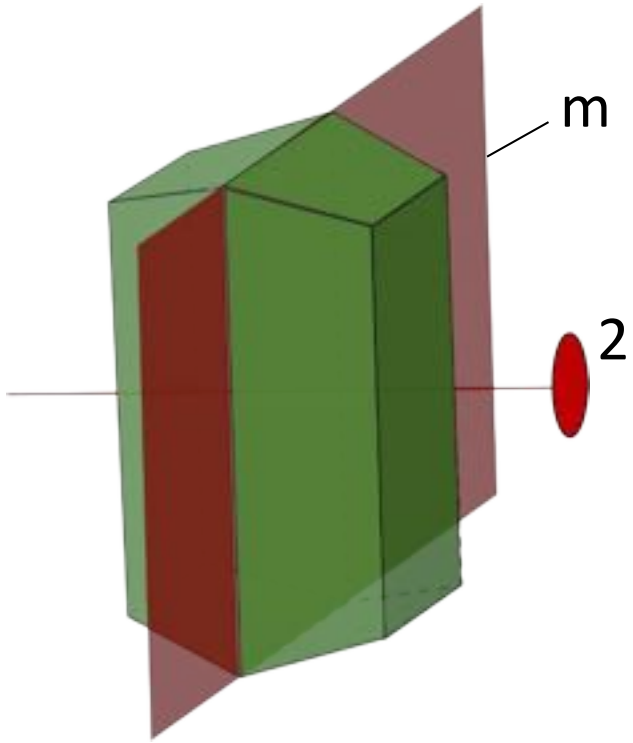
→ one 2 perpendicular to m

$\frac{2}{m}$ ← "perpendicular to"

speak: '2 over m'

crystal class 2/m





http://webmineral.com/data/Gypsum.shtml

Source: Frank Hoffmann

Classify Crystal into Classes

2nd Example

→ one m

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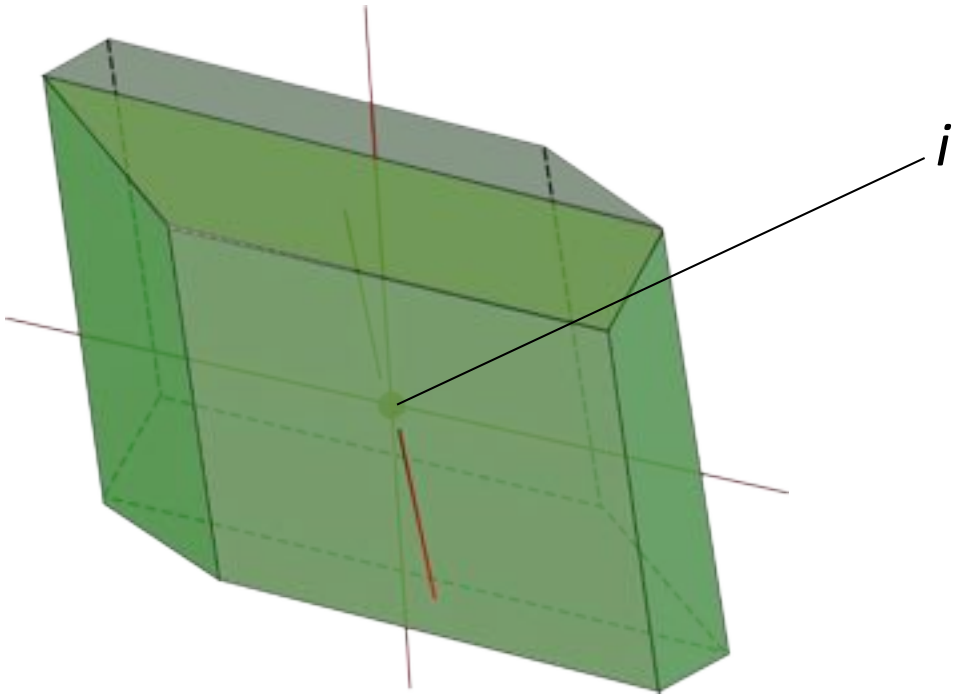

crystal class 2/m

→ there is also a center of inversion, however this is not a 'unique' SE

→ it is automatically generated by 2/m!

http://webmineral.com/data/Gypsum.shtml

Source: Frank Hoffmann

Classify Crystal into Classes

2nd Example

→ one m

→ one 2 perpendicular to m

$\frac{2}{m}$ ← "perpendicular to"

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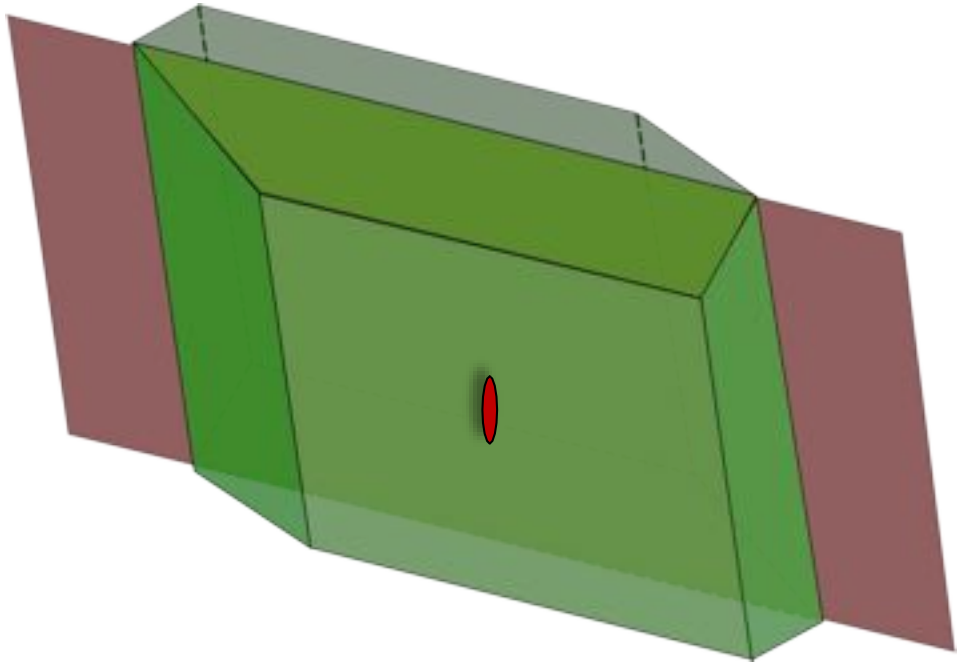
crystal class 2/m



prismatic

$CaSO_4 \cdot 2\,H_2O$

Gypsum

http://webmineral.com/data/Gypsum.shtml

azurite, chlorite, clinopyroxene, epidote, malachite, kaolinite, orthoclase, and talc

Source: Frank Hoffmann

Classify Crystal into Classes

2nd Example

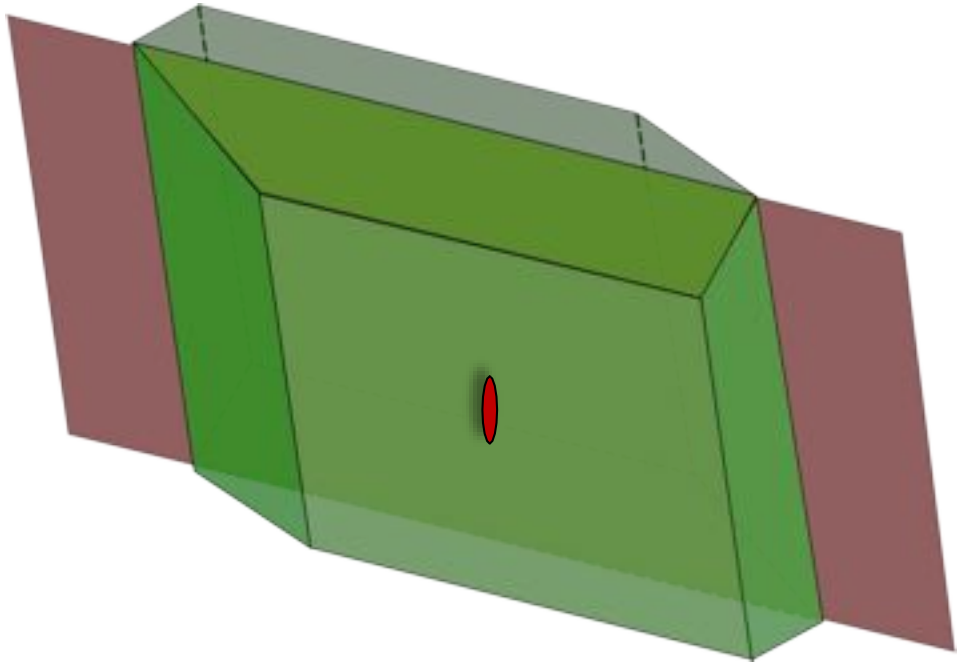
→ one m

→ one 2 perpendicular to m

$\frac{2}{m}$ ← "perpendicular to"

speak: '2 over m'

crystal class 2/m



http://webmineral.com/data/Gypsum.shtml

prismatic

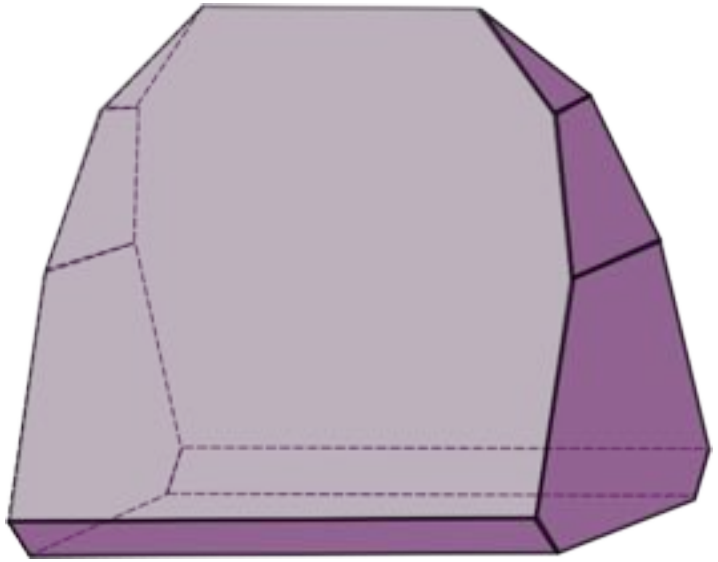
$Fe_3(PO_4)_2 \cdot 8H_2O$
Vivianite

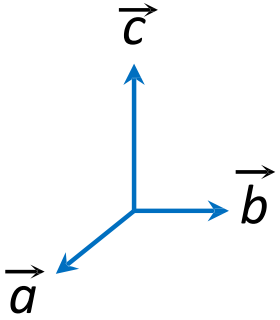
azurite, chlorite, clinopyroxene, epidote, malachite, kaolinite, orthoclase, and talc

Source: Frank Hoffmann

Classify Crystal into Classes

3rd Example



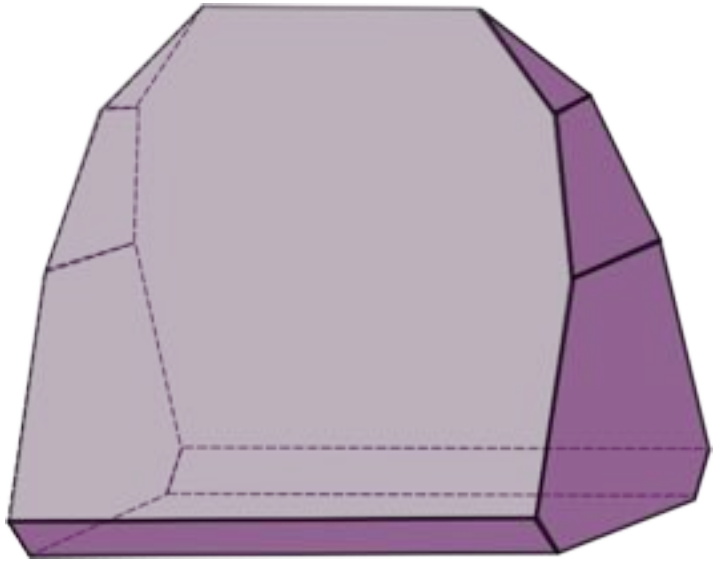


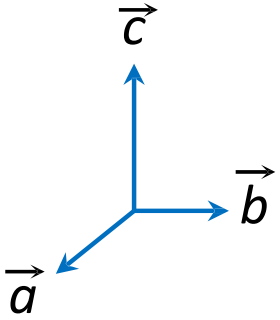
Source: Frank Hoffmann

Classify Crystal into Classes

3rd Example

Introducing viewing directions, here a b c

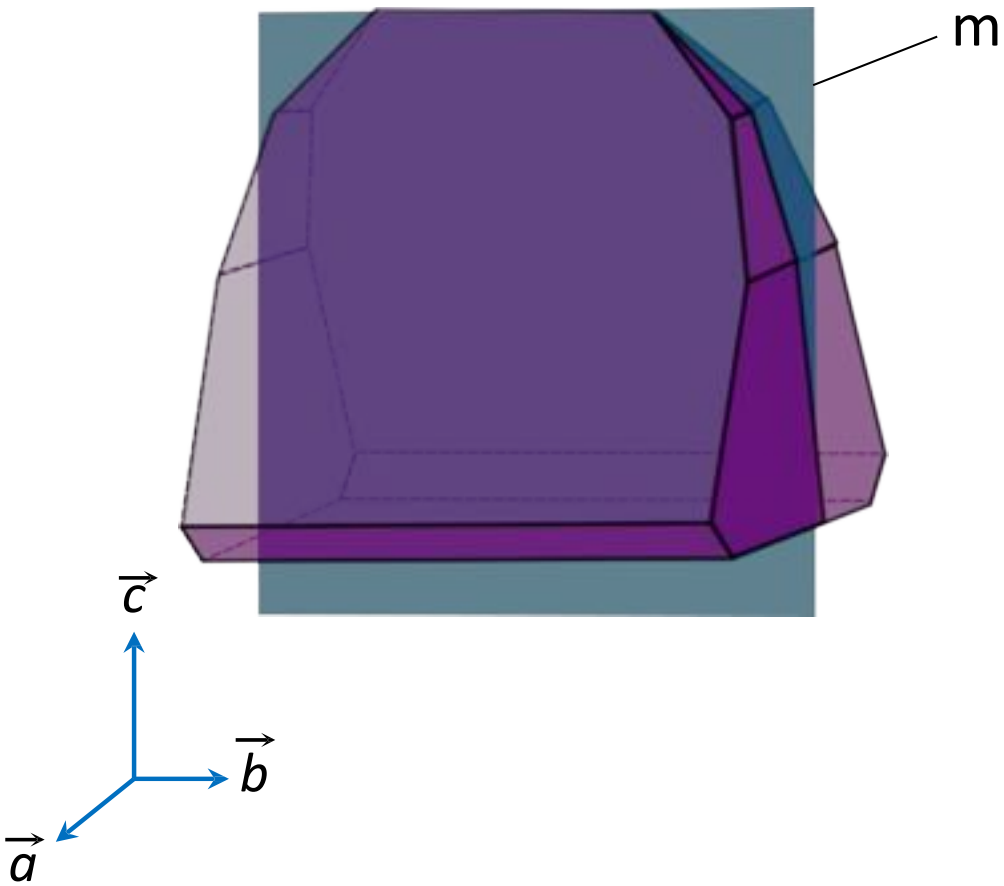




Source: Frank Hoffmann

Classify Crystal into Classes

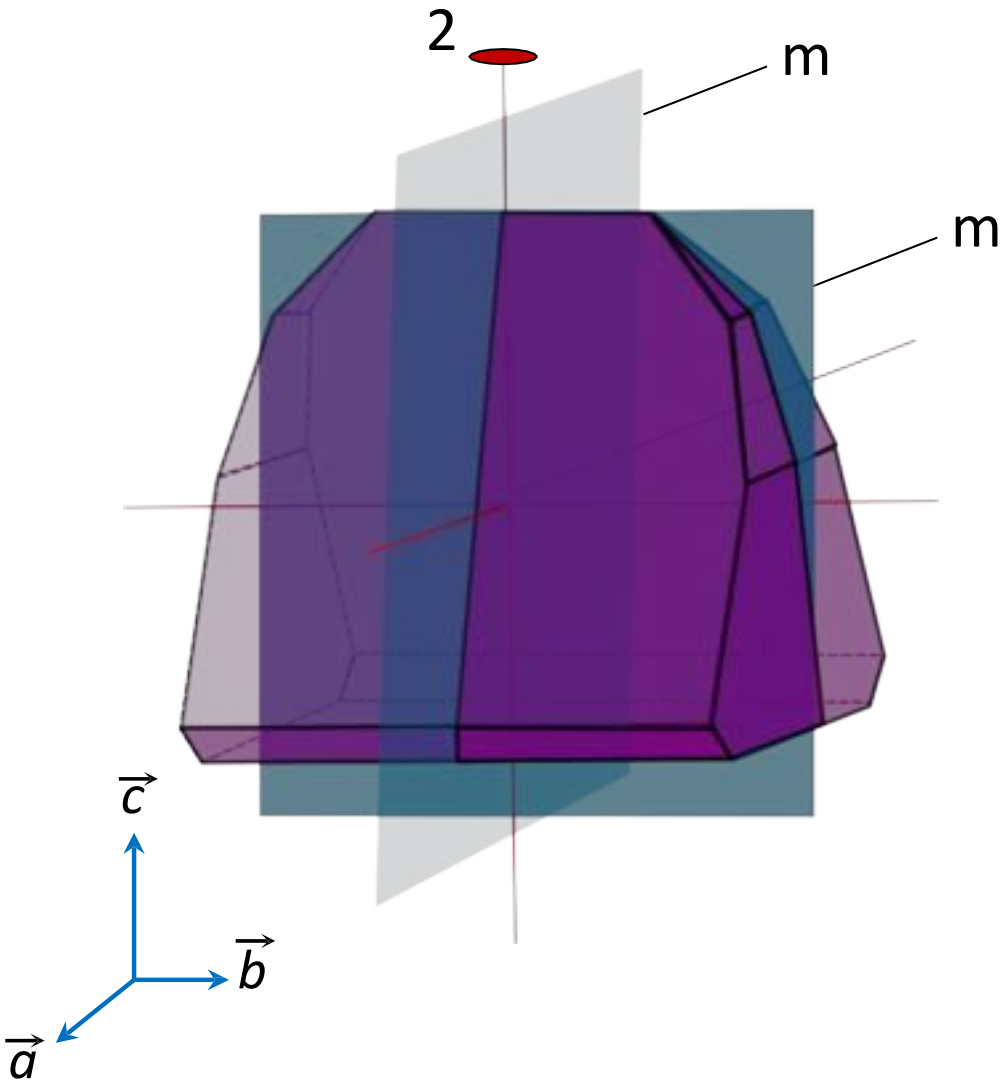
3rd Example



Source: Frank Hoffmann

Classify Crystal into Classes

3rd Example



symmetry elements 2 m m

crystal class m m 2 ← by convention

a b c

(ortho)rhombic-pyramidal

$MgNH_4PO_4 \cdot 6\,H_2O$

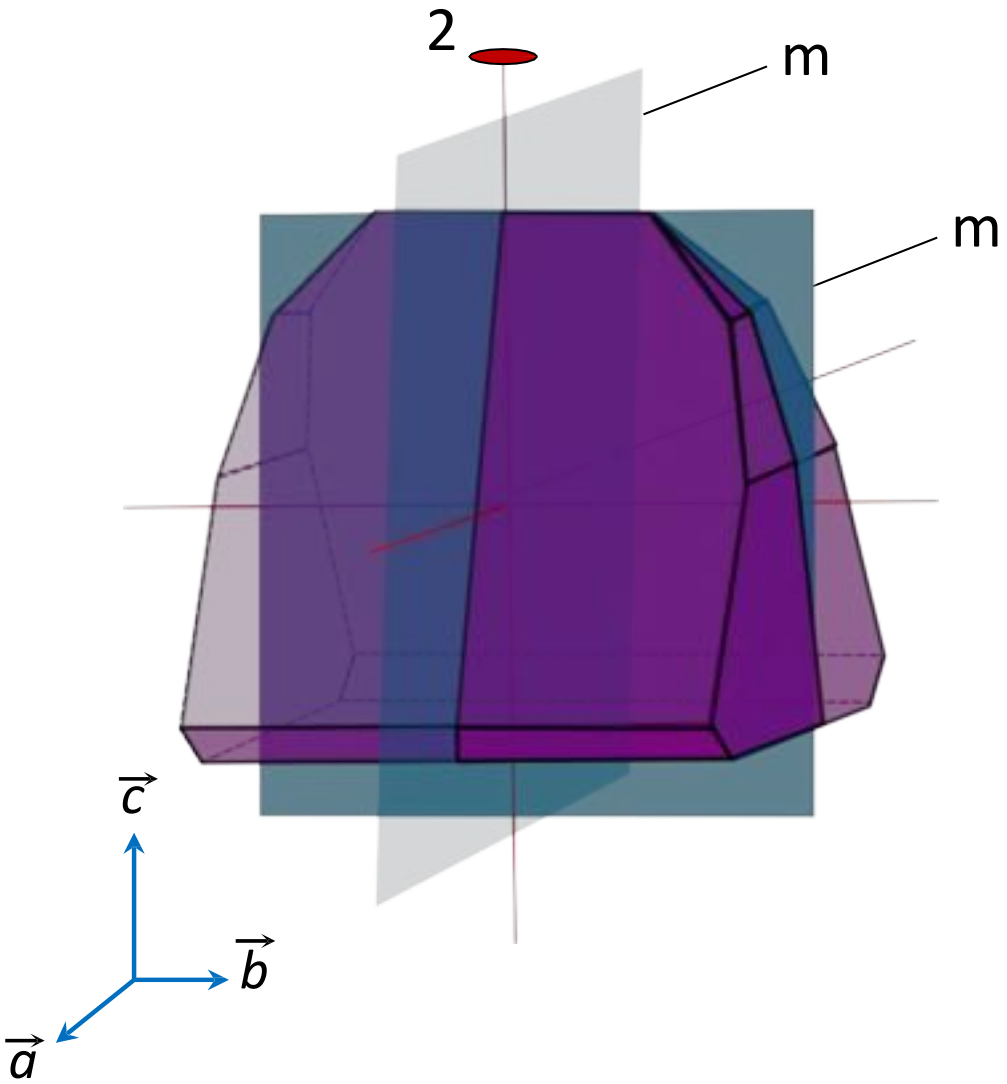
Struvite

http://webmineral.com/data/Struvite.shtml

Source: Frank Hoffmann

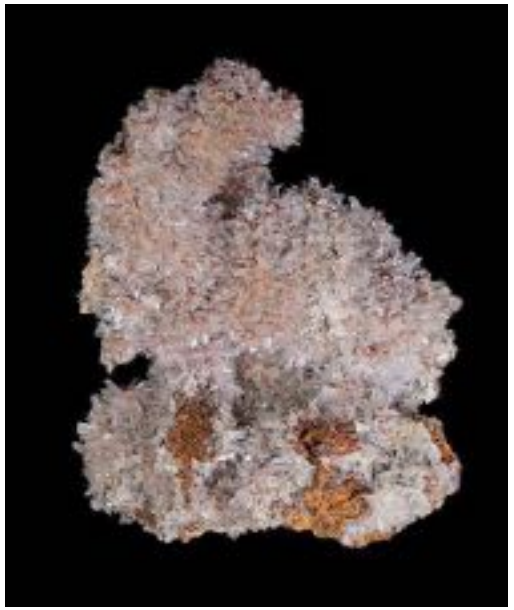
Classify Crystal into Classes

3rd Example



crystal class mm2

(ortho)rhombic-pyramidal



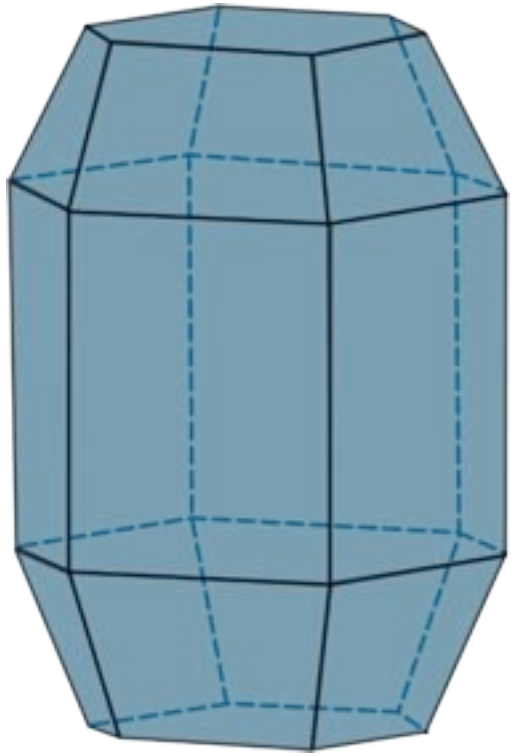
$Zn_4Si_2O_7(OH)_2 \cdot H_2O$

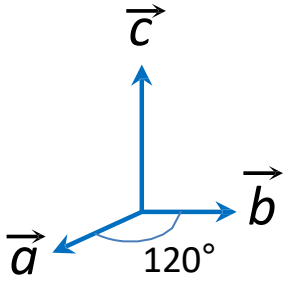
Hemimorphite

Source: Frank Hoffmann

Classify Crystal into Classes

4th Example



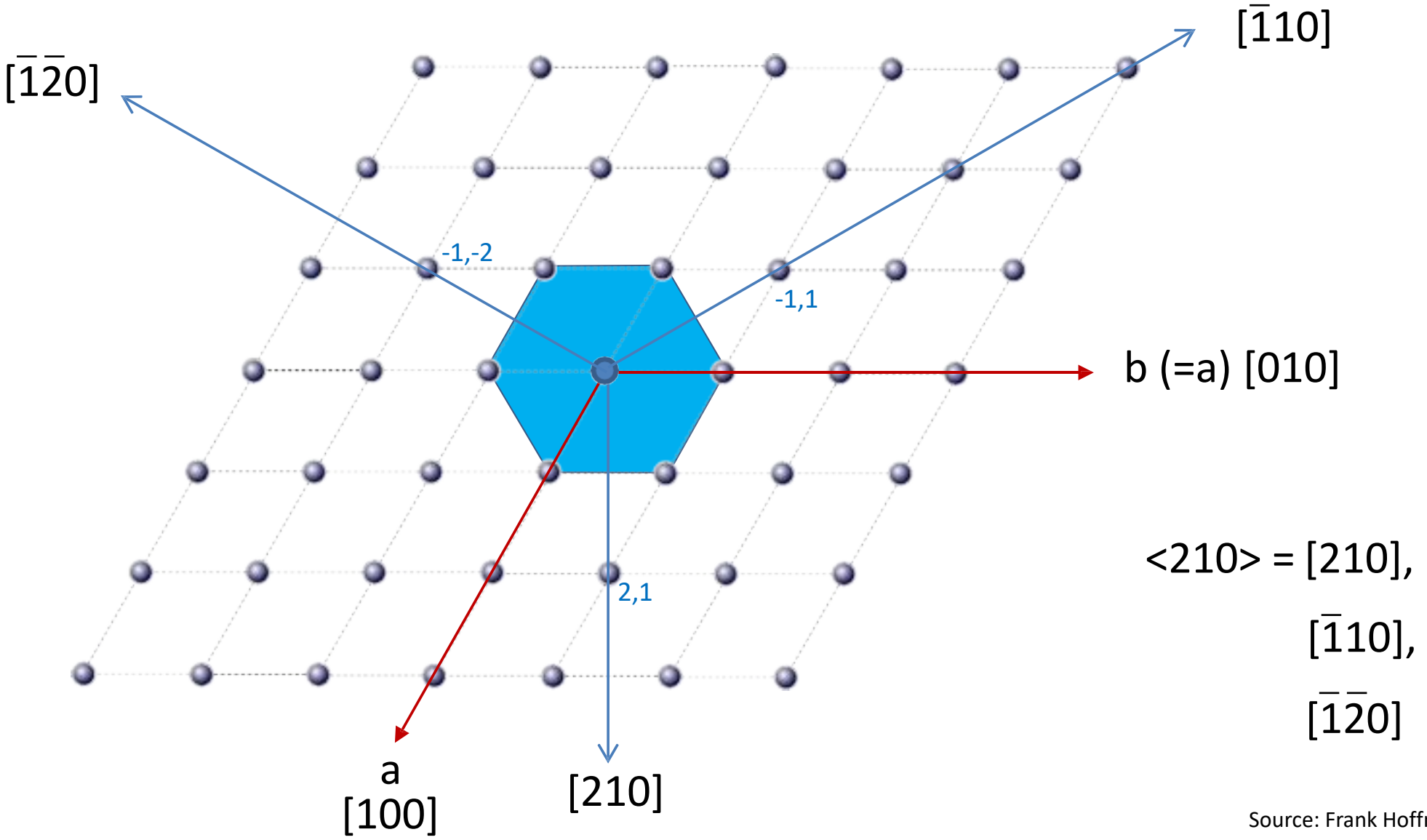


viewing directions
(hexagonal crystal system)

c a [210]

Source: Frank Hoffmann

Lattice Directions

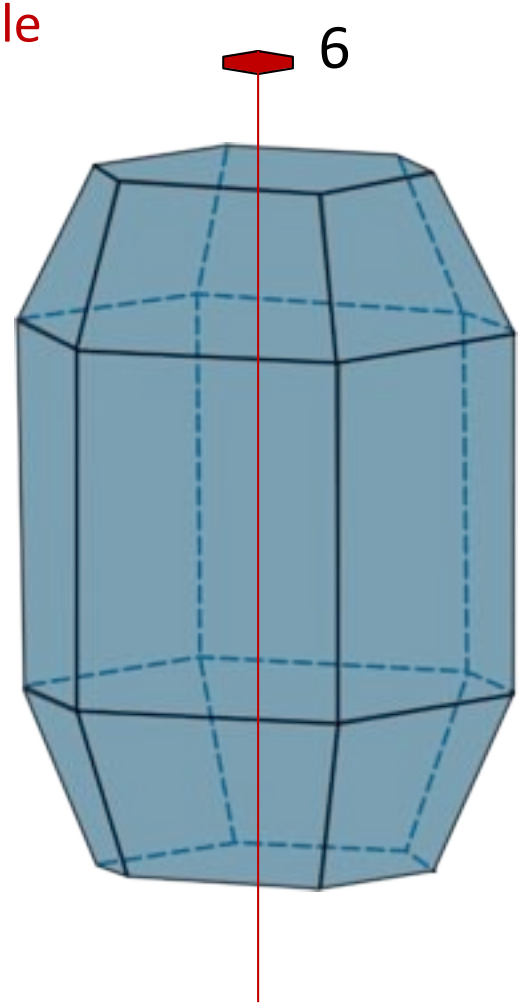


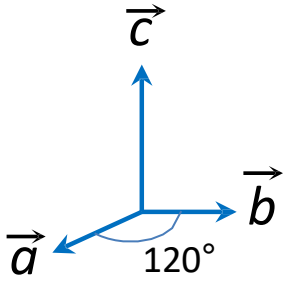
<210> = [210],
[$\bar{1}$10],
[$\bar{1}\bar{2}$0]

Source: Frank Hoffmann

Classify Crystal into Classes

4th Example





viewing directions
(hexagonal crystal system)

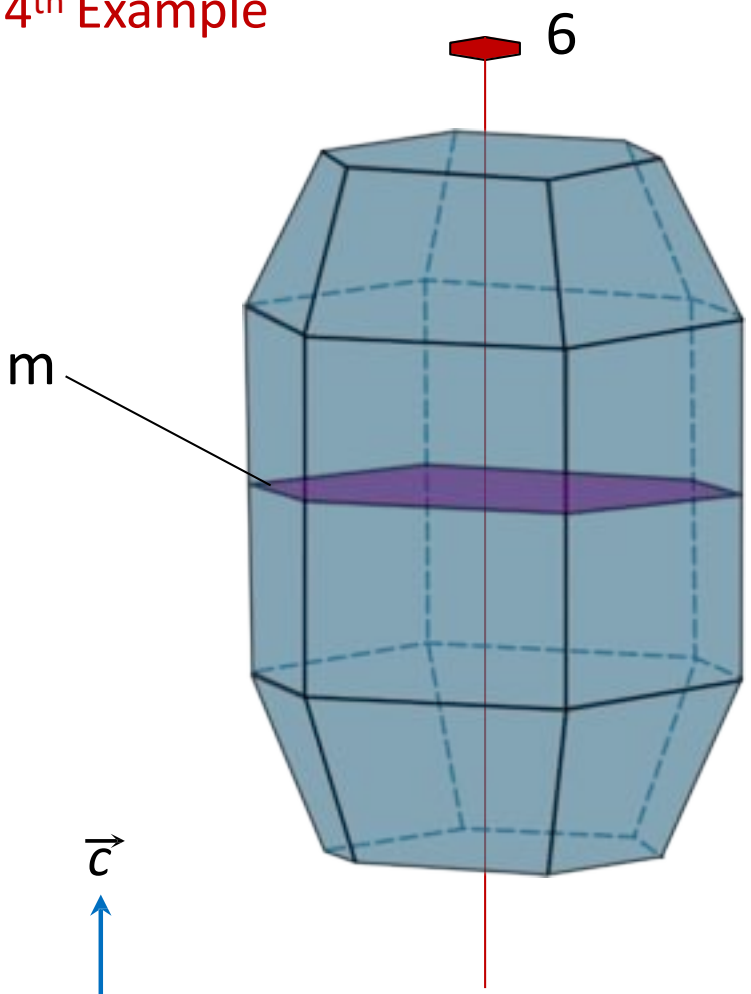
c a [210]

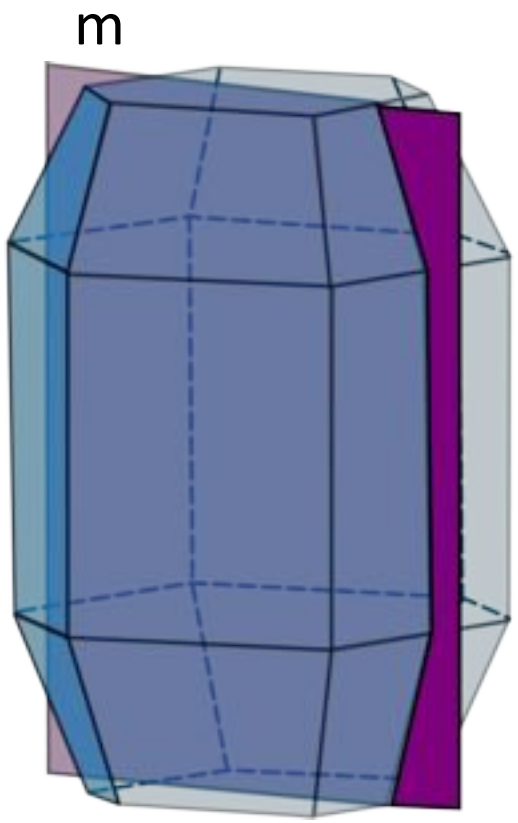
6

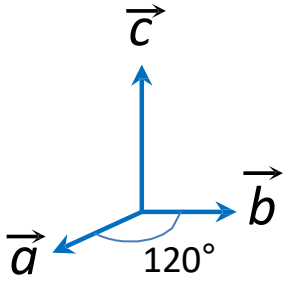
Source: Frank Hoffmann

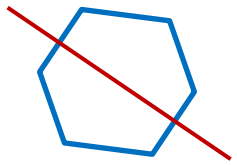
Classify Crystal into Classes

4th Example









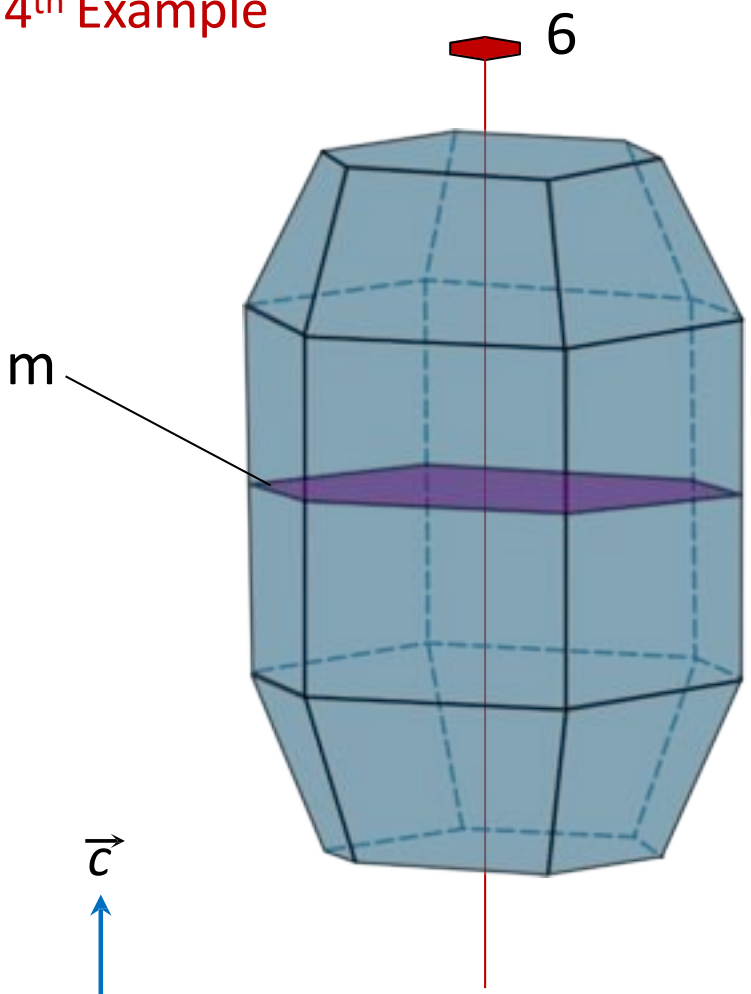
viewing directions
(hexagonal crystal system)

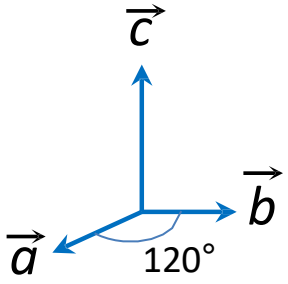
c	a	[210]
$\frac{6}{m}$	m	

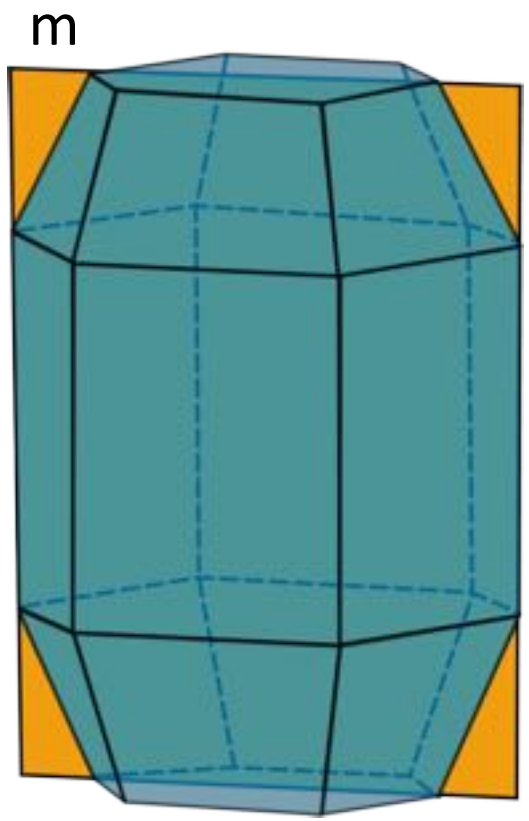
Source: Frank Hoffmann

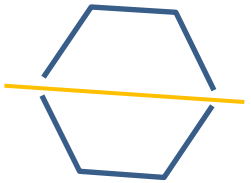
Classify Crystal into Classes

4th Example









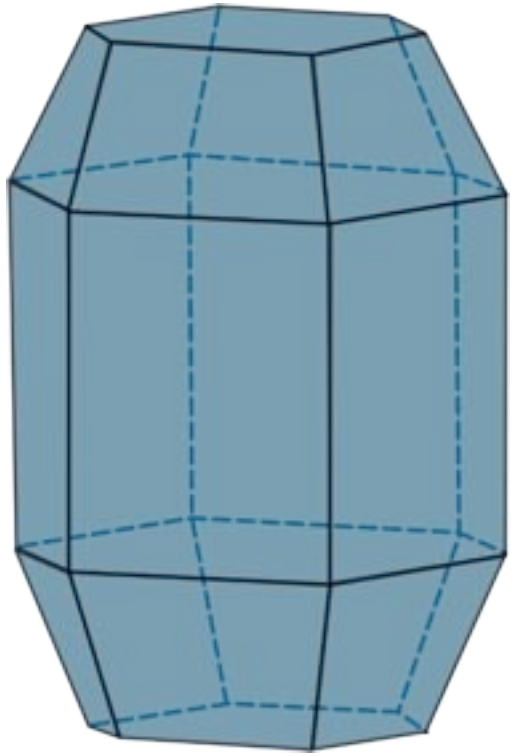
viewing directions
(hexagonal crystal system)

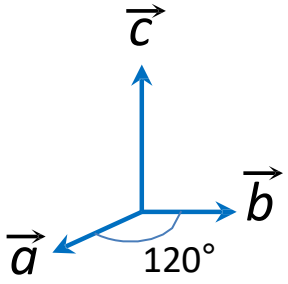
c	a	[210]
$\frac{6}{m}$	m	m

Source: Frank Hoffmann

Classify Crystal into Classes

4th Example





crystal class 6/mmm

dihexagonal-dipyramidal

CuS

Covellite

(Mg, Graphite, Nickeline)

Systematization of Crystal Structures

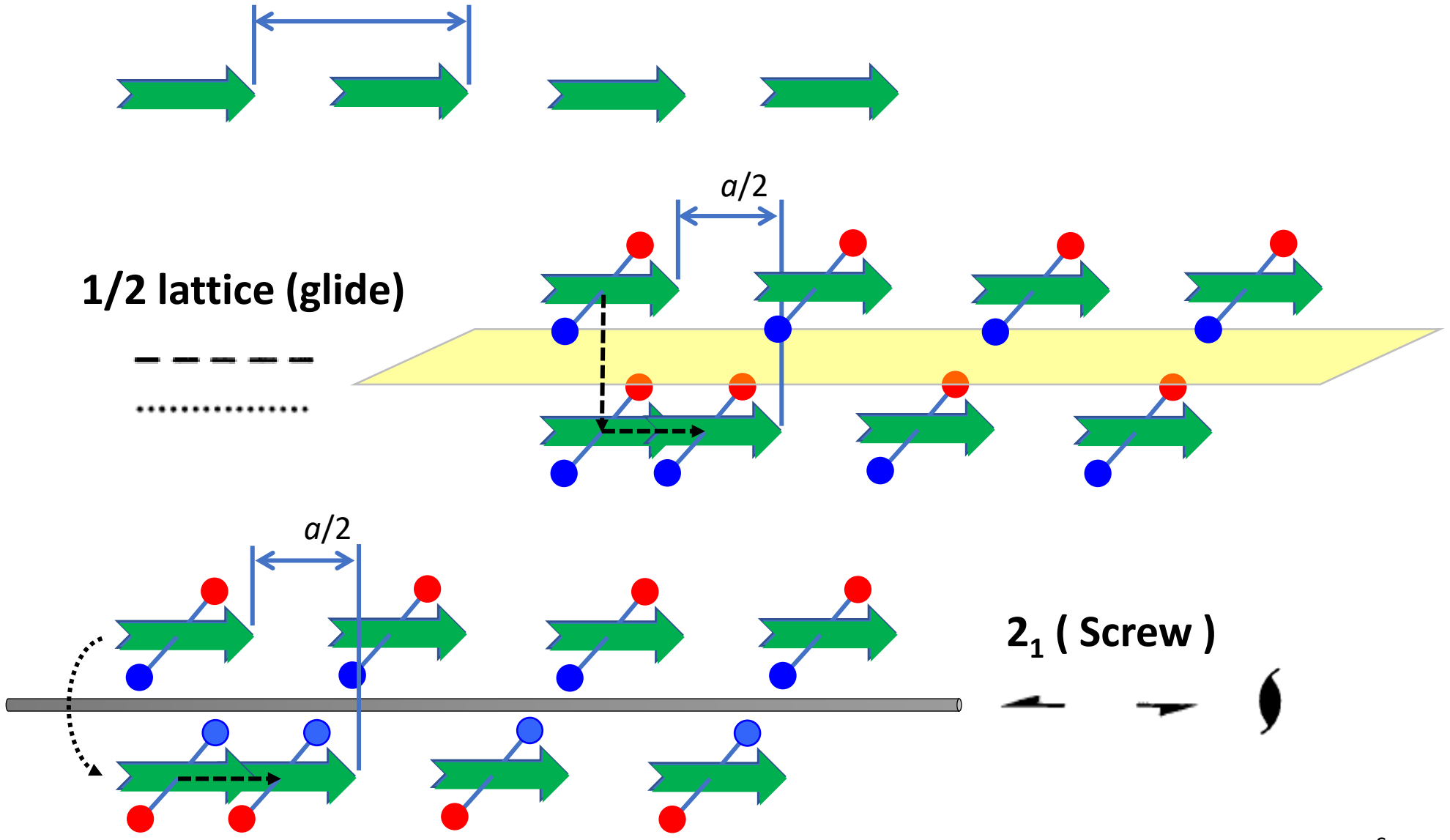
4. Step: Space groups — 230
   complete symmetry

3. Step: Crystal classes — 32
   crystallographic PG

2. Step: Bravais lattices — 14
   primitive + centered

1. Step: Crystal systems — 7
   metric + symmetry of the UC

Translation – Glide – Screw axis

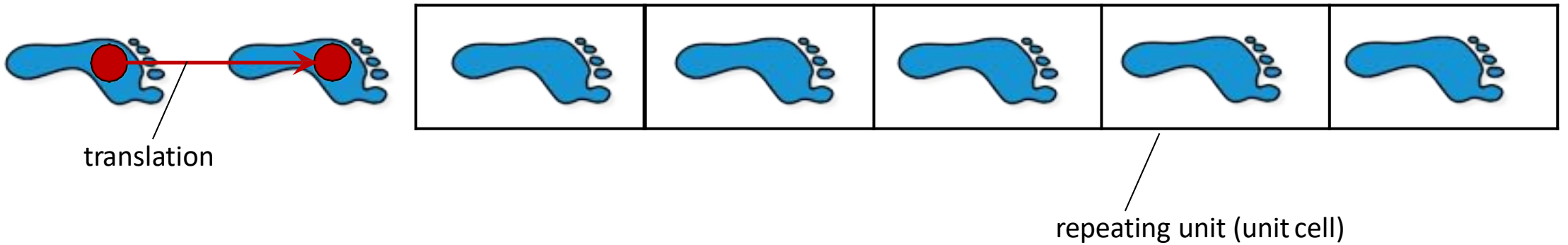


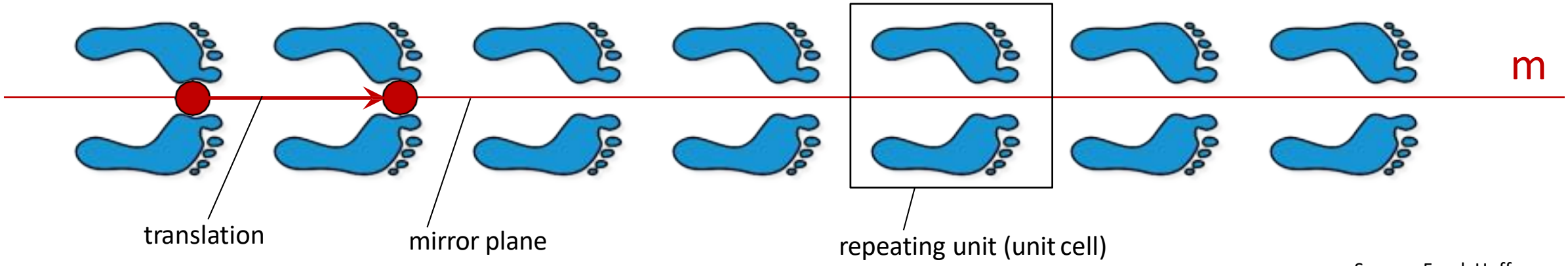
Source: Frank Hoffmann

Translational Symmetry

- There are three symmetry elements, which have a translational component

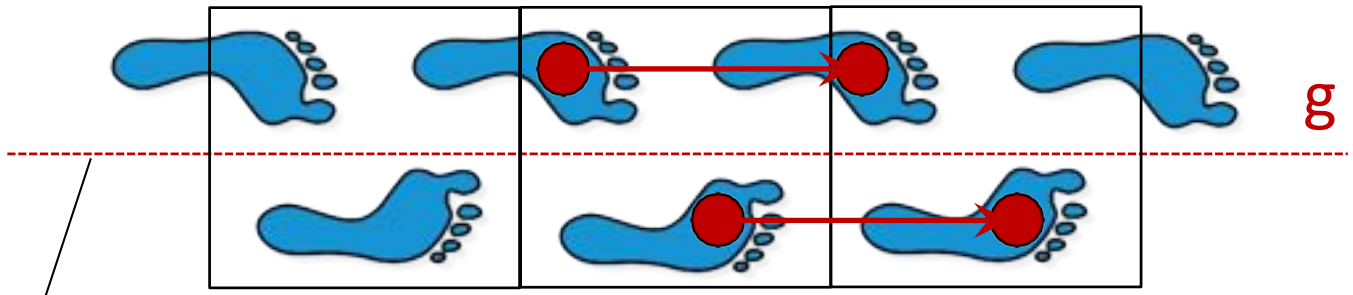
1. Translation (in units of whole unit cells along the lattice vectors)





Source: Frank Hoffmann

Glide Planes/Lines



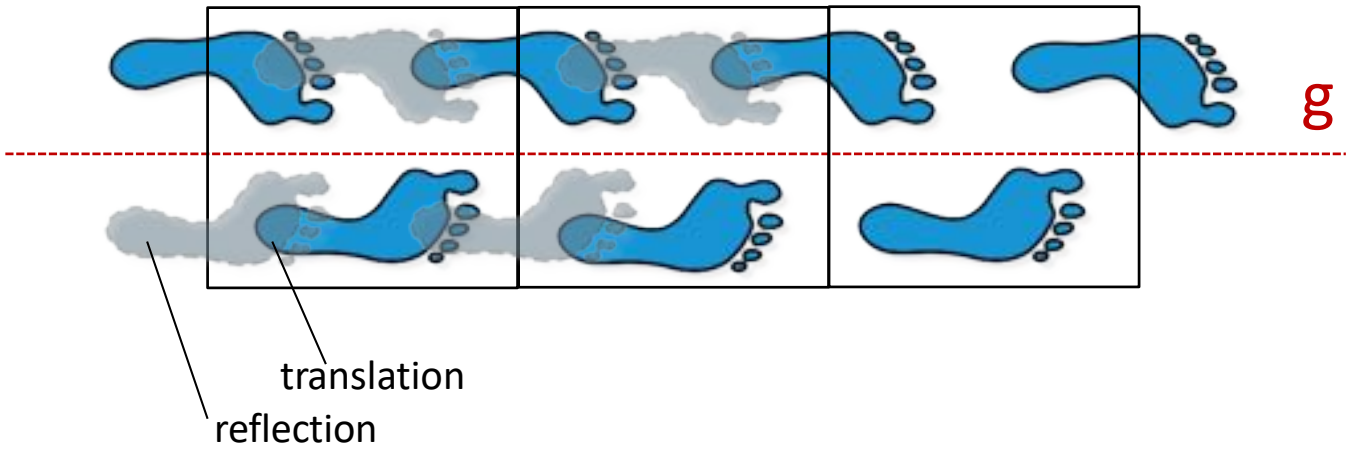
glide line

glide reflection →

(a) reflection at a plane / line
(b) translation (usually by $^1/_2$ of the unit cell)

Source: Frank Hoffmann

Glide Planes/Lines



glide reflection →

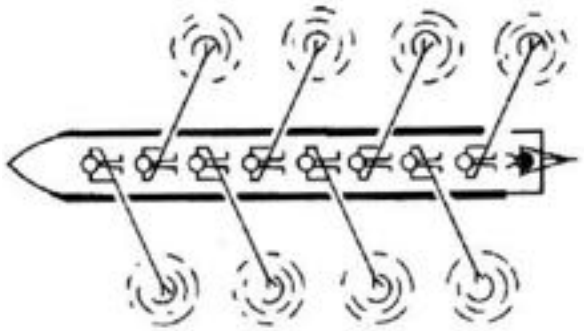
(a) reflection at a plane / line
(b) translation (usually by $^1/_2$ of the unit cell)

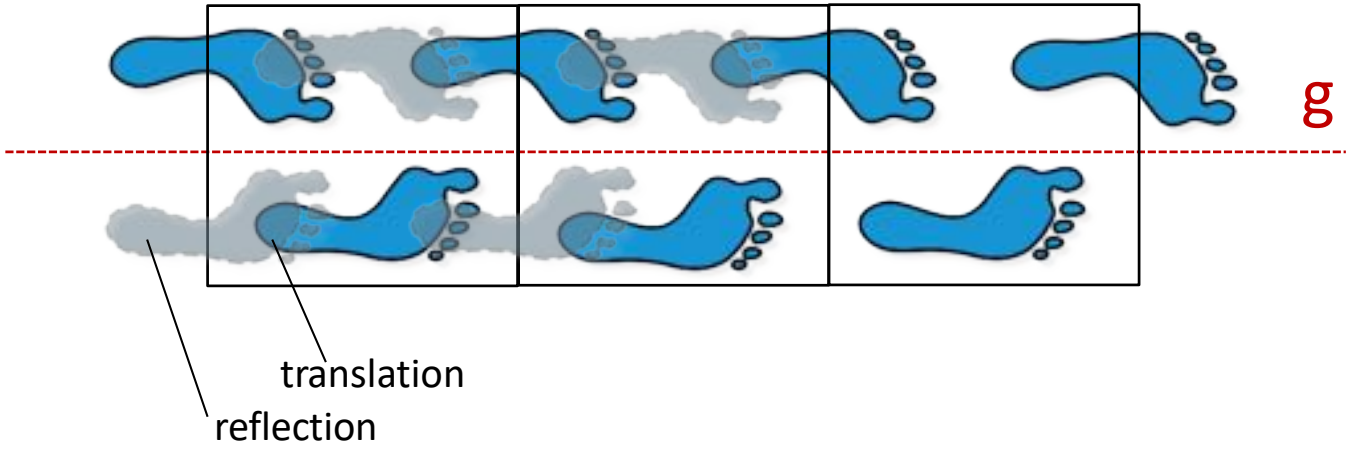
Source: Frank Hoffmann

Glide Planes/Lines

- There are three symmetry elements, which have a translational component

1. Translations (in units of whole unit cells along the lattice vectors)
2. Glide planes / glide axes
3. Screw axes





Kaiser's spotted newt

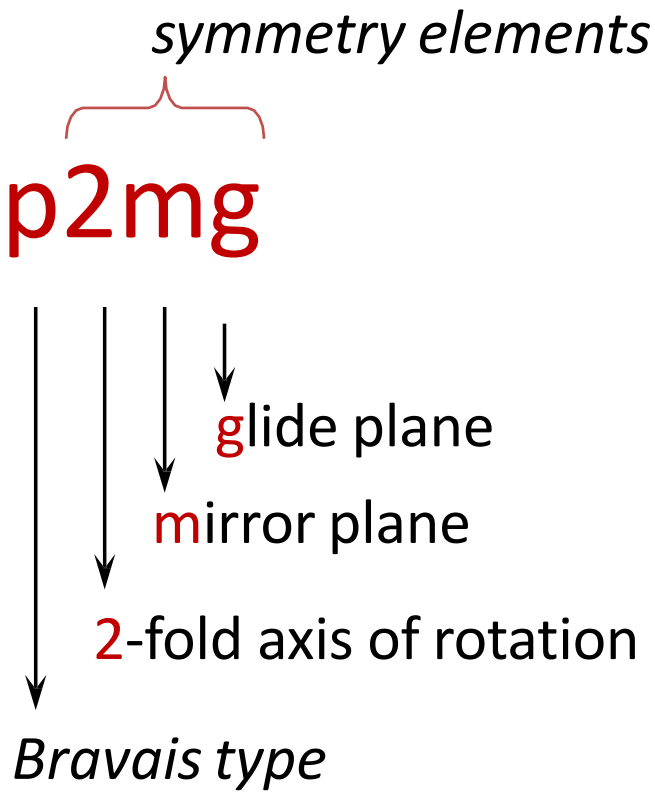
glide reflection →

(a) reflection at a plane / line
(b) translation (usually by $^1/_2$ of the unit cell)

Source: Frank Hoffmann

Notation of Plane Groups

- Notation of Wallpaper groups
  - in full notation always 4 symbols
  - begins with **p** or **c** according to the Bravais lattice type
  - followed by the digit **n** indicating the rotational symmetry order
  - plus two symbols indicating mirrors (**m**), glides (**g**) perpendicular to a) the *x*-axis and b) the *y*-axis
    - if there are no such operators a (**1**) is denoted



Source: Frank Hoffmann

Notation of Plane Groups

- Full and Short Notation of Wallpaper groups

  the short notation drops digits **n** or a **m**
  that can be deduced, so long as that leaves
  no confusion with another plane group

p2mg

Optional assignment: Overlay this pattern with the unit cell and the respective graphical symbols of the symmetry elements at their correct positions within this pattern!

Full	p111	p1m1	p1g1	c1m1	p211	p2mm	p2mg	p2gg	c2mm	p311	p3m1	p31m	p411	p4mm	p4gm	p611	p6mm
Short	p1	pm	pg	cm	p2	pmm	pmg	pgg	cmm	p3	p3m1	p31m	p4	p4m	p4g	p6	p6m

Glade Plane in Crystals

Symmetry operation (SO) ⟷ Symmetry element (SE)

glide reflection — *glide plane*

→ (a) reflection at a plane
(b) translation by $^1/_2$ or $^1/_4$ of the unit cell

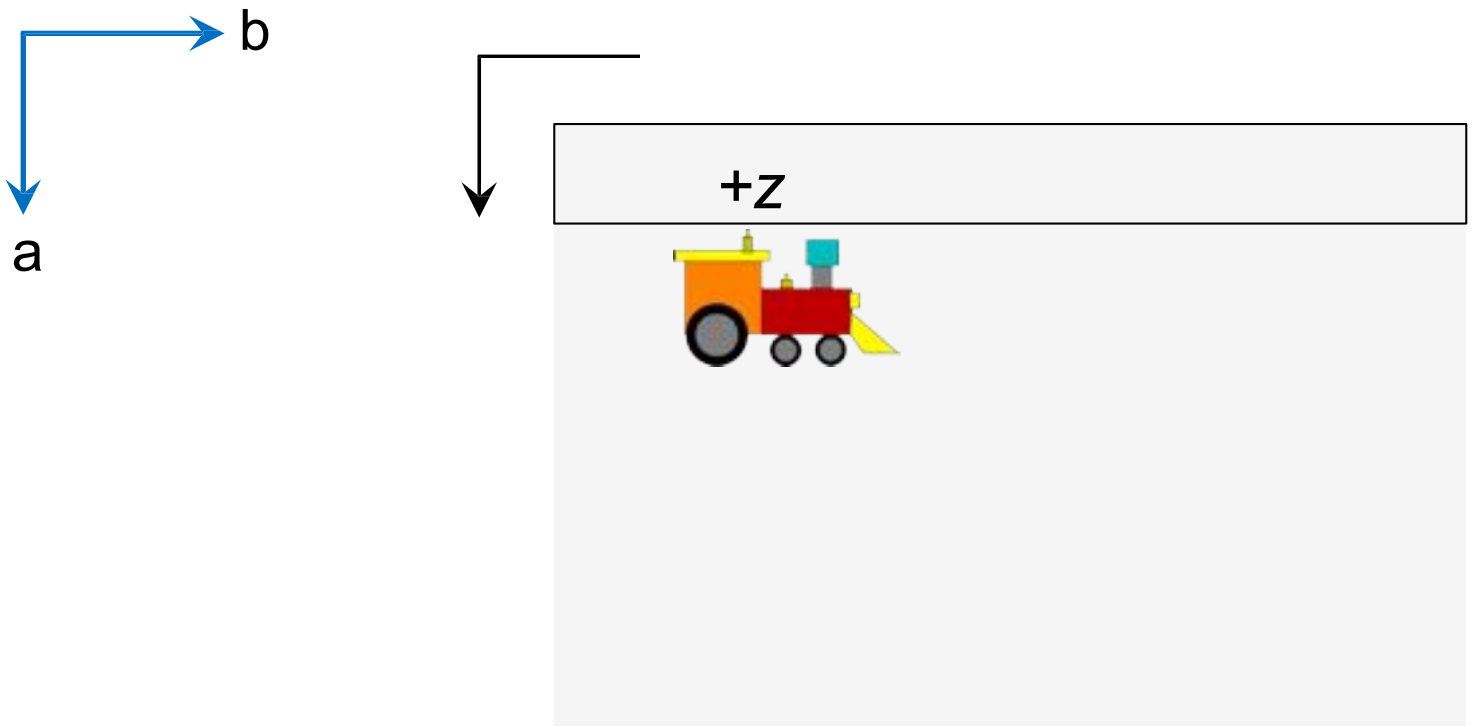
a, b, c, *n, d, e*

characters indicate
the translation direction

Source: Frank Hoffmann

Glade Plane - a

- glide plane *a* ⟶ translation direction = a ⟶ x + ½

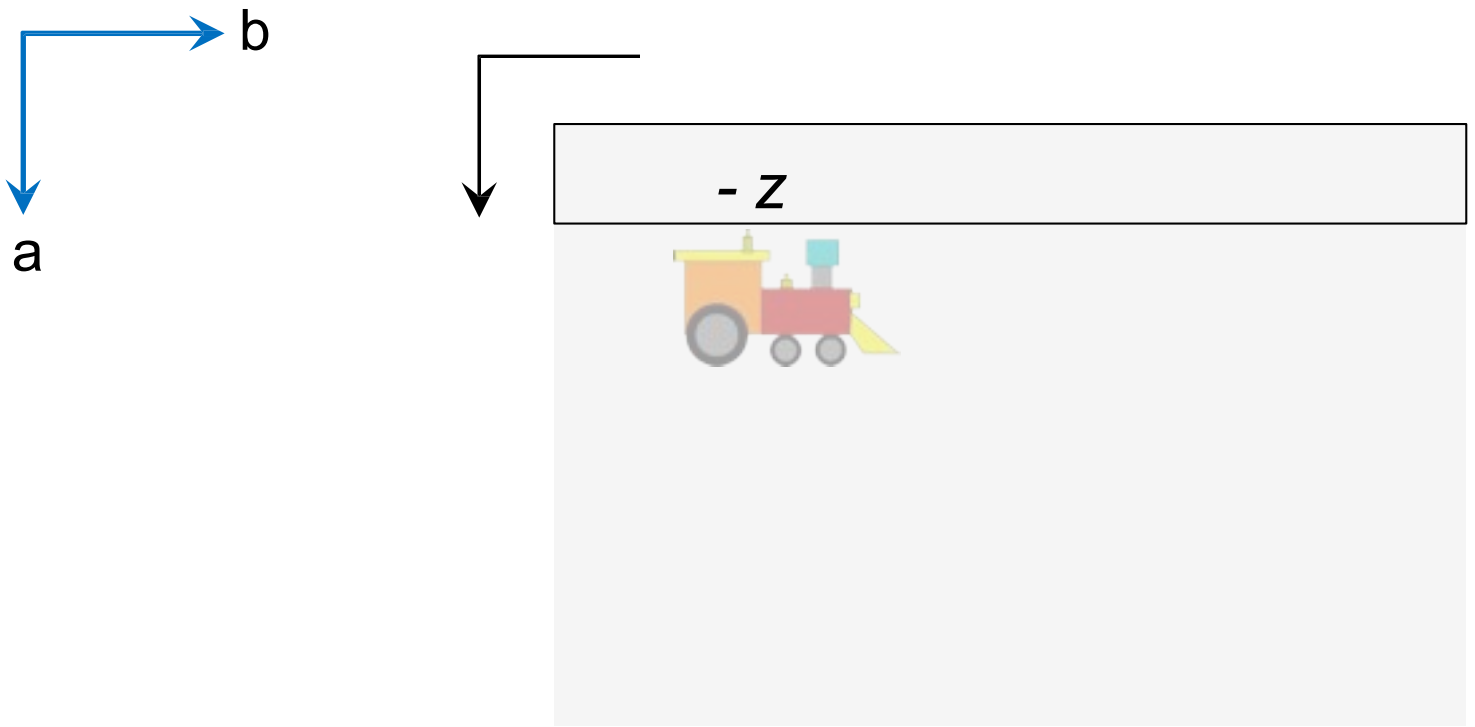


- mirror plane runs parallel to the drawing layer
- additional symbol that indicates the direction of the transition

Source: Frank Hoffmann

Glade Plane - a

- glide plane *a* ⟶ translation direction = a ⟶ x + ½

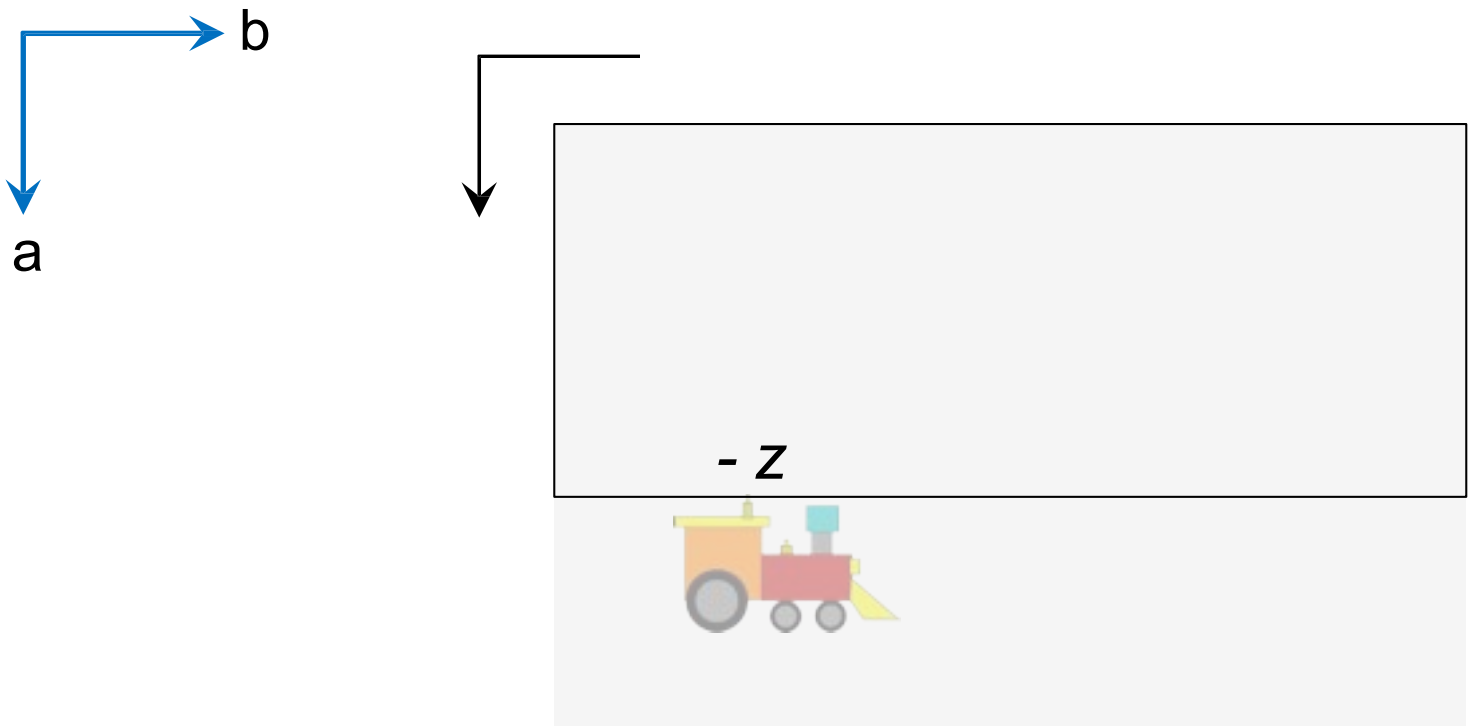


- mirror plane runs parallel to the drawing layer
- additional symbol that indicates the direction of the transition

Source: Frank Hoffmann

Glade Plane - a

- glide plane *a* ⟶ translation direction = a ⟶ x + ½

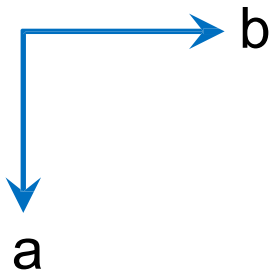


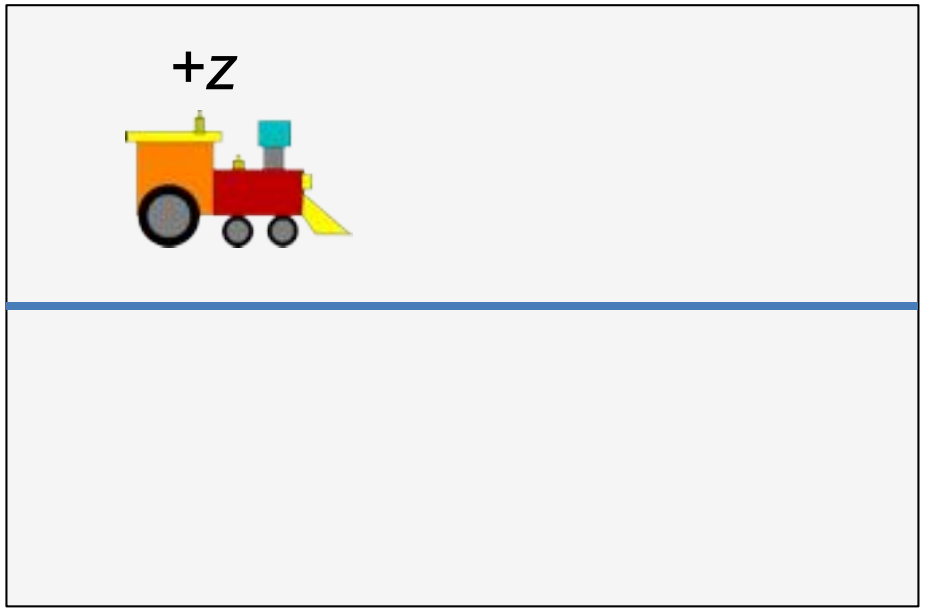
- mirror plane runs parallel to the drawing layer
- additional symbol that indicates the direction of the transition

Source: Frank Hoffmann

Glade Plane - b

- glide plane *b* ⟶ translation direction = b ⟶ y + ½



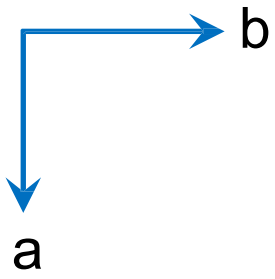


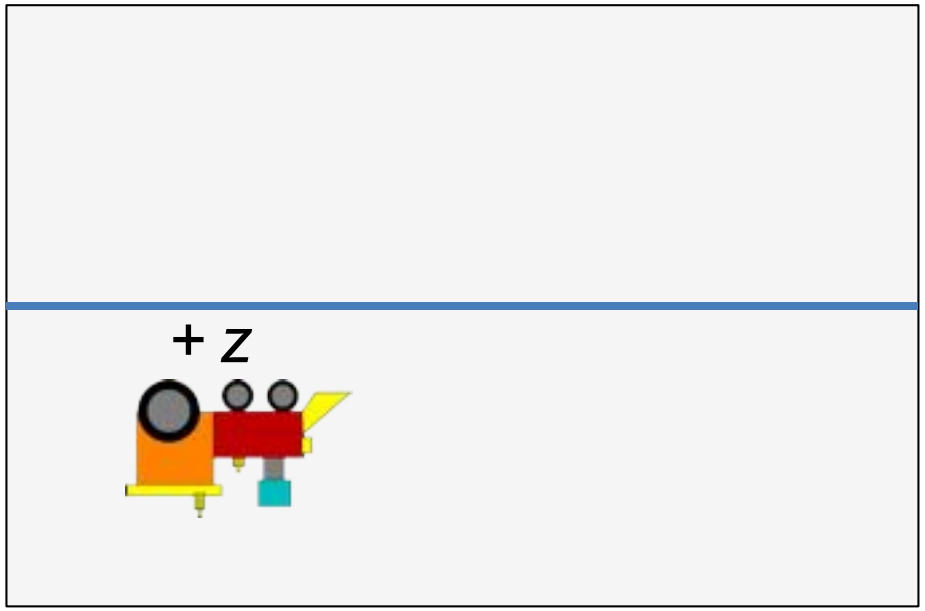
- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane - b

- glide plane *b* → translation direction = b → y + ½



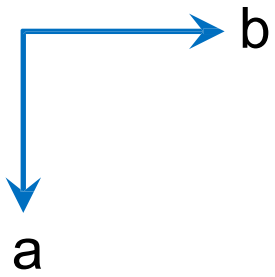


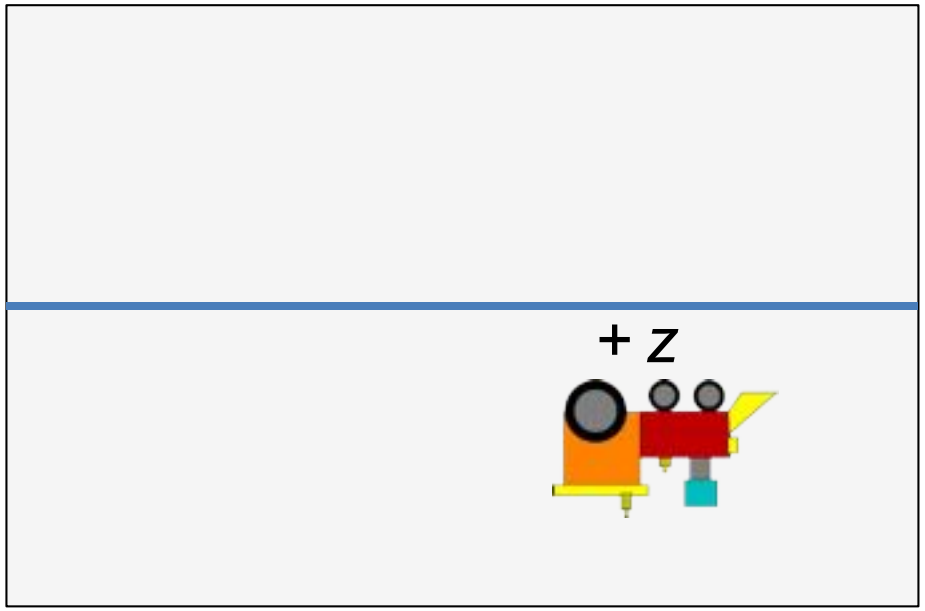
- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane - b

- glide plane *b* ⟶ translation direction = b ⟶ y + ½



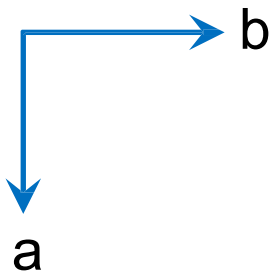


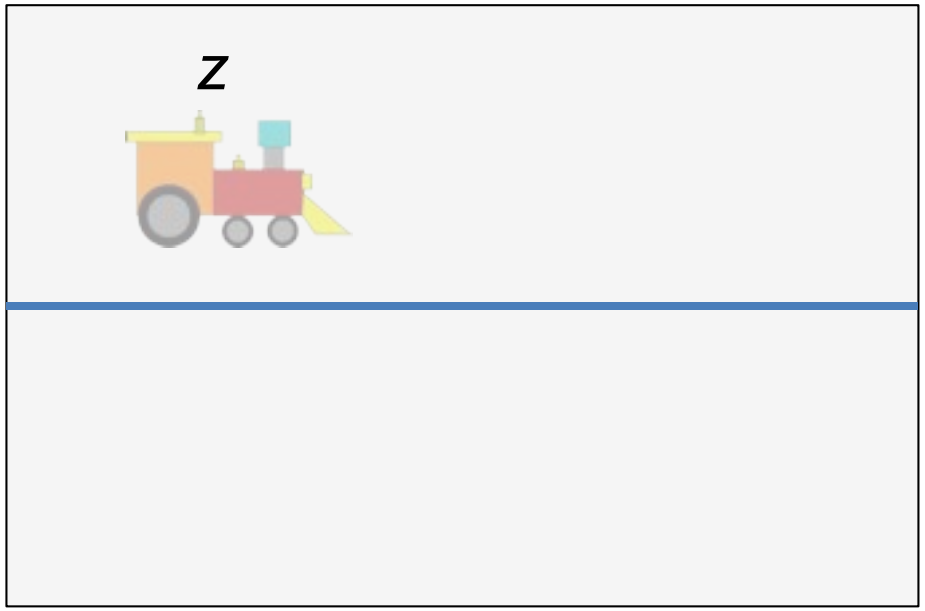
- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane - c

- glide plane *c* ⟶ translation direction = c ⟶ z + ½



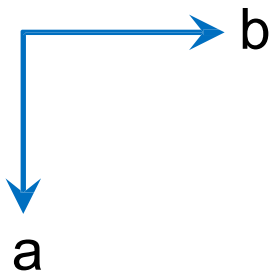


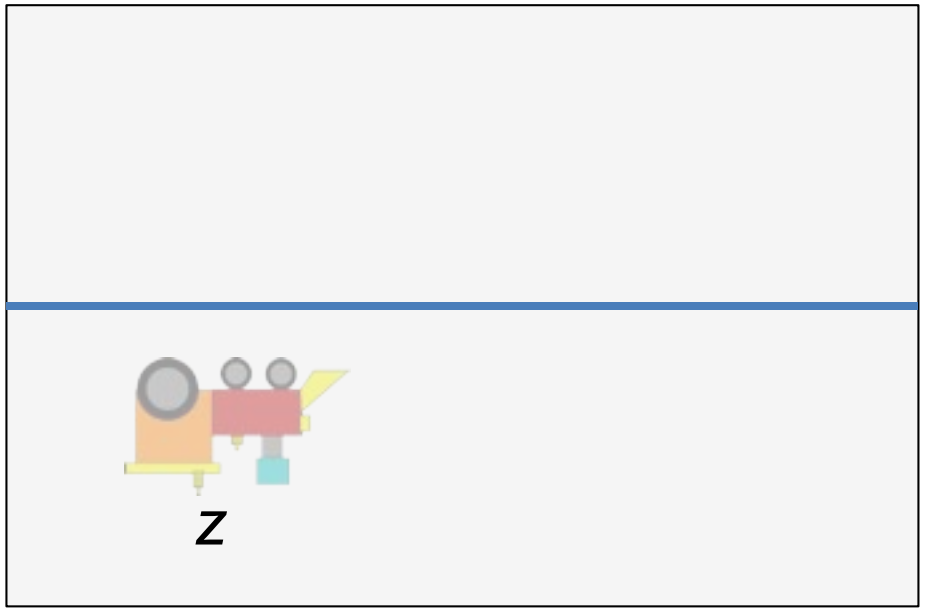
- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane - c

- glide plane *c* ⟶ translation direction = c ⟶ z + ½



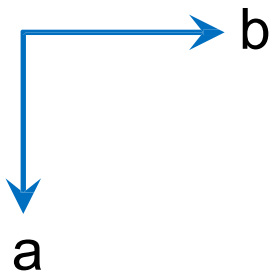


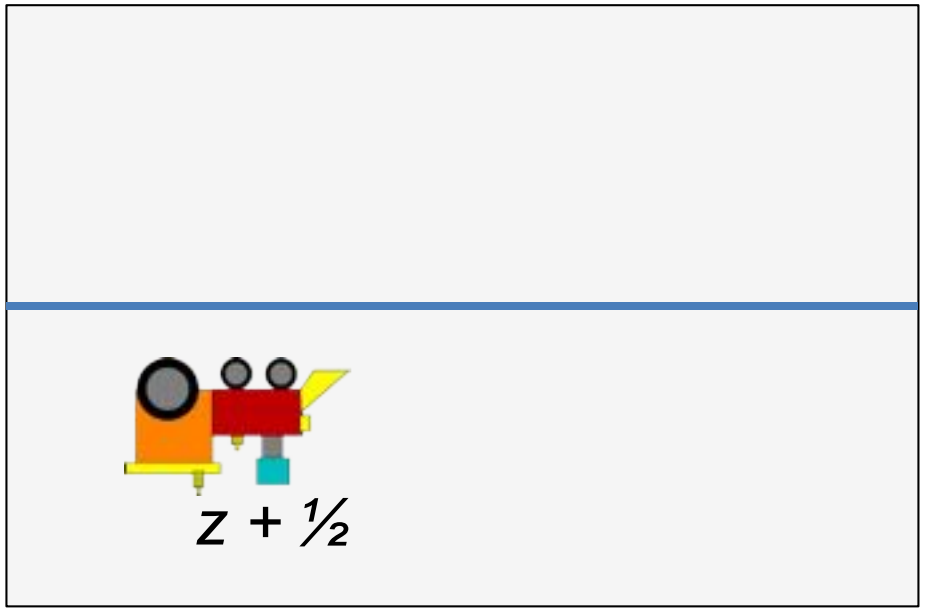
- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane - c

- glide plane *c* ⟶ translation direction = c ⟶ z + ½





- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

Glade Plane in Crystals

Symmetry operation (SO) ⟷ Symmetry element (SE)

glide reflection — *glide plane*

→ (a) reflection at a plane
(b) translation by $^1/_2$ or $^1/_4$ of the unit cell

a, b, c, ***n, d, e***

Source: Frank Hoffmann

diagonal Glade Plane - n

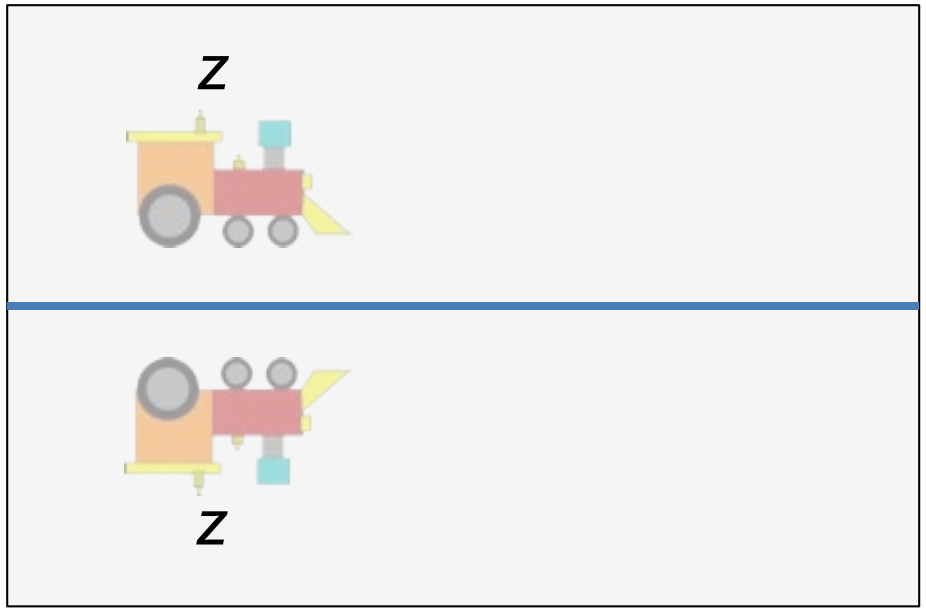
- glide plane *n* ⟶ translation direction = diago*n*al

⟶ y + ½

b ⟶ z + ½

i.e. in the (*b*,*c*) plane

a



- mirror plane perpendicular to the drawing layer

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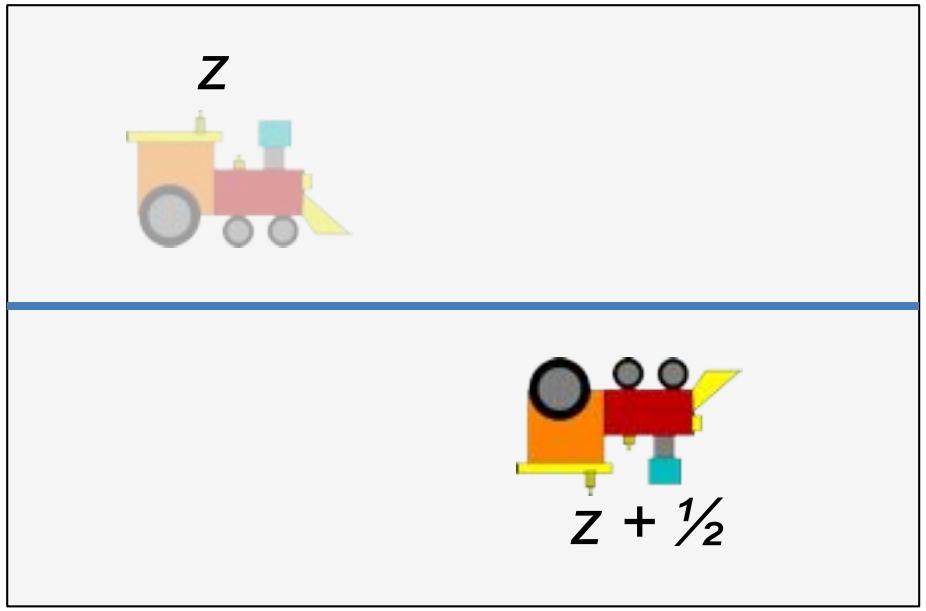

- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

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⟶ y + ½

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i.e. in the (*b*,*c*) plane

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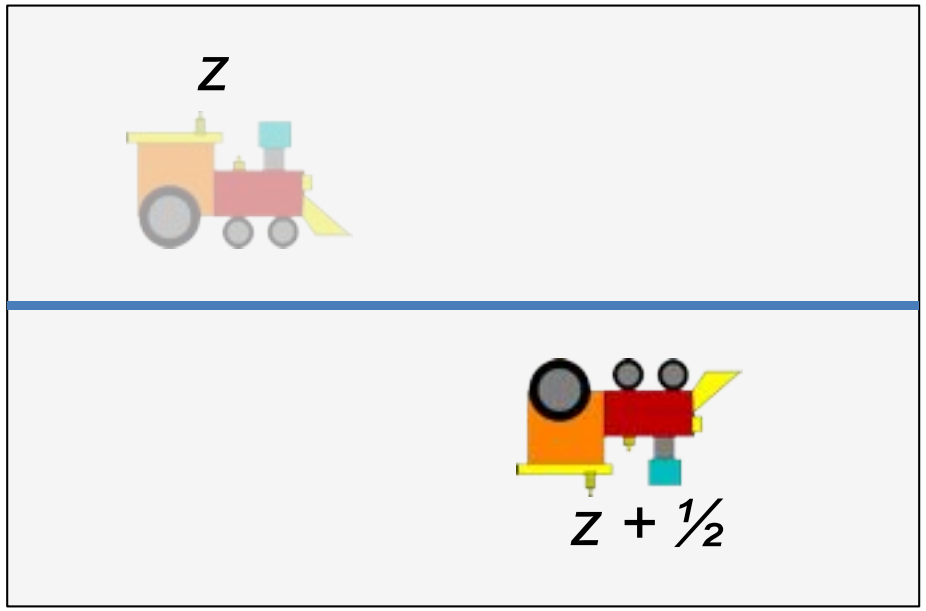
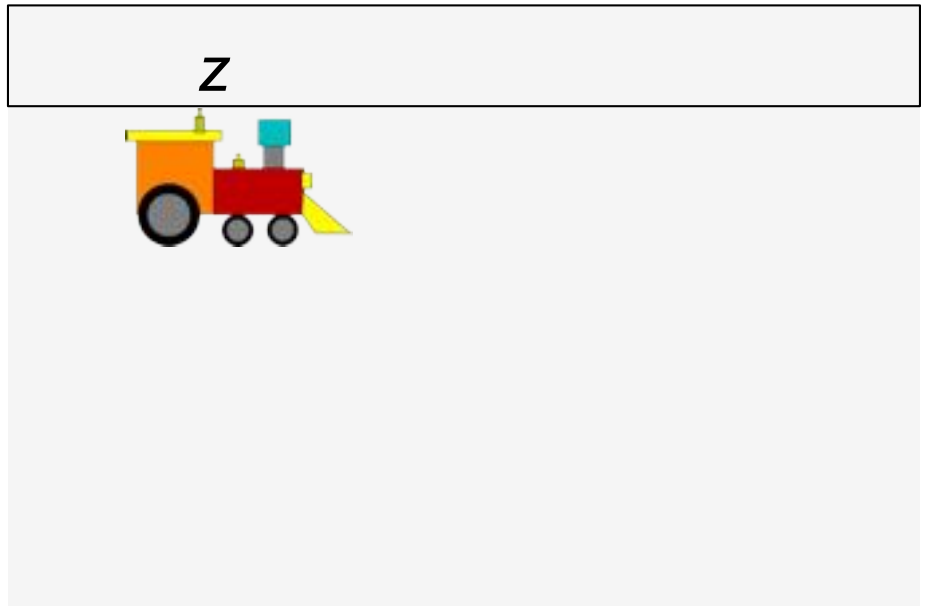


- mirror plane perpendicular to the drawing layer

⟶ x + ½

⟶ y + ½

i.e. in the (*a*,*b*) plane



- mirror plane runs parallel to the drawing layer

diagonal Glade Plane - n

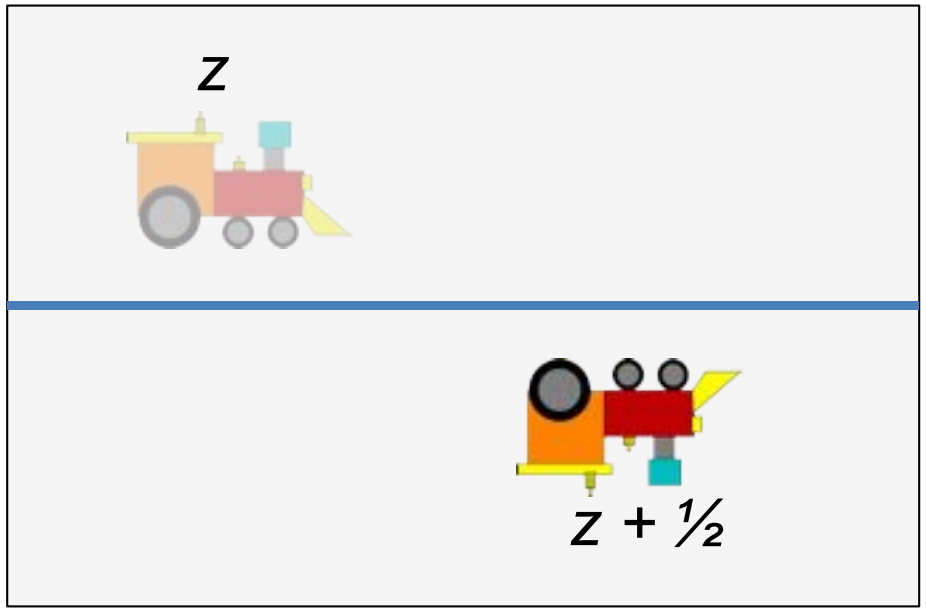
- glide plane *n* → translation direction = diago*n*al

→ y + ½
→ z + ½

b

a

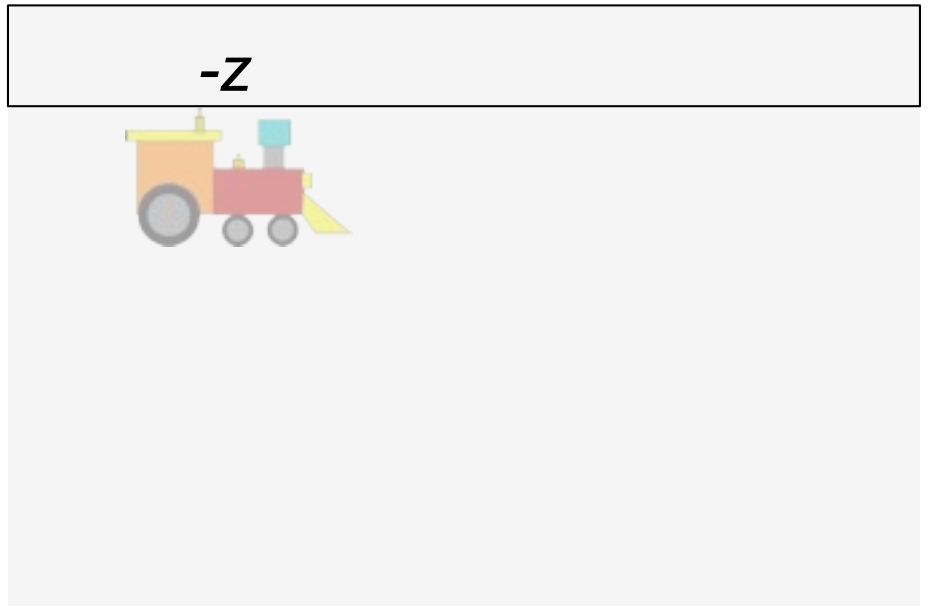
i.e. in the (*b*,*c*) plane



- mirror plane perpendicular to the drawing layer

→ x + ½
→ y + ½

i.e. in the (*a*,*b*) plane



- mirror plane runs parallel to the drawing layer

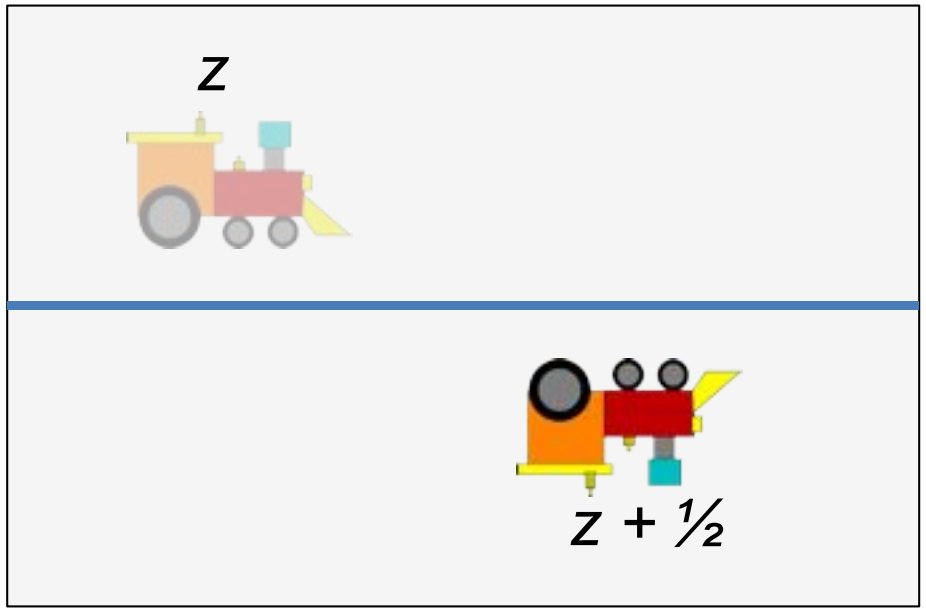
diagonal Glade Plane - n

- glide plane *n* ⟶ translation direction = diago*n*al

⟶ y + ½
b ⟶ z + ½

i.e. in the (*b*,*c*) plane

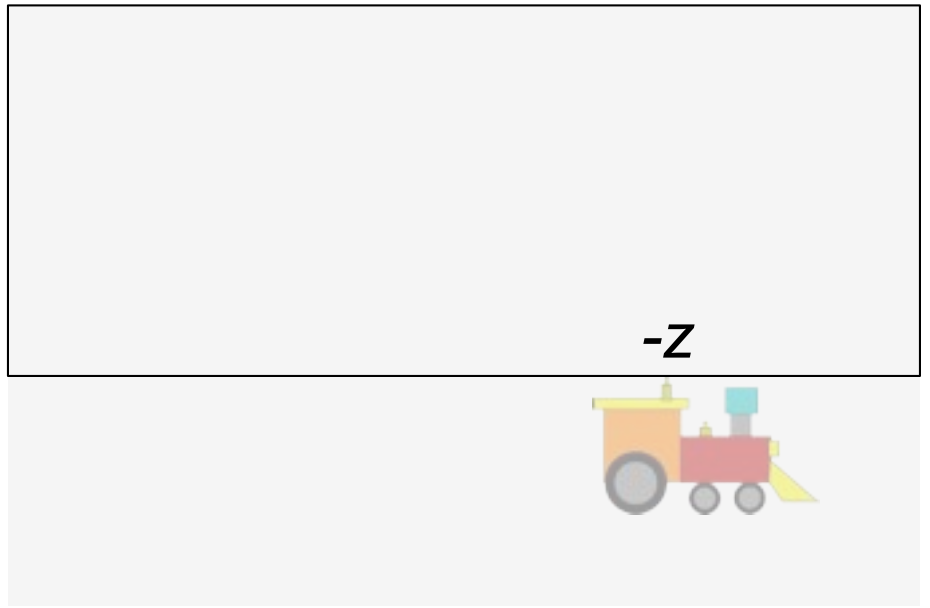
a



- mirror plane perpendicular to the drawing layer

⟶ x + ½
⟶ y + ½

i.e. in the (*a*,*b*) plane

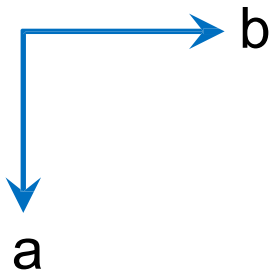


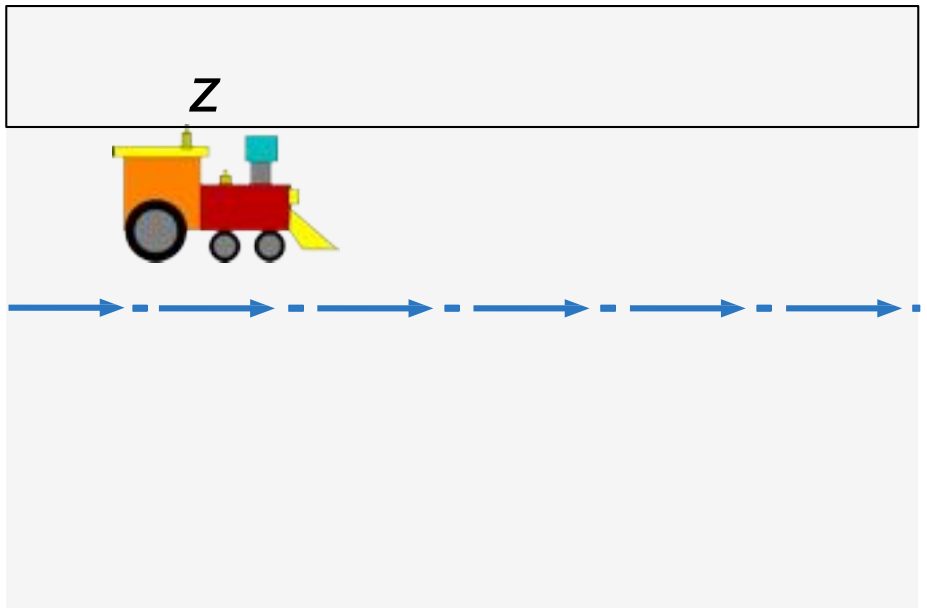
- mirror plane runs parallel to the drawing layer

diamond like Glade Plane - d

- glide plane *d* → translation direction = *d*iagonal as in *d*iamond
  - → y + ¼ (!)
  - → z + ¼ (!)

i.e. in the (*b*,*c*) plane





- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

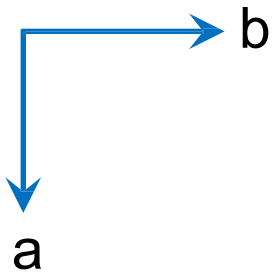
diamond like Glade Plane - d

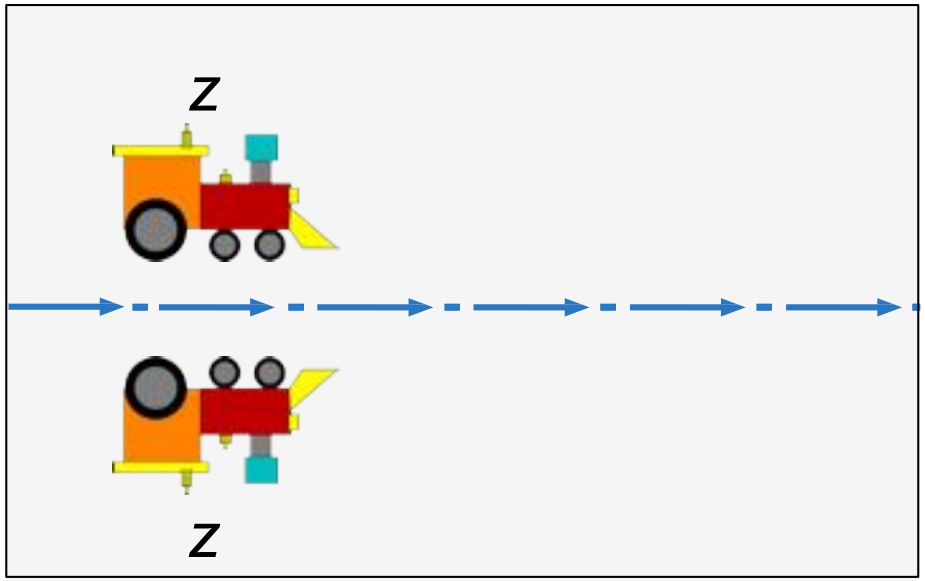
- glide plane *d* ⟶ translation direction = *d*iagonal as in *d*iamond

⟶ y + ¼ (!)

⟶ z + ¼ (!)

i.e. in the (*b*,*c*) plane





- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

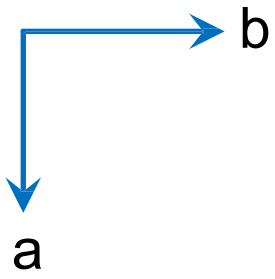
diamond like Glade Plane - d

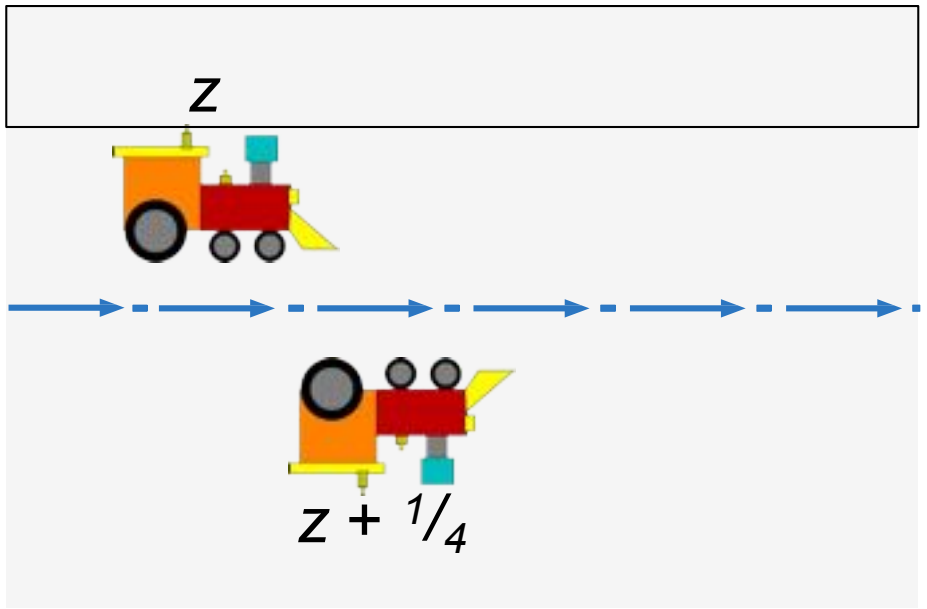
- glide plane *d* ⟶ translation direction = *d*iagonal as in *d*iamond

⟶ y + ¼ (!)

⟶ z + ¼ (!)

i.e. in the (*b*,*c*) plane





- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

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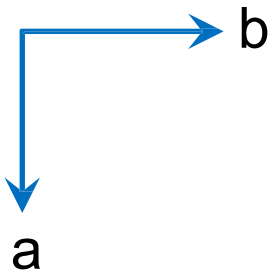
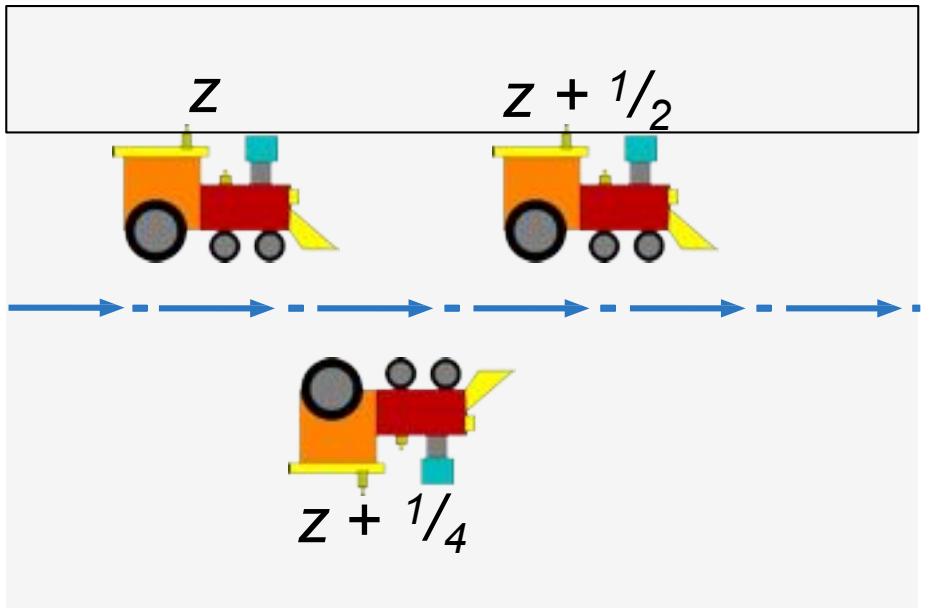
- glide plane *d* ⟶ translation direction = *d*iagonal as in *d*iamond

⟶ y + ¼ (!)

⟶ z + ¼ (!)

i.e. in the (*b*,*c*) plane





- mirror plane perpendicular to the drawing layer

Source: Frank Hoffmann

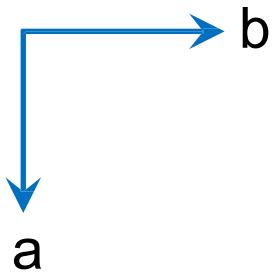
diamond like Glade Plane - d

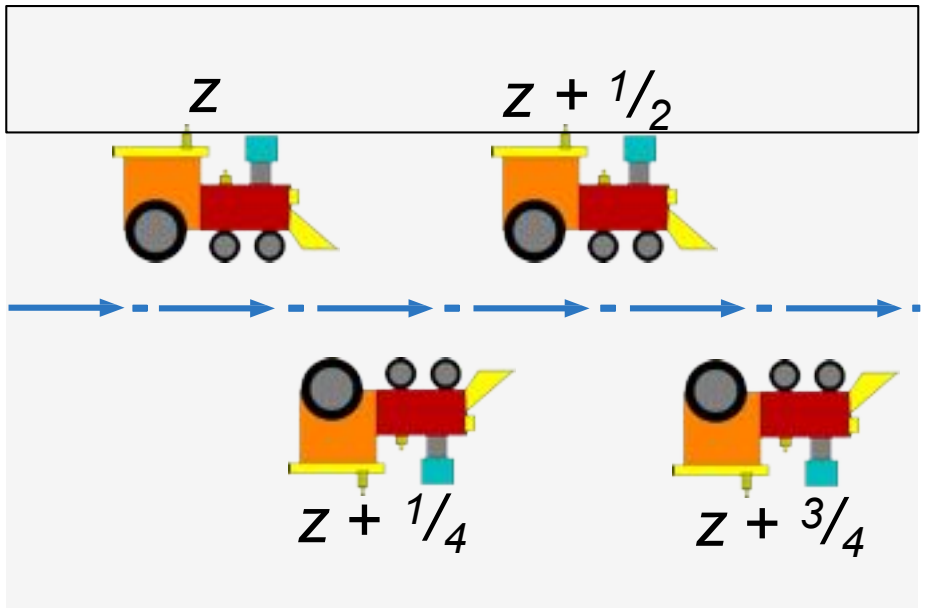
- glide plane *d* ⟶ translation direction = *d*iagonal as in *d*iamond

⟶ y + ¼ (!)

⟶ z + ¼ (!)

i.e. in the (*b*,*c*) plane





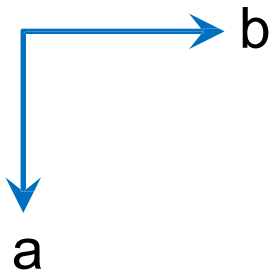
- mirror plane perpendicular to the drawing layer

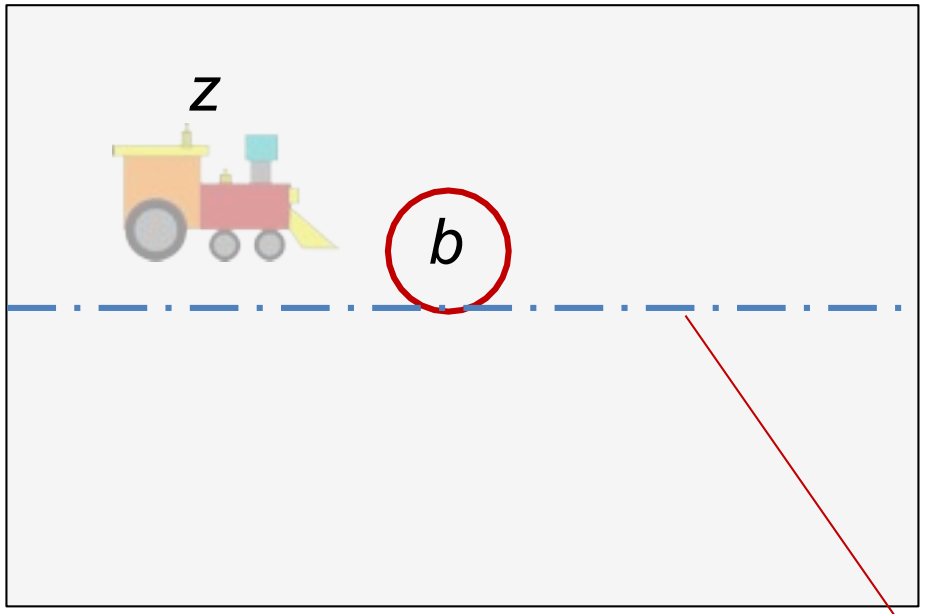
Source: Frank Hoffmann

Double Glide Plane - e

- glide plane *e* → translation direction = b *and* c
  - → y + ½
  - → z + ½

i.e. in the (*b*,*c*) plane





- mirror plane perpendicular to the drawing layer
- there are two glide planes at once with two glide directions perpendicular to each other

these are two glide planes, both equally oriented!

Source: Frank Hoffmann

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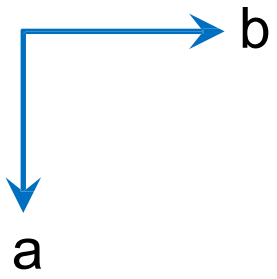
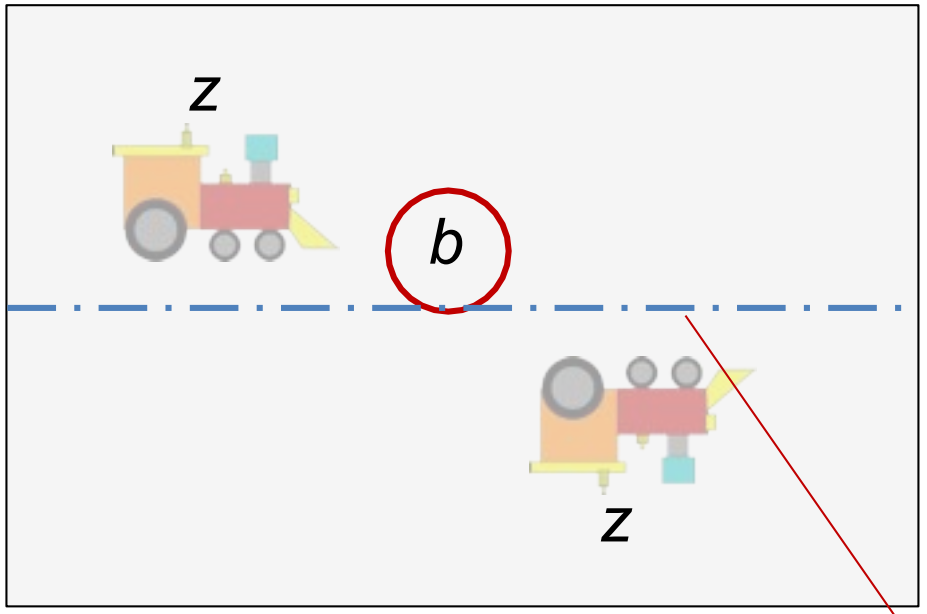
i.e. in the (*b*,*c*) plane





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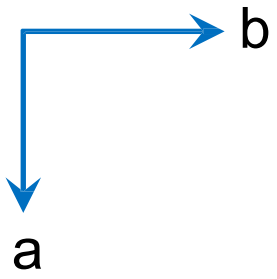

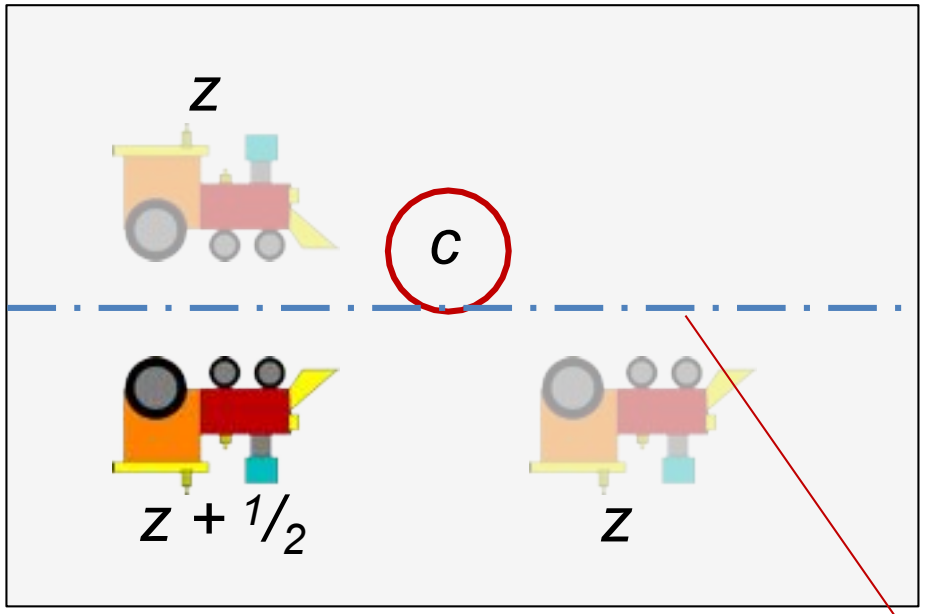

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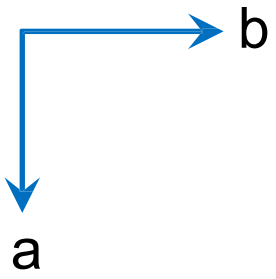

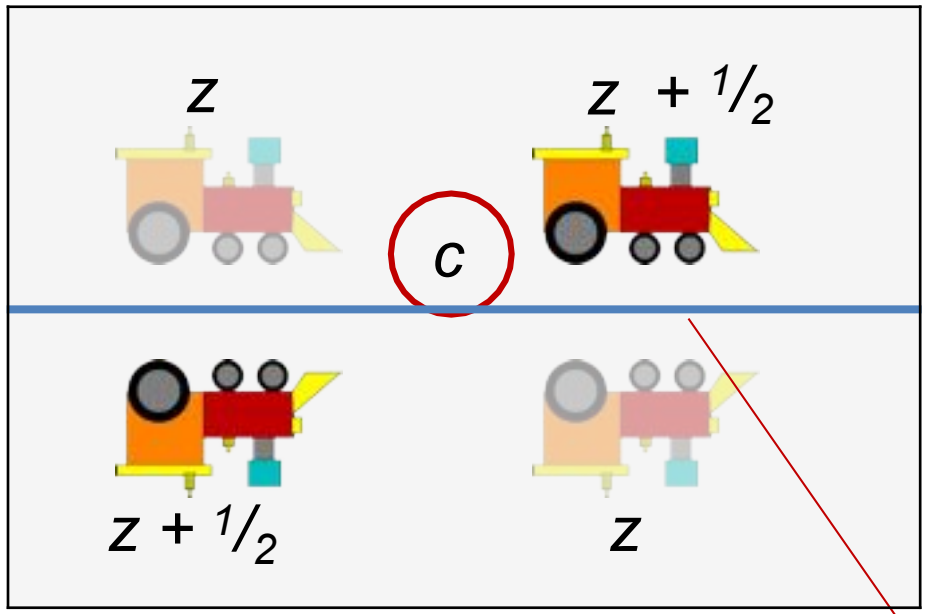

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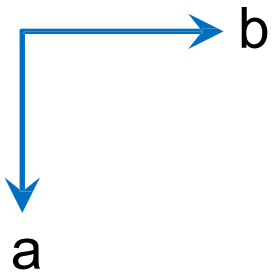

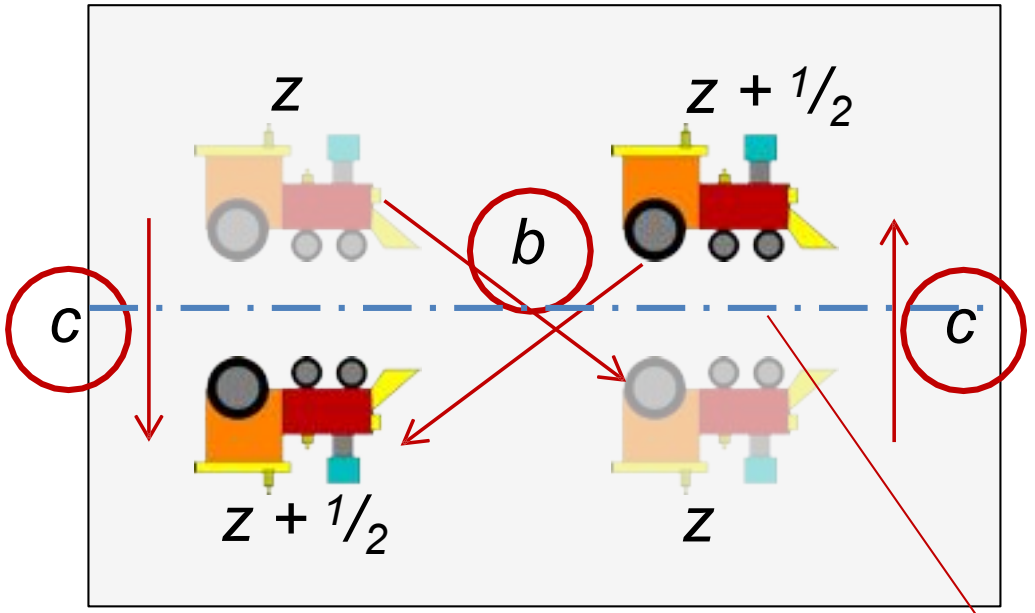

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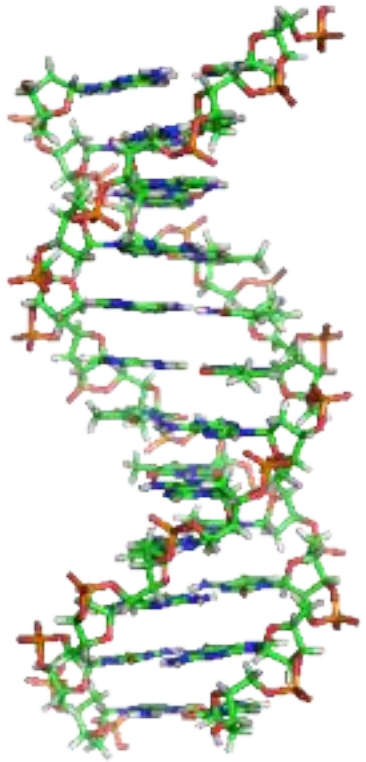
Source: Frank Hoffmann

Double Helices



B-DNA
double helix

double spiral staircase

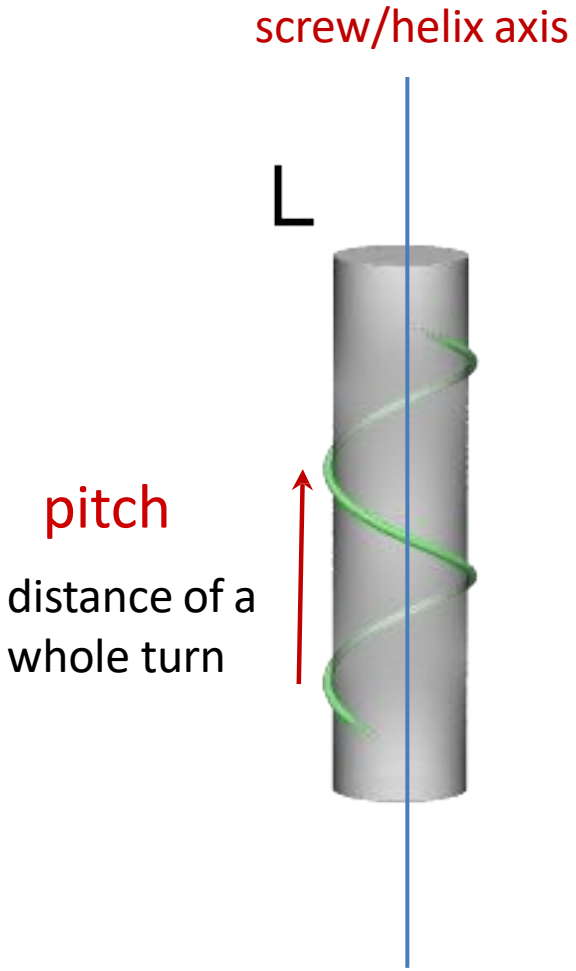
http://www.olafureliasson.net/

climber plant

screw

Source: Frank Hoffmann

Characteristics of Helices



Source: Frank Hoffmann

Characteristics of Helices

handedness

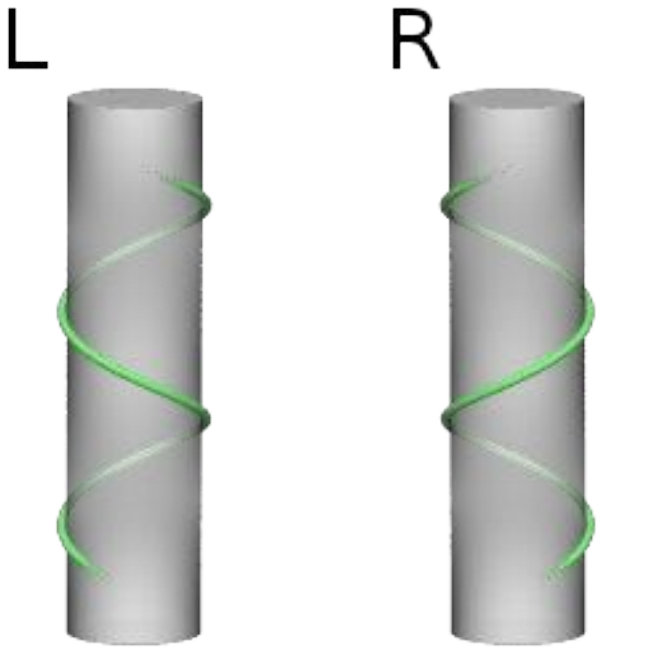


image mirror image

chiral objects

with the viewing direction along axis of the helix…

→ …if a clockwise screwing motion moves the helix away from the observer, then it is called a right- handed helix

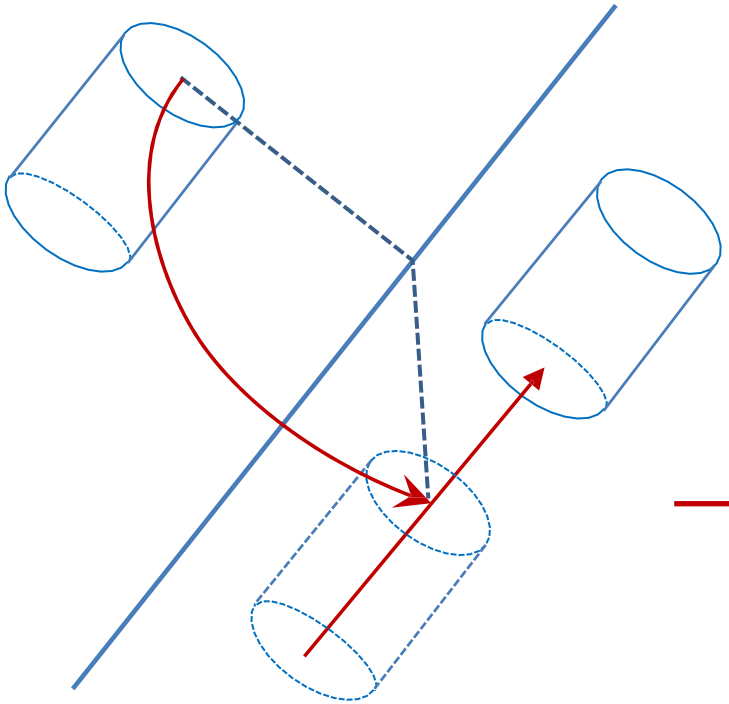
→ …if a counter-clockwise screwing motion moves the helix away from the observer, then it is called a left-handed helix

Source: Frank Hoffmann

Screw Axes

Symmetry operation (SO) ⟷ Symmetry element (SE)

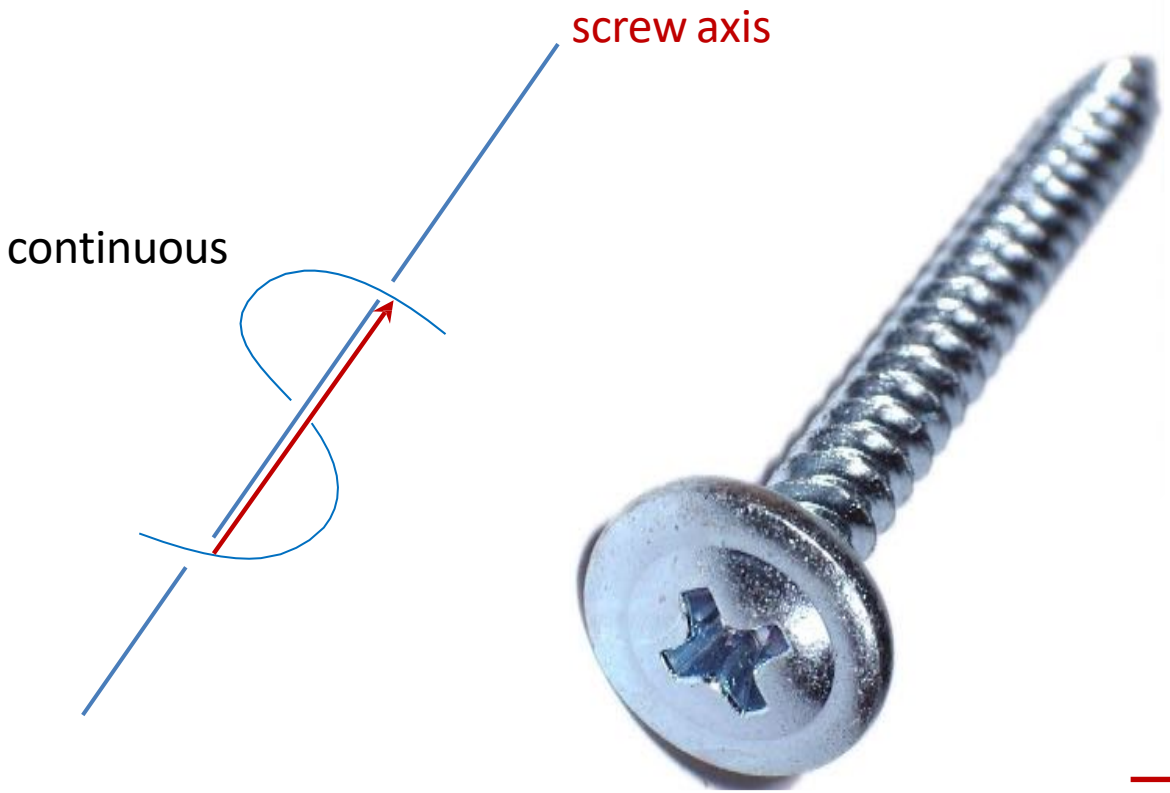
screw rotation *screw axis*

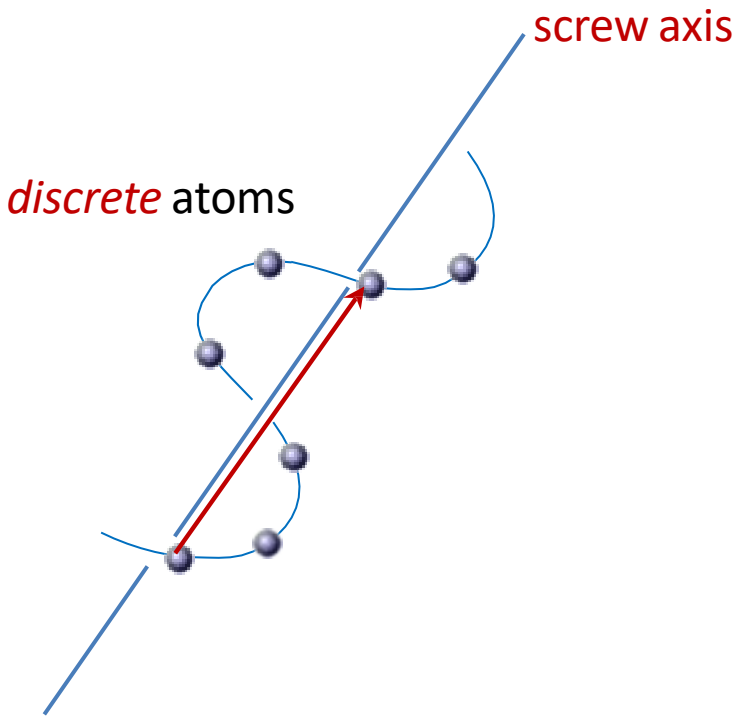


(a) rotation around the axis
(b) translation parallel to the axis

Source: Frank Hoffmann

Characteristics of Helices





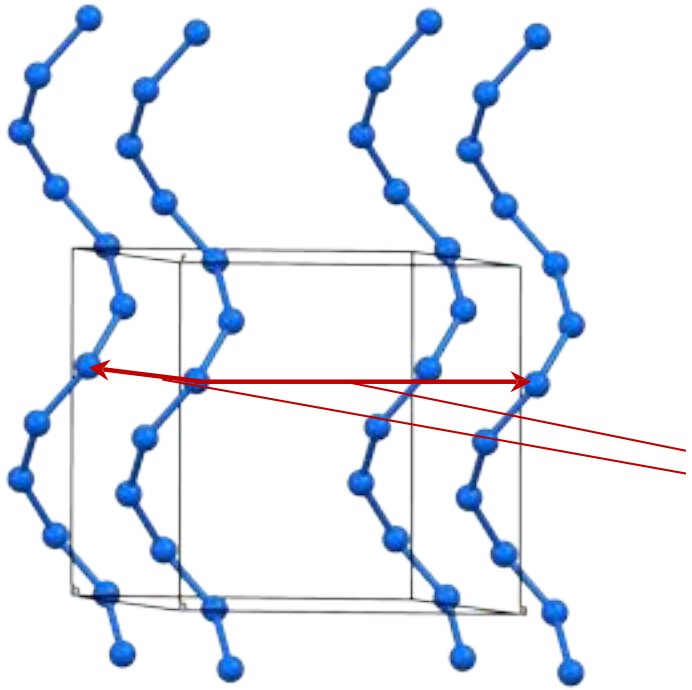
→ rotational order = ∞

→ rotational part limited

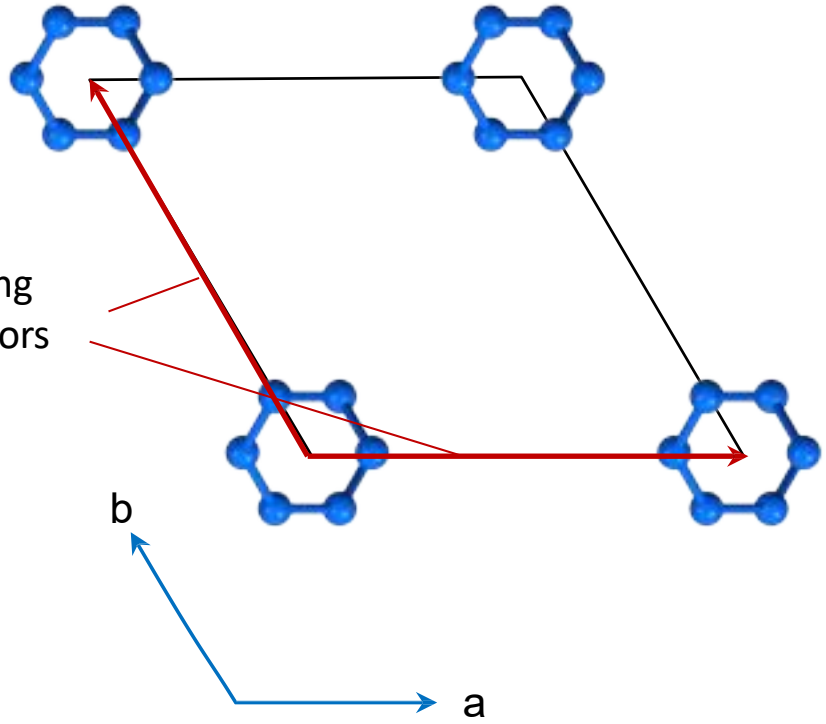
→ rotational order is restricted to 1 to 4 and 6!

Source: Frank Hoffmann

Screw Axes in Crystal Structure



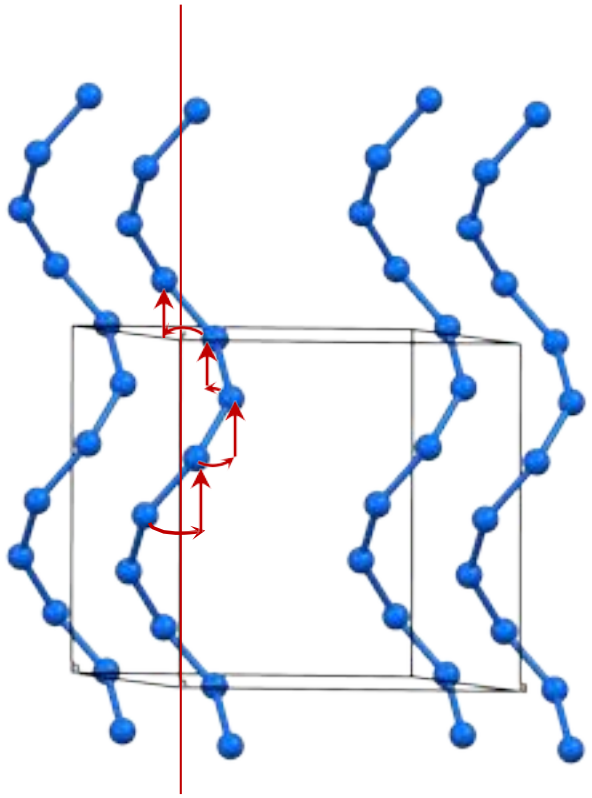
translation along
the lattice vectors

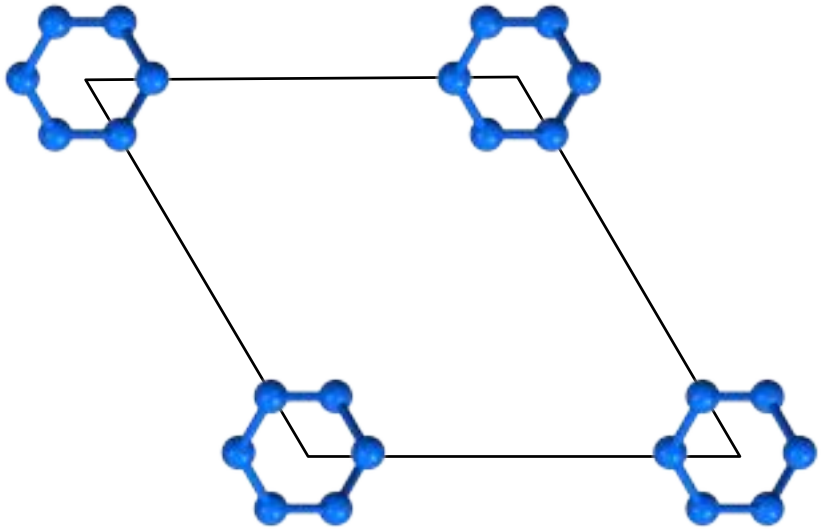


Source: Frank Hoffmann

Screw Axes in Crystal Structure

screw axis





→ (a) rotation by 360°/6 = 60°
(b) translation by $^1/_6$ of the unit cell

→ 6-fold screw axis → 6_1 → translational component = 1/6

Source: Frank Hoffmann

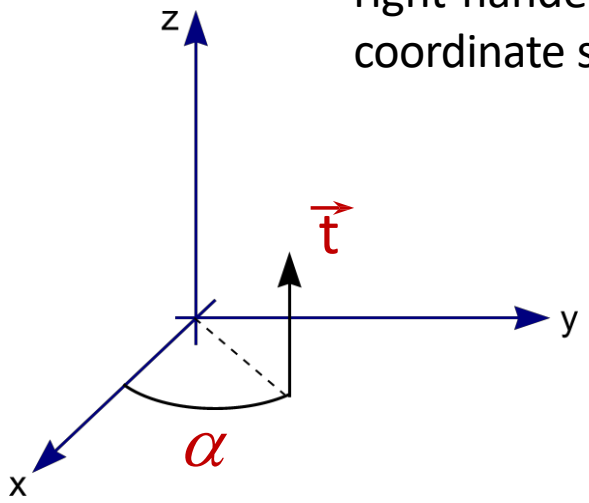
Screw Axes in Crystal Structure

- Screw Axis n_m ; where m < n

  ⟶ rotation by an angle α of 360°/n

  ⟶ n = order of the axis = 360° / n

  ⟶ translation of m/n of the whole unit cell parallel to the screw axis



right-handed coordinate system

$\vec{t}$ = translation element = m / n

α = rotation angle

Source: Frank Hoffmann

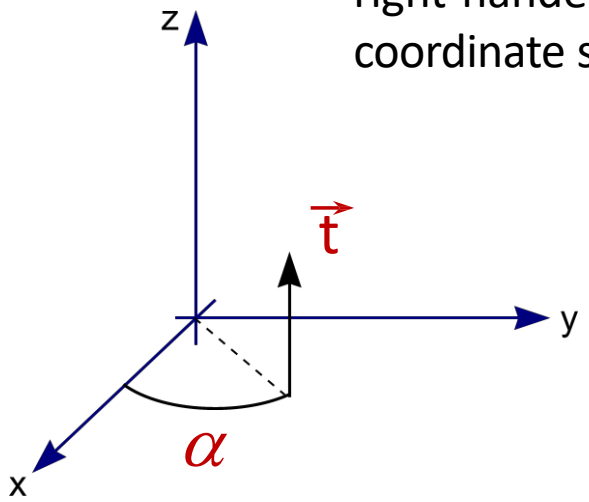
Screw Axes in Crystal Structure

- Screw Axis n_m ; where m < n

a 3_2 screw axis (n=3, m=2) means

⟶ rotation by 360°/3 = 120°

⟶ translation of m/n, i.e. $^2/_3$ of the whole unit cell parallel to the screw axis



right-handed coordinate system

$\vec{t}$ = translation element = m / n

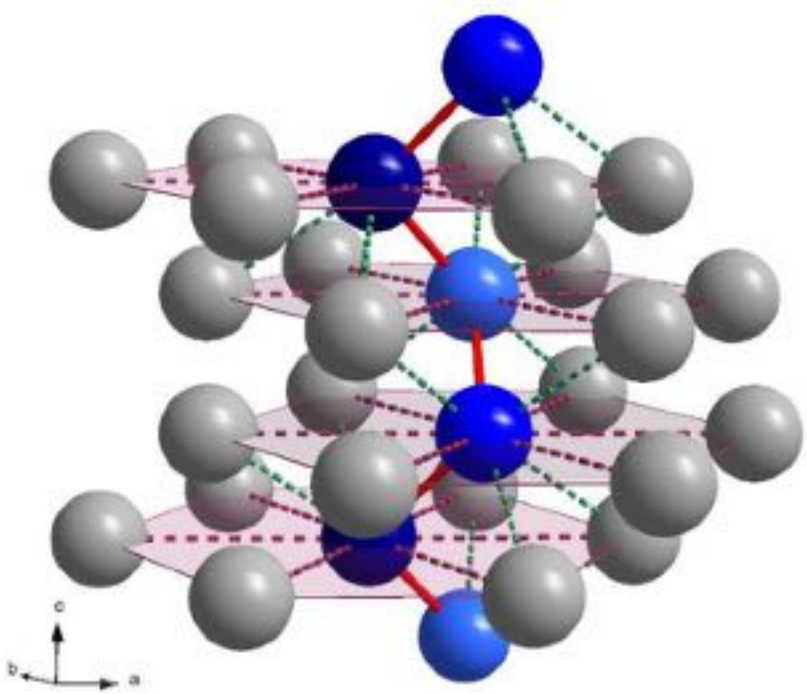
α = rotation angle

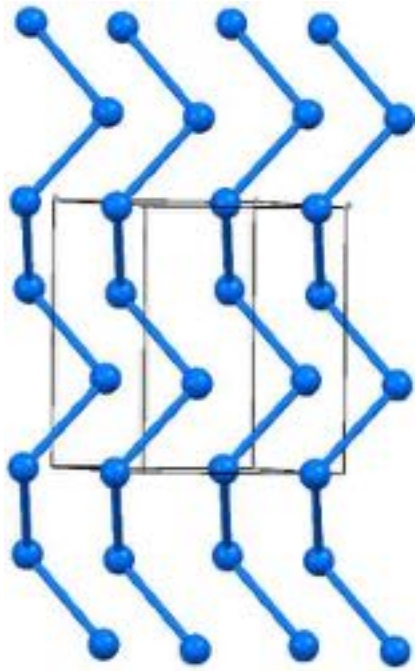
the possible screw axes are 2_1, 3_1, 4_1, 4_2, 6_1, 6_2, and 6_3, and the enantiomorphous 3_2, 4_3, 6_4, and 6_5.

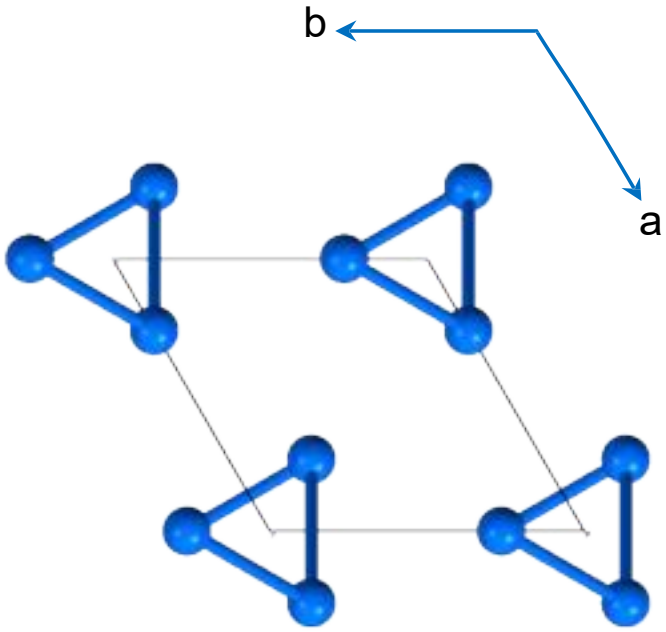
Source: Frank Hoffmann

Screw Axes in Tellurium

3_1 screw axis







→ trigonal crystal system

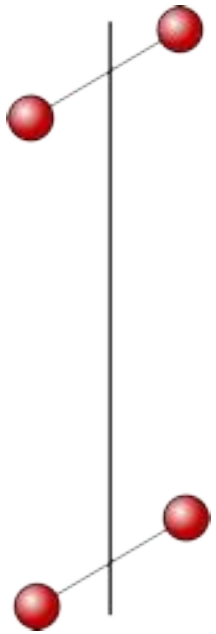
→ space group $P3_121$

Source: Frank Hoffmann

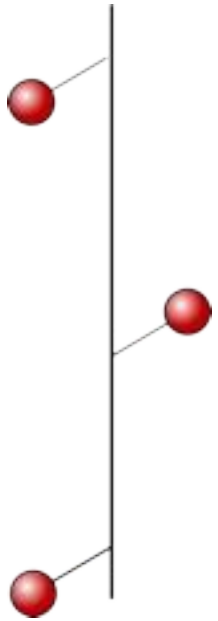
2-fold Screw Axes

n_m

order *n*	*m*	*t*	*symbol*
2	0	0	2
	1	1/2	2_1
	2	1	2



2_0



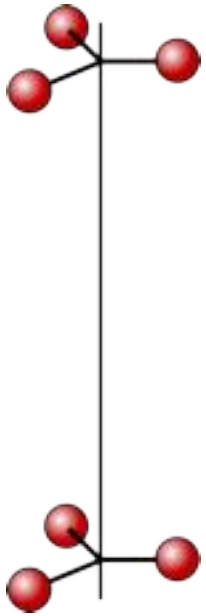
2_1

Source: Frank Hoffmann

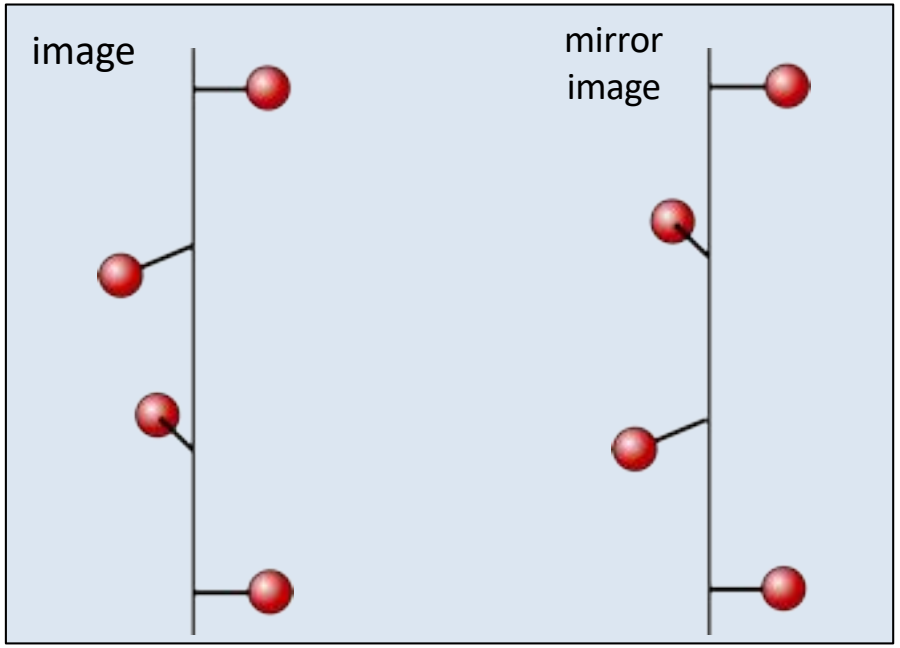
3-fold Screw Axes

n_m

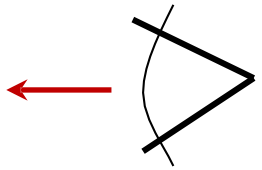
order *n*	*m*	*t*	*symbol*
3	0	0	3
	1	1/3	3_1
	2	2/3	3_2
	3	1	3



3_0

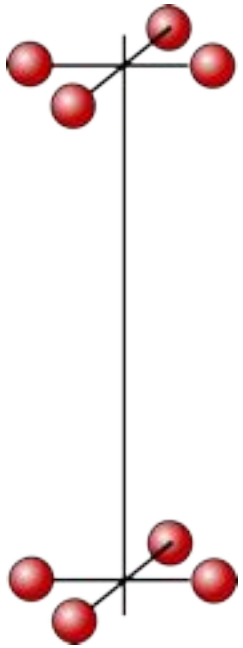


3_1 3_2

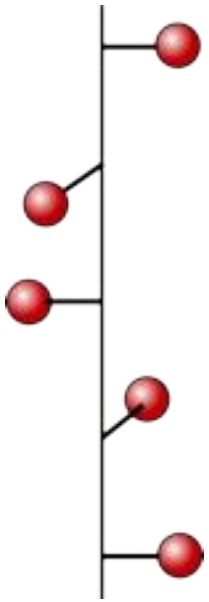


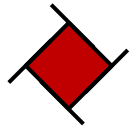
Source: Frank Hoffmann

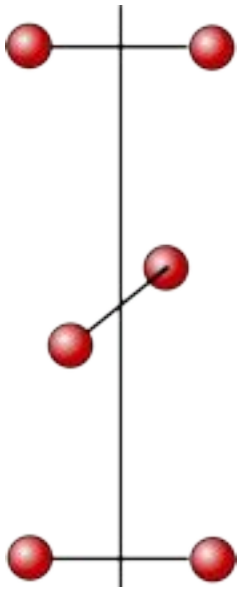
4-fold Screw Axes

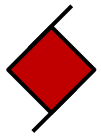


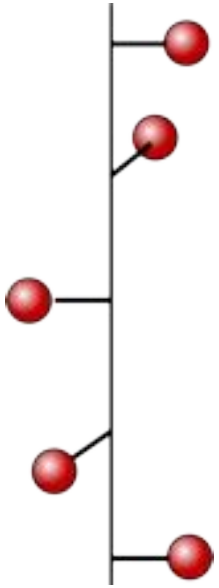
4_0 

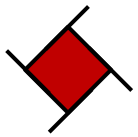


4_1 

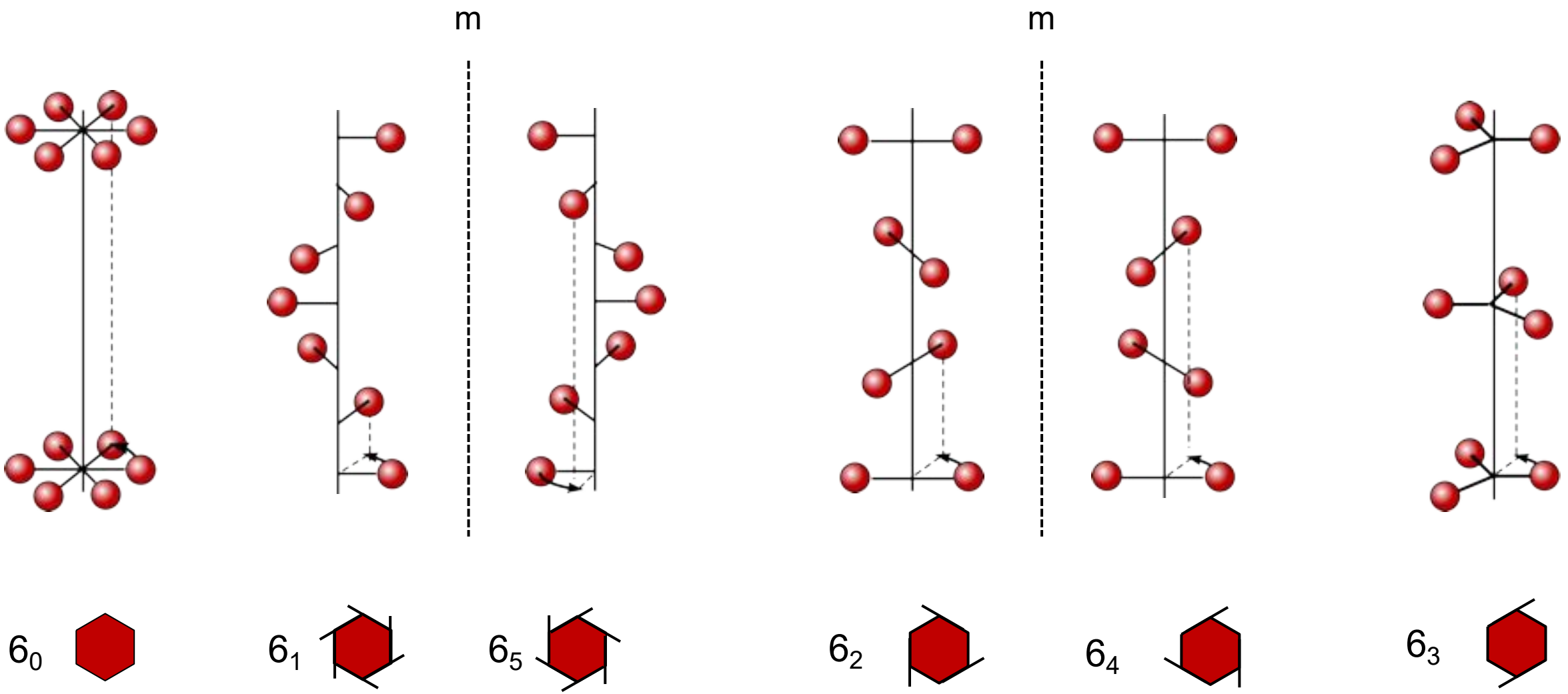


4_2 



4_3 

6-fold Screw Axes



Systematization of Crystal Structures

4. Step: Space groups — 230
   complete symmetry

3. Step: Crystal classes — 32
   crystallographic PG

2. Step: Bravais lattices — 14
   primitive + centered

1. Step: Crystal systems — 7
   metric + symmetry of the UC

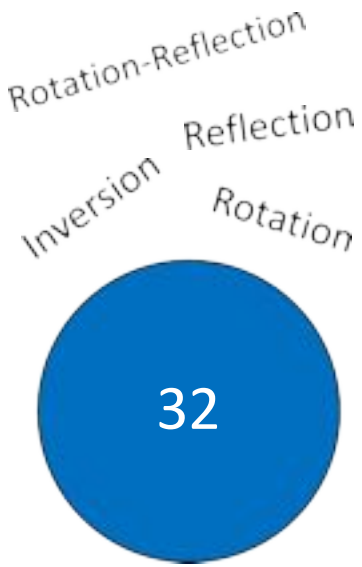
Space Groups

Combination of

14

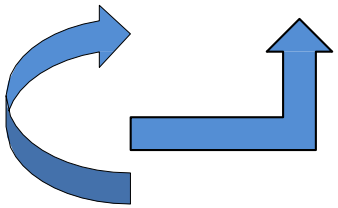
Bravais lattices

with



Point groups

and



screw and glide symmetry

gives

230

Space groups

dimensions	1	2	3	4	5	6
no. of 'space' groups	2	17	230	4894	~220 k	~29 mill

Source: Frank Hoffmann

International Tables for Crystallography

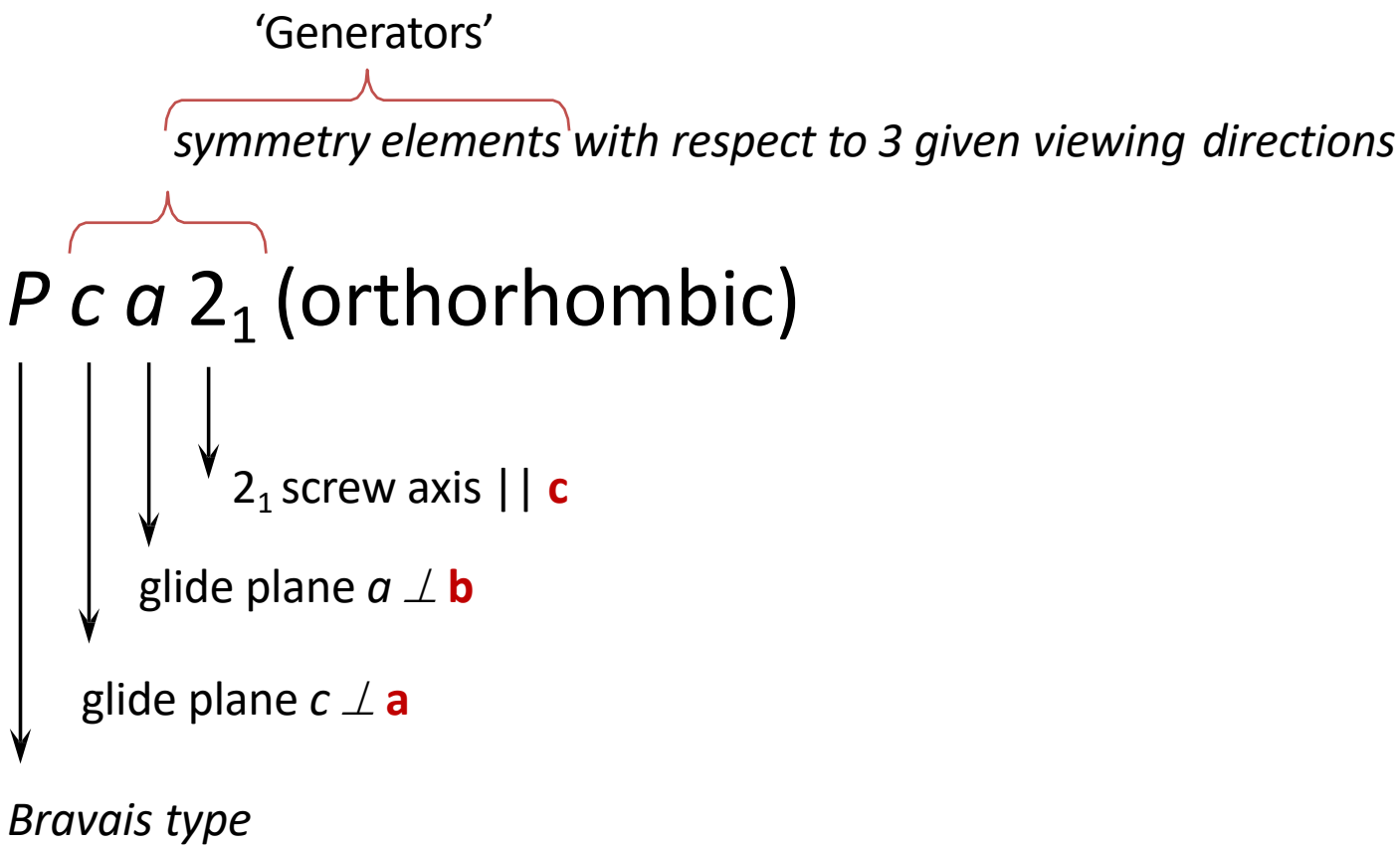
International Tables for Crystallography
Volume A: Space-group symmetry

Definition and Nomenclature of Space Groups

Space group

Set of symmetry elements (and respective operations), which completely describes the spatial arrangement of a 3D periodic pattern.

Nomenclature



Source: Frank Hoffmann

Crystallographic Viewing Directions

- monoclinic: determined by convention
- tetragonal, trigonal, hexagonal: rotational axis of highest order is by definition || to the *c*-axis and the first viewing direction
- rule of thumb: look for something new!

	crystal system	*viewing directions*		
	triclinic	—		
	monoclinic	*b*		
	orthorhombic	*a*	*b*	*c*
a = b	tetragonal	*c*	*a*	[110]
a = b	trigonal	*c*	*a*	[210]
a = b	hexagonal	*c*	*a*	[210]
	cubic	*a*	[111]	[110]

Source: Frank Hoffmann

Space groups to Point groups (Crystal class)

- Derivation of the crystal class from the space group

1) Leave out the Bravais type

2) Convert all SEs with translational components into their respective SEs *without* translation symmetry

   → Glide planes are converted into simple mirror planes

   → Screw Axes are converted into simple axes of rotation

3) Axes of rotation, rotoinversion axes and mirror planes remain unchanged

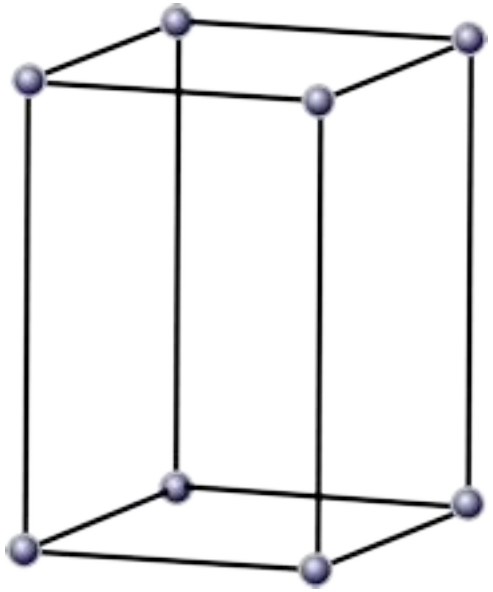
space group $P\,2_1/n$ → *crystal class* $2/m$

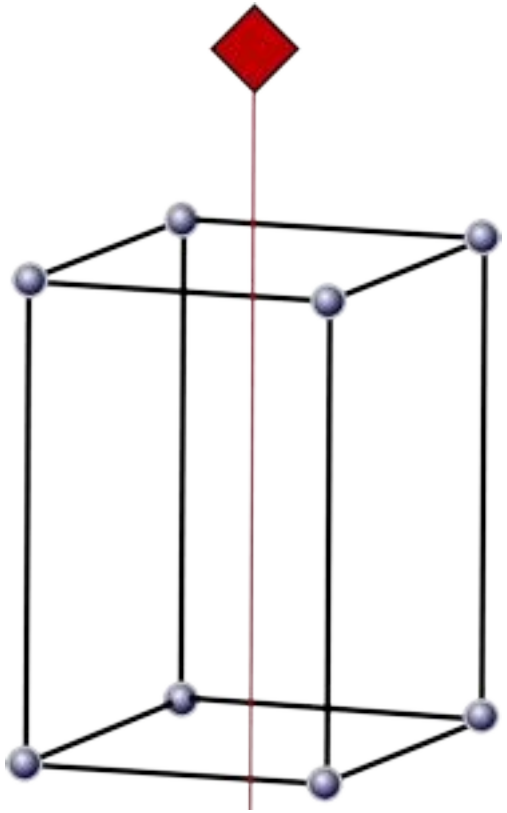
Crystal system – Crystal class – Space group

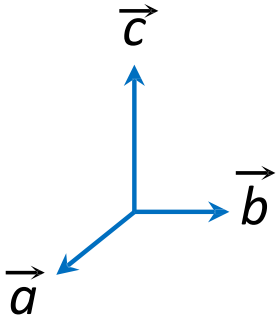
tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$







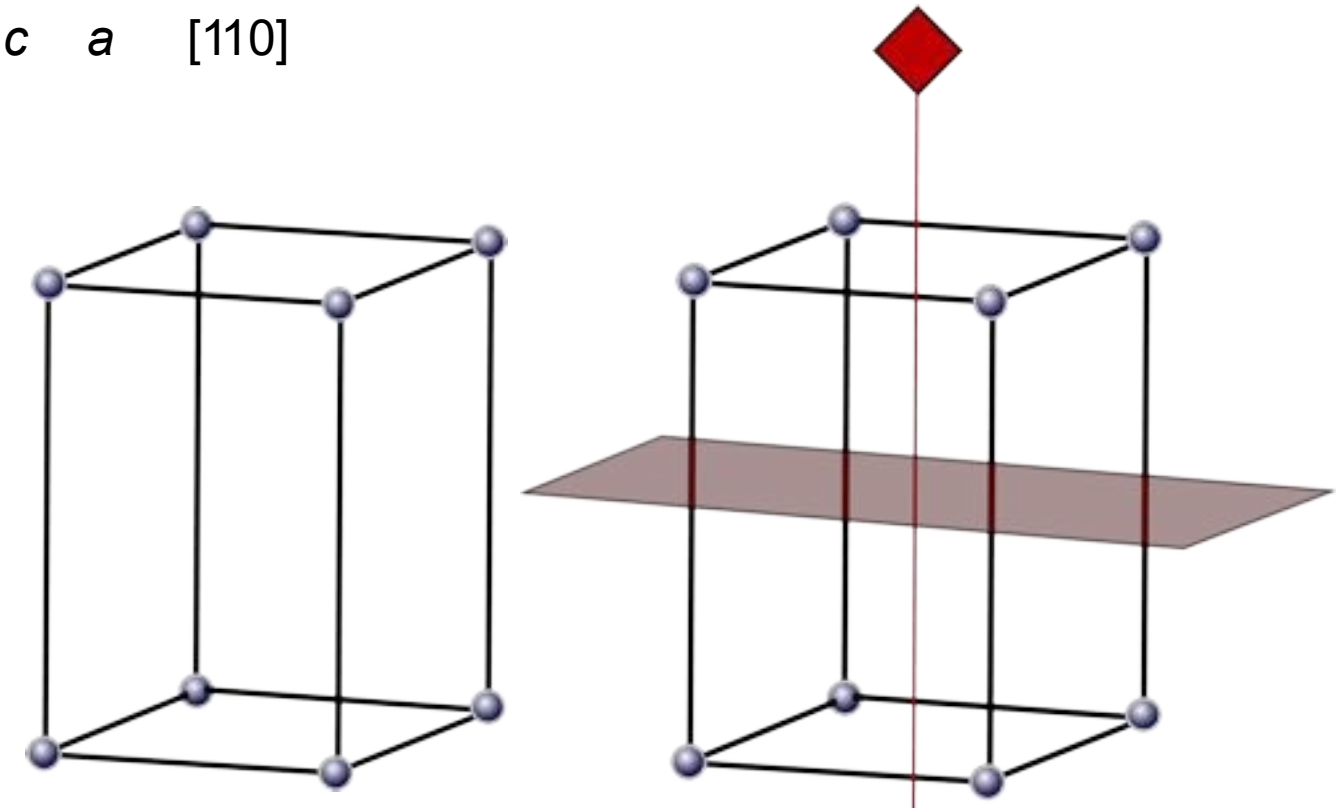
Source: Frank Hoffmann

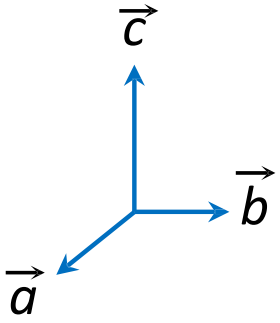
Crystal system – Crystal class – Space group

tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$





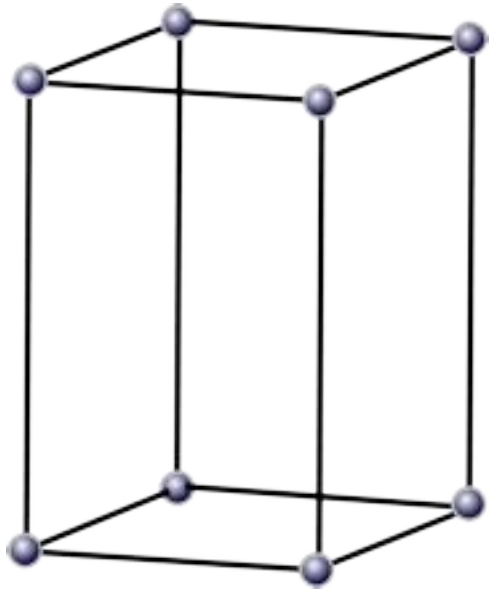
Source: Frank Hoffmann

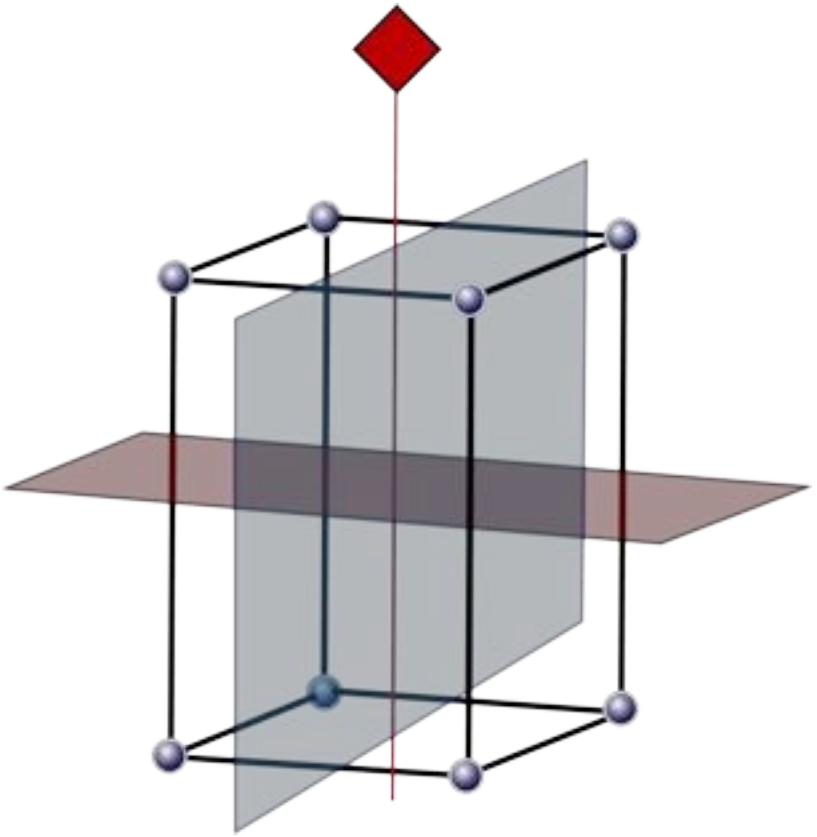
Crystal system – Crystal class – Space group

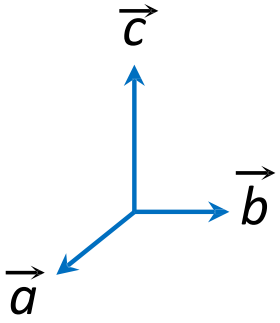
tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$







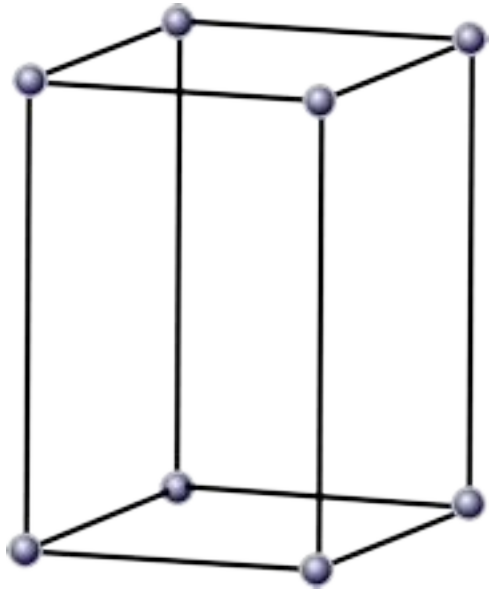
Source: Frank Hoffmann

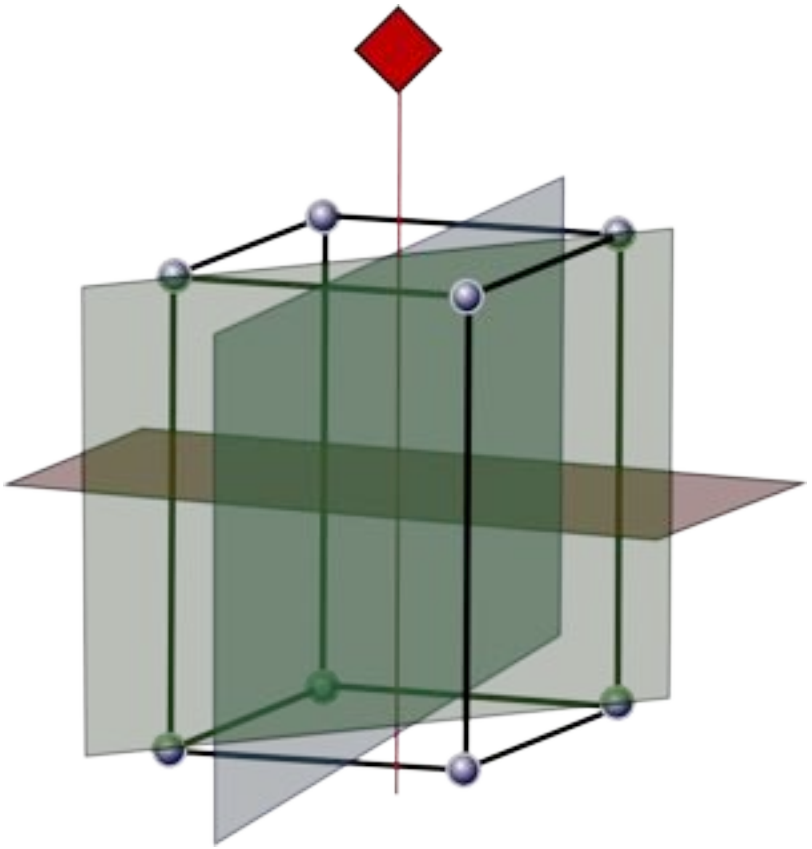
Crystal system – Crystal class – Space group

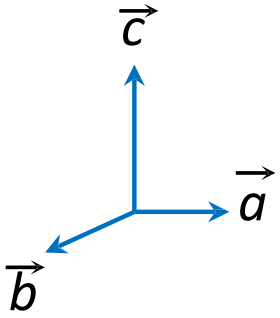
tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$







4/mmm

P4/mmm

c *a* [110]

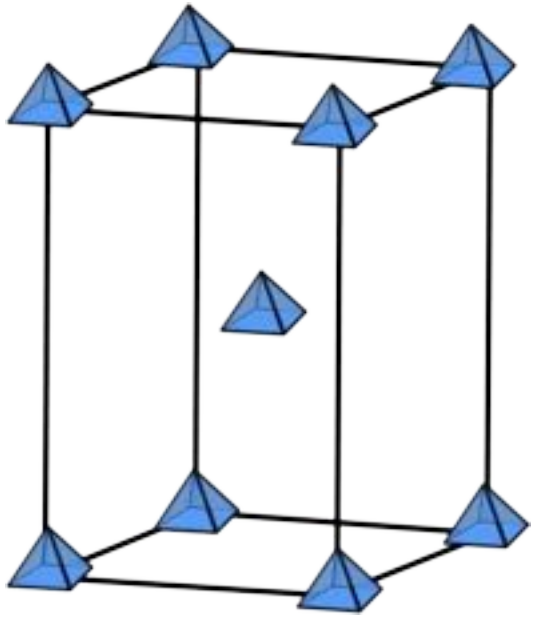
Source: Frank Hoffmann

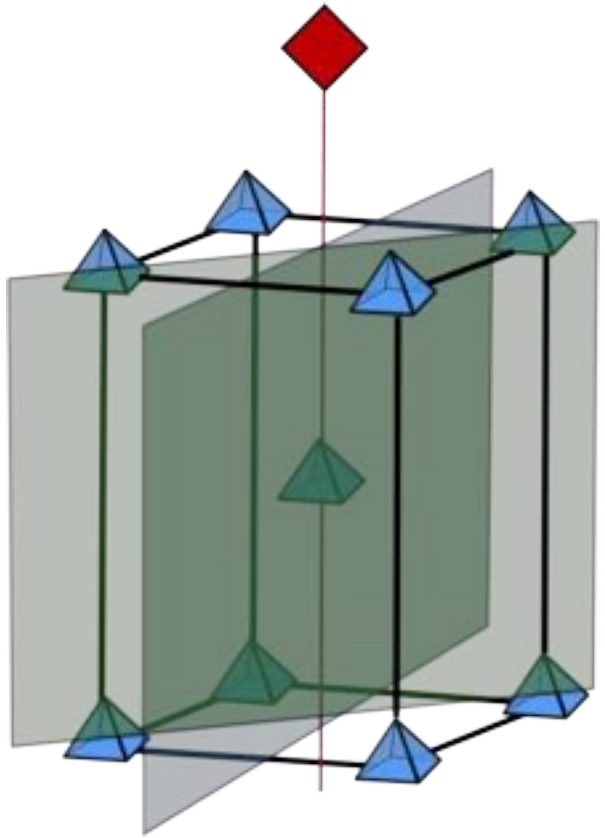
Crystal system – Crystal class – Space group

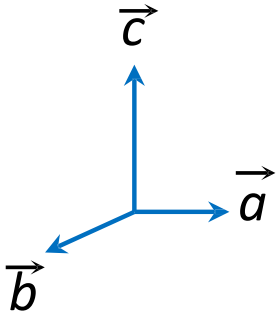
tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$







4mm

I4mm

c a [110]

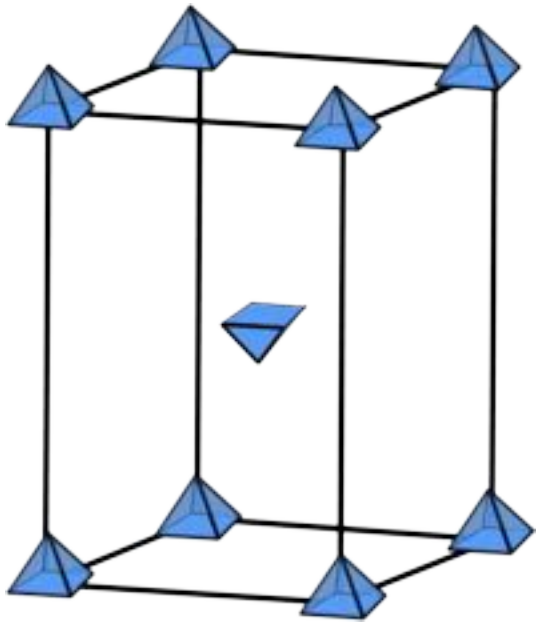
Source: Frank Hoffmann

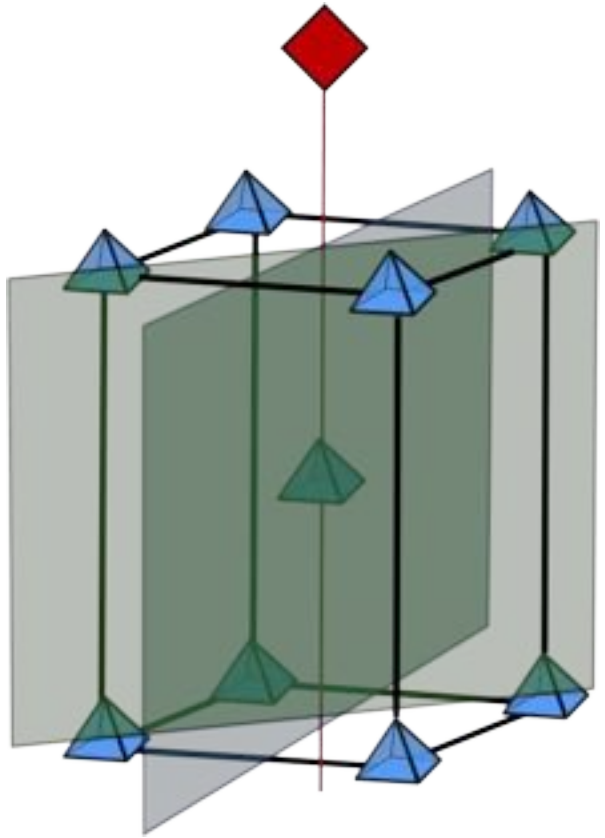
Crystal system – Crystal class – Space group

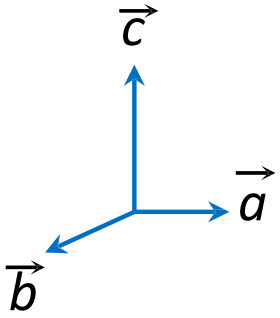
tetragonal → *c* *a* [110]

a = b

$\alpha = \beta = \gamma = 90°$







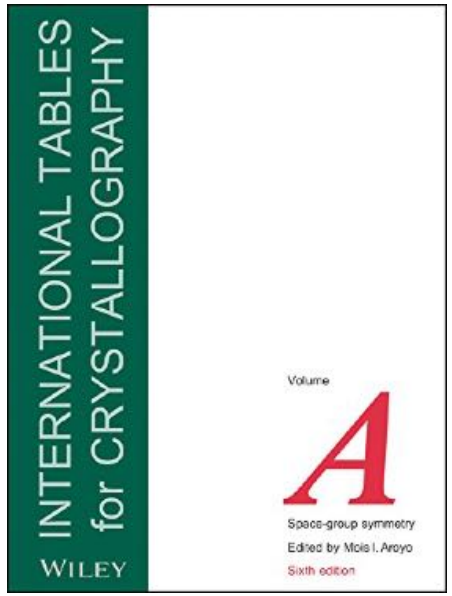
4mm

P4mm

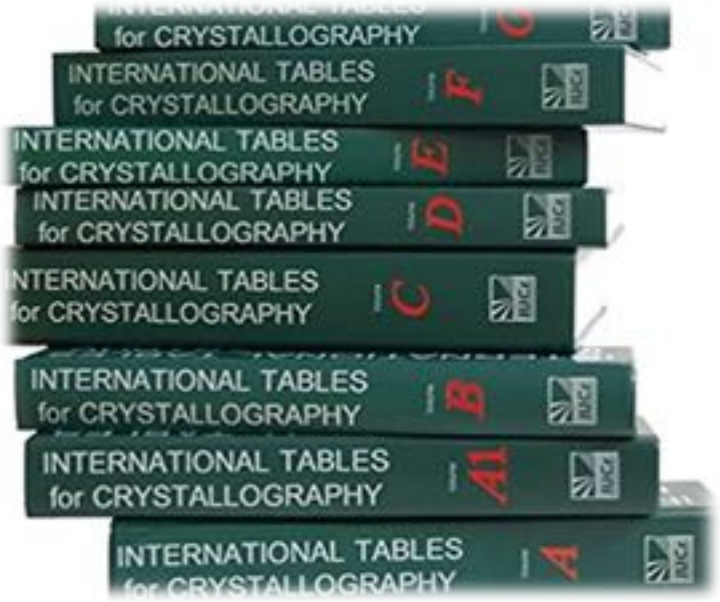
c a [110]

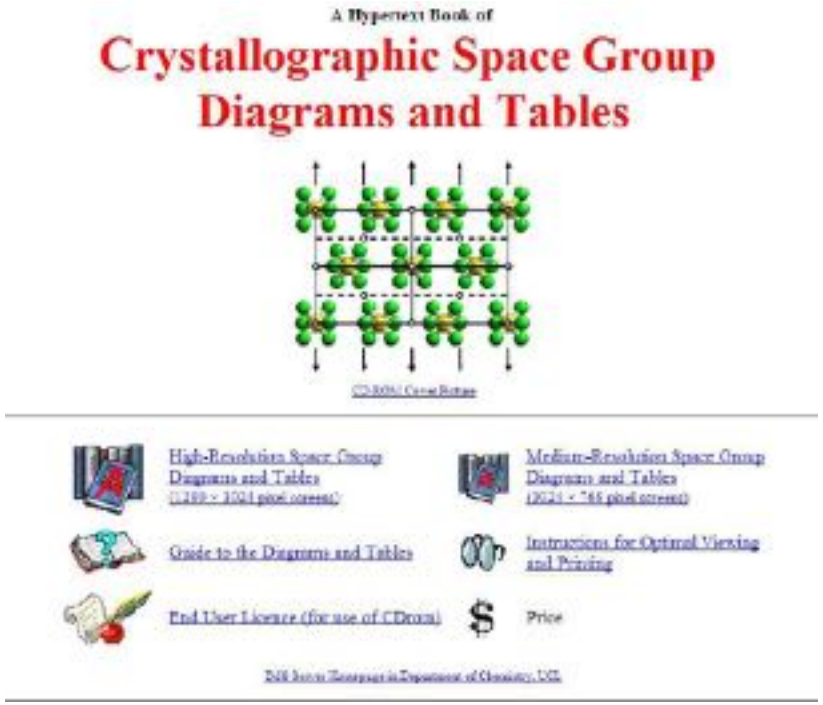
Source: Frank Hoffmann

International Table for Crystallography



International Tables for Crystallography
Volume A: Space-group symmetry





http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

Source: Frank Hoffmann

International Table for Crystallography

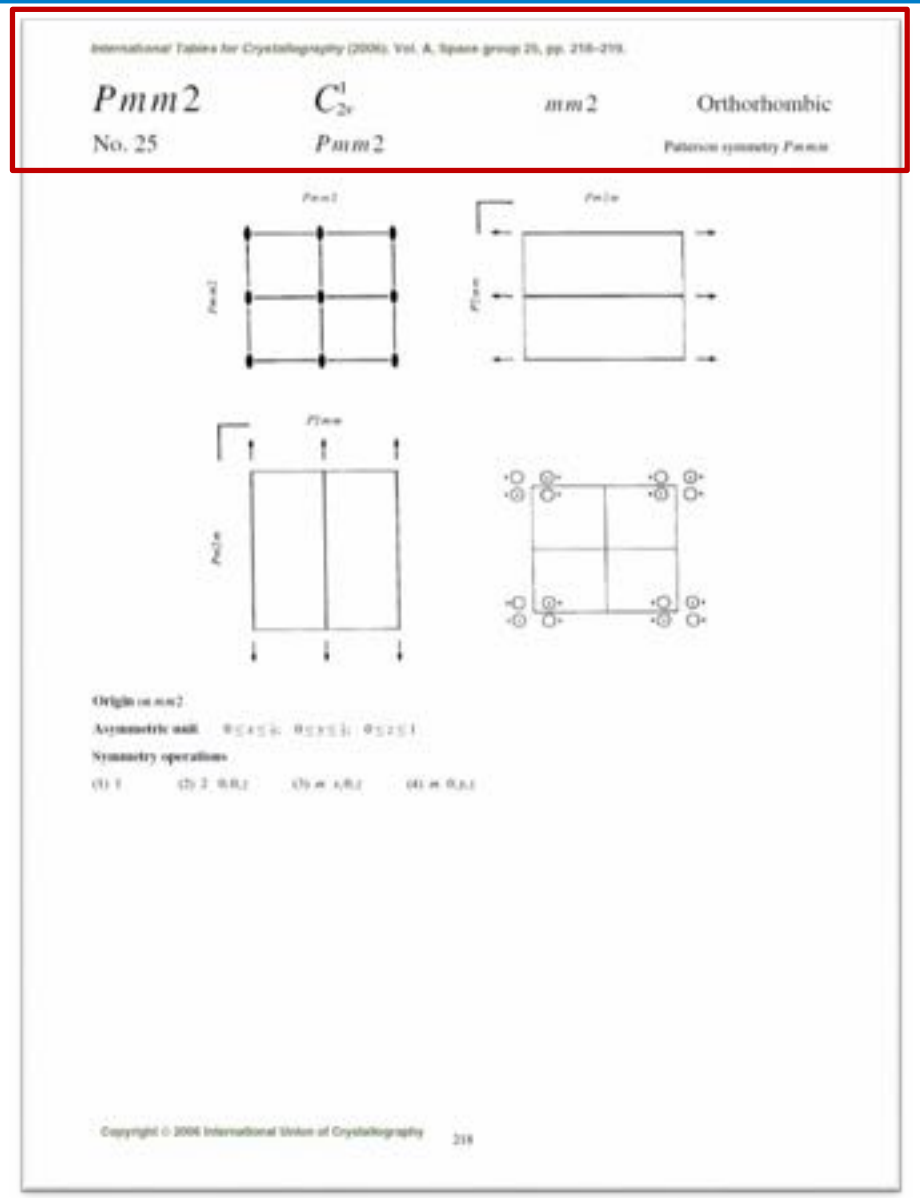
- Systematic listing of the 17 plane groups and 230 space groups
- Space group symbol in short and full notation as well as an unique #
- Indication of the crystal system and the crystal class in both systems of nomenclature (H.-M. and Schoenflies)
- Diagrams of the position of the SEs
- General position diagram
- Listing of all SOs as coordination transformations
- Multiplicity, Wyckoff letters, Site symmetry
- …and some more (“incomprehensible”) things ☺

group theory / X-ray diffraction

Source: Frank Hoffmann

Space group Pmm2

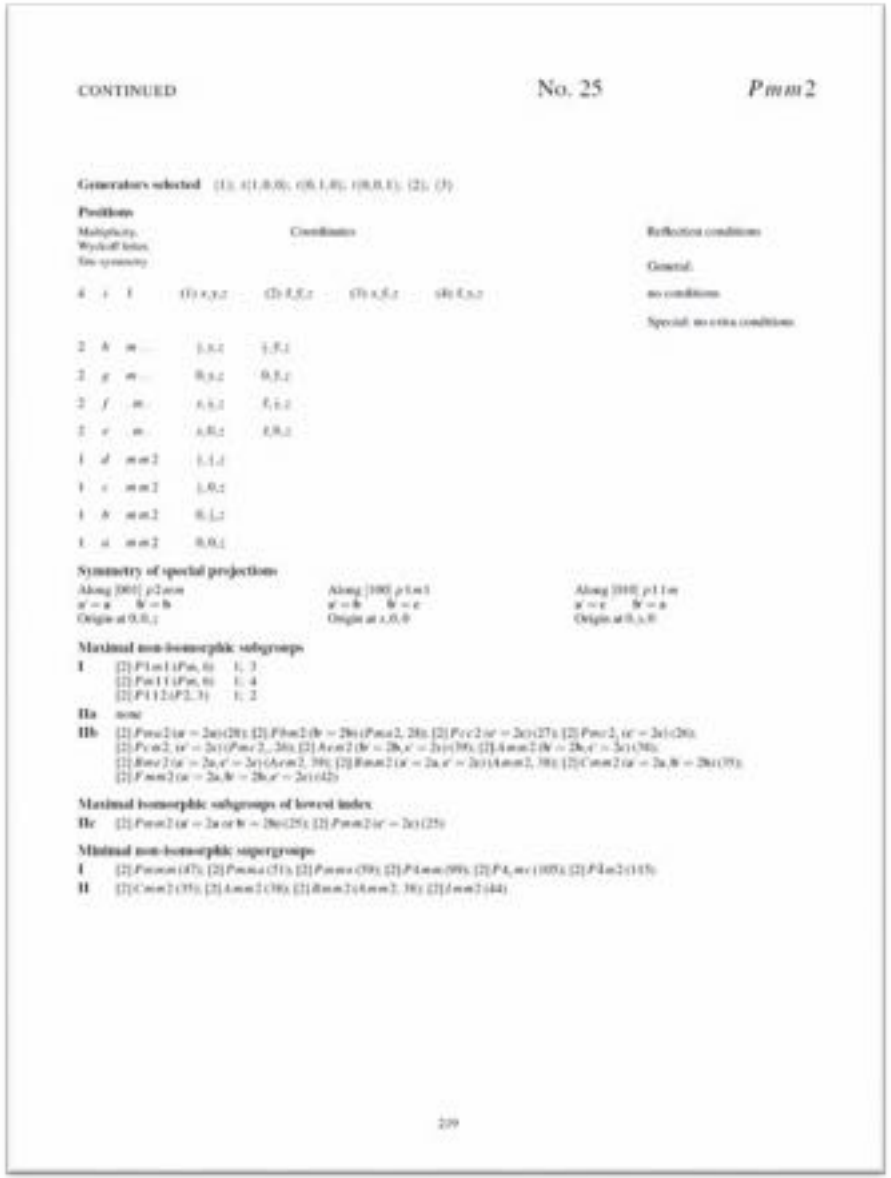
Header



International Tables for Crystallography (2006). Vol. A. Space group 25, pp. 218–219.

Pmm2 C_{2v}^{1} *mm2* Orthorhombic

No. 25 *Pmm2* Patterson symmetry *Pmmm*



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 i 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$ no conditions

Special: no extra conditions

2 h m.. $\frac{1}{2},y,z$ $\frac{1}{2},\bar{y},z$

2 g m.. $0,y,z$ $0,\bar{y},z$

2 f m.. $x,\frac{1}{2},z$ $\bar{x},\frac{1}{2},z$

2 e m.. $x,0,z$ $\bar{x},0,z$

1 d mm2 $\frac{1}{2},\frac{1}{2},z$

1 c mm2 $\frac{1}{2},0,z$

1 b mm2 $0,\frac{1}{2},z$

1 a mm2 $0,0,z$

Symmetry of special projections

Along [001] $p2mm$ $a' = a$ $b' = b$ Origin at $0,0,z$

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

Along [010] $p1m1$ $a' = c$ $b' = a$ Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pmc2_1$ ($a' = 2a$) (26); [2] $Pbm2$ ($b' = 2b$) ($Pmc2_1$, 26); [2] $Pcc2$ ($a' = 2a$) (27); [2] $Pmc2_1$ ($c' = 2c$) (26); [2] $Pcc2$ ($a' = 2a$) ($Pmc2_1$, 26); [2] $Amm2$ ($b' = 2b$, $c' = 2c$) (38); [2] $Amm2$ ($b' = 2b$, $c' = 2c$) (38); [2] $Bmm2$ ($a' = 2a$, $c' = 2c$) (A$mm2$, 38); [2] $Bmm2$ ($a' = 2a$, $c' = 2c$) (A$mm2$, 38); [2] $Cmm2$ ($a' = 2a$, $b' = 2b$) (35); [2] $Fmm2$ ($a' = 2a$, $b' = 2b$, $c' = 2c$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($a' = 2a$ or $b' = 2b$) (25); [2] $Pmm2$ ($c' = 2c$) (25)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pmma$ (51); [2] $Pnnn$ (58); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}2c$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($A$$mm2$, 38); [2] $Imm2$ (44)

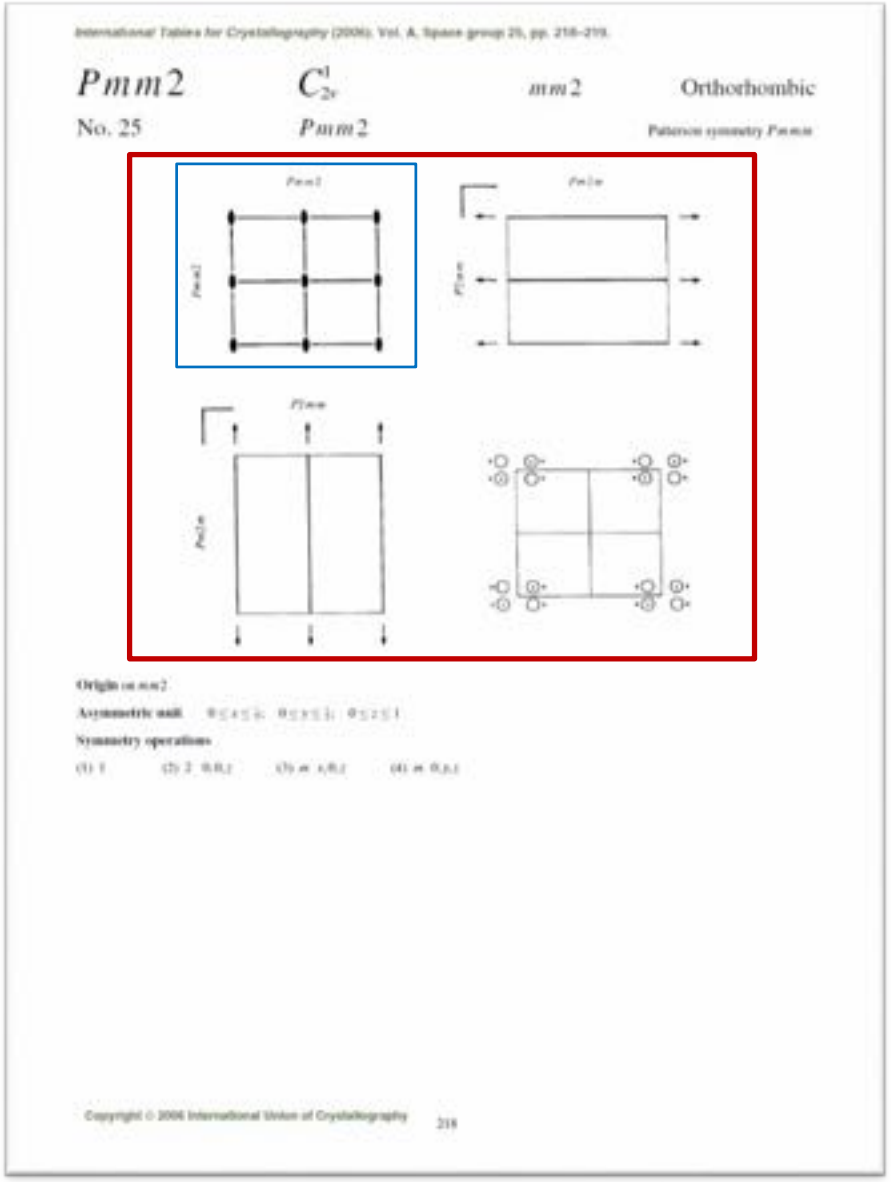
Source: Frank Hoffmann

Space group Pmm2 - Header

			Schoenflies	H.-M.		
Short symbol	$Pmm2$	*Crystal class*	C_{2v}^{1}	$mm2$	*Crystal system*	Orthorhombic
Number	No. 25	*Full symbol*	$Pmm2$			Patterson Symmetry $Pmmm$

Source: Frank Hoffmann

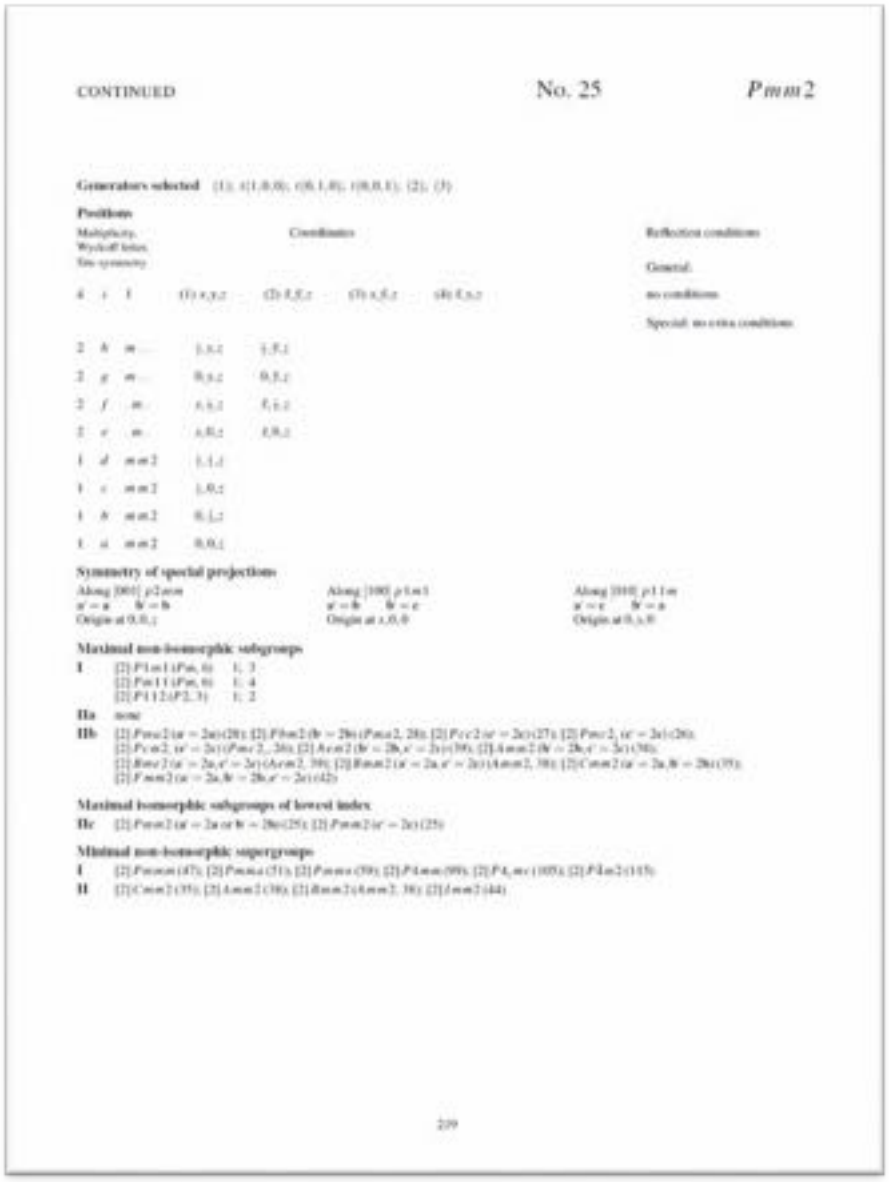
Space group Pmm2



International Tables for Crystallography (2006). Vol. A. Space group 25, pp. 218–219.

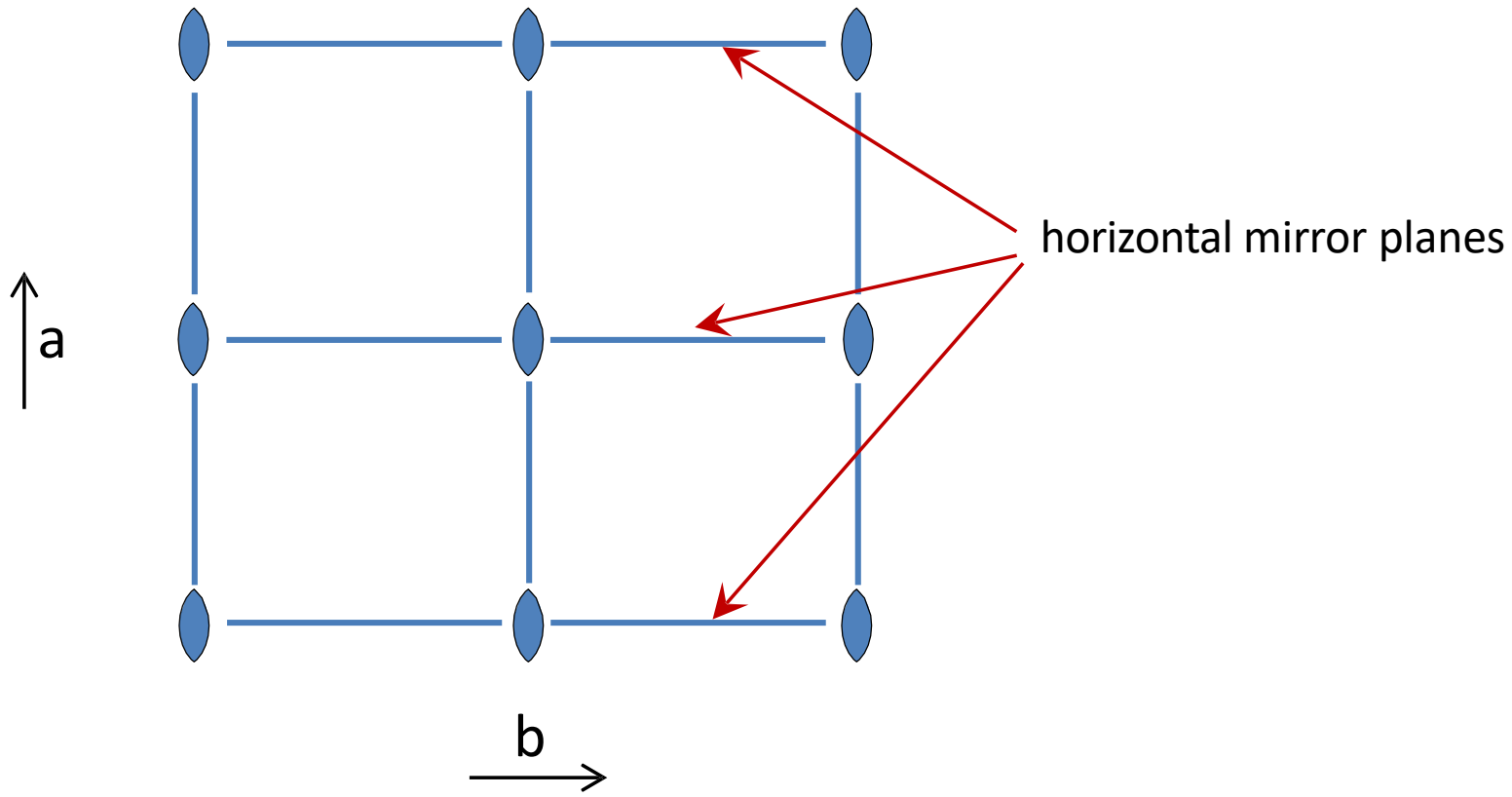
*Pmm*2 C_{2v}^{1} *mm*2 Orthorhombic

No. 25 *Pmm*2 Patterson symmetry *Pmmm*



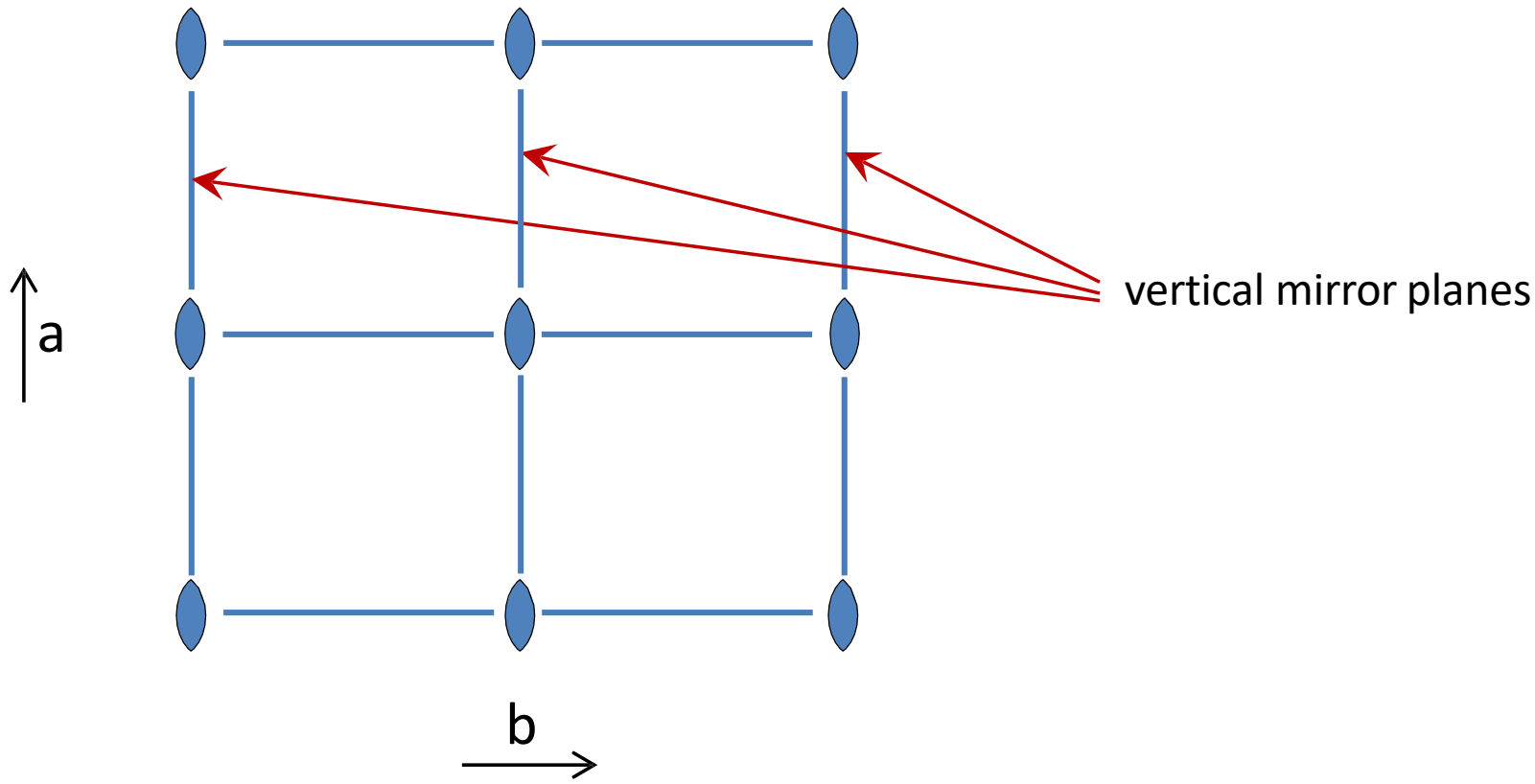
Source: Frank Hoffmann

Space group Pmm2 - Diagram of the Symmetry elements



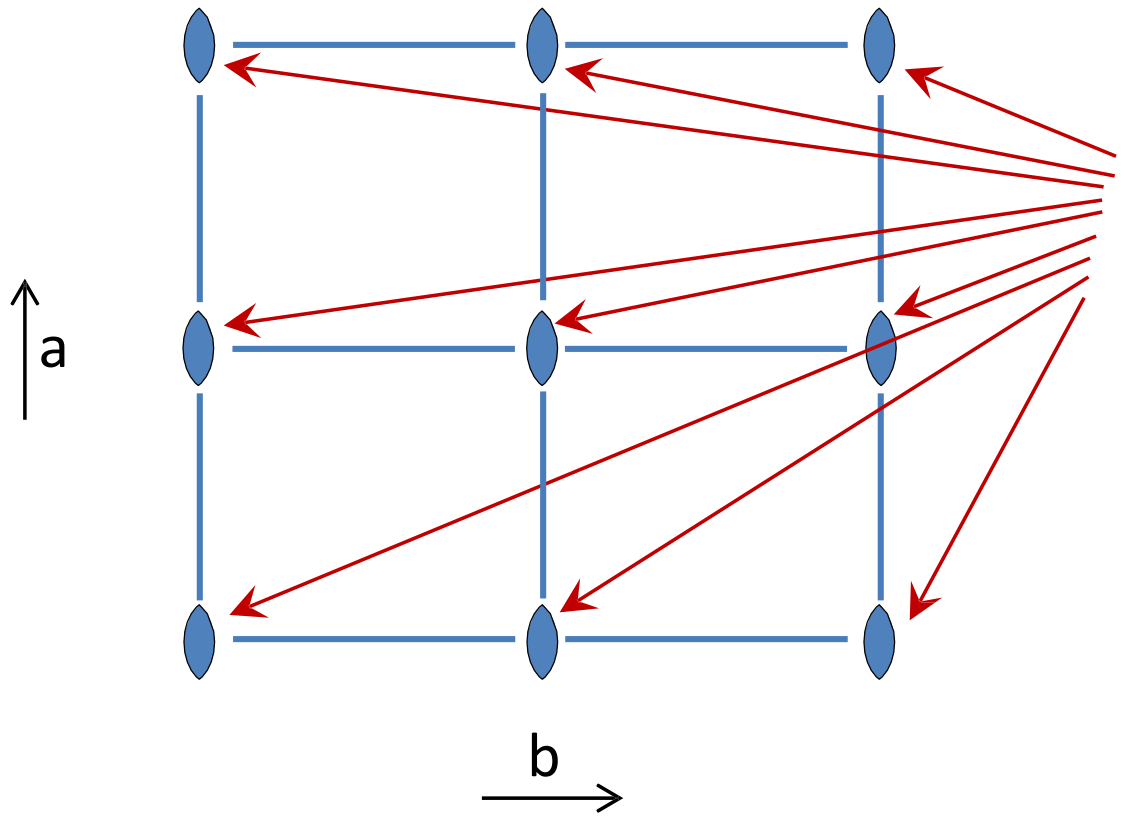
Source: Frank Hoffmann

Space group Pmm2 - Diagram of the Symmetry elements



Source: Frank Hoffmann

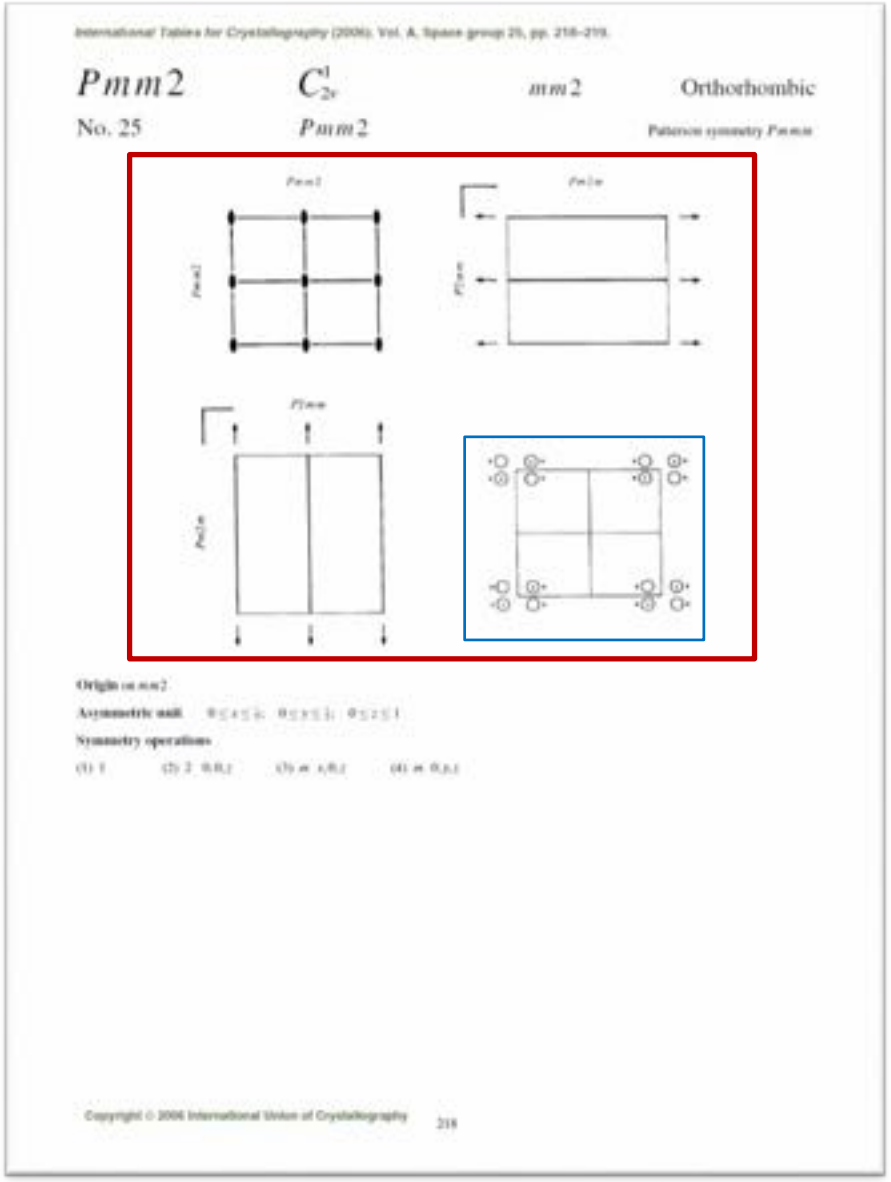
Space group Pmm2 - Diagram of the Symmetry elements



2-fold axes of rotation

Source: Frank Hoffmann

Space group Pmm2



International Tables for Crystallography (2006). Vol. A. Space group 25, pp. 218–219.

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$

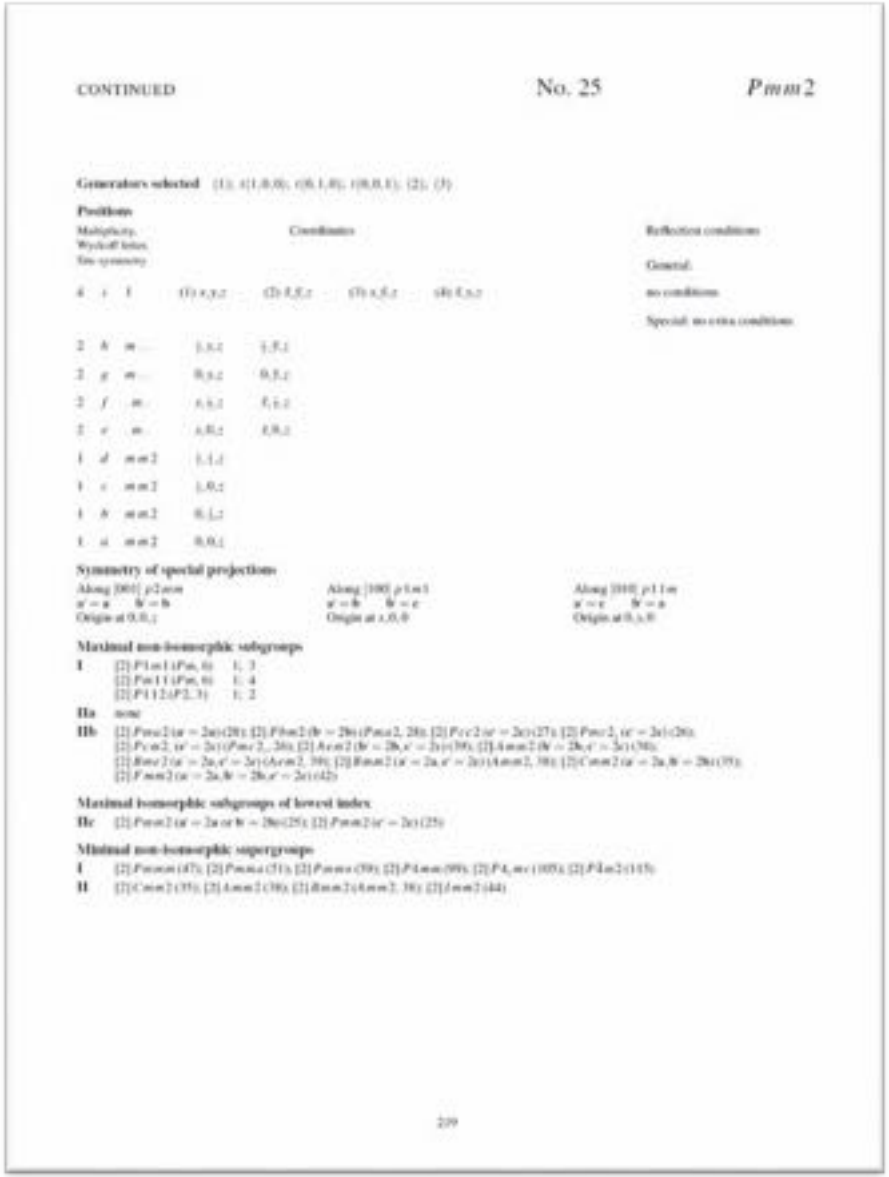
Patterson symmetry $Pmmm$

Origin on $mm2$

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) m x,0,z (4) m 0,y,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
4 i 1	(1) x,y,z (2) $\bar{x}$,$\bar{y}$,z (3) x,$\bar{y}$,z (4) $\bar{x}$,y,z	General: no conditions
2 h m..	½,y,z ½,$\bar{y}$,z	Special: no extra conditions
2 g m..	0,y,z 0,$\bar{y}$,z	
2 f m..	x,½,z $\bar{x}$,½,z	
2 e m..	x,0,z $\bar{x}$,0,z	
1 d $mm2$	½,½,z	
1 c $mm2$	½,0,z	
1 b $mm2$ 0,½,z		
1 a $mm2$ 0,0,z		

Symmetry of special projections

Along [001] $p2mm$ $a' = a$ $b' = b$ Origin at 0,0,z

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

Along [010] $p1m1$ $a' = c$ $b' = a$ Origin at 0,y,0

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pmm2$ ($a' = 2a$) (28); [2] $Pbm2$ ($b' = 2b$) ($Pmm2$, 28); [2] $Pcc2$ ($a' = 2a$) (27); [2] $Pmc2_1$ ($a' = 2a$) (26); [2] $Pcm2_1$ ($a' = 2a$) ($Pmc2_1$, 26); [2] $Amm2$ ($b' = 2b$, $a' = 2a$) (38); [2] $Aem2$ ($b' = 2b$, $c' = 2a$) (39); [2] $Ama2$ ($b' = 2b$, $c' = 2a$) (40); [2] $Abm2$ ($a' = 2a$, $c' = 2a$) ($Aem2$, 39); [2] $Fmm2$ ($a' = 2a$, $b' = 2b$) ($Ammm$, 38); [2] $Fdd2$ ($a' = 2a$, $b' = 2b$) (43); [2] $Imm2$ ($a' = 2a$, $b' = 2b$, $c' = 2c$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmm2$ ($a' = 2a$ or $b' = 2b$) (25); [2] $Pmm2$ ($a' = 2a$) (25)

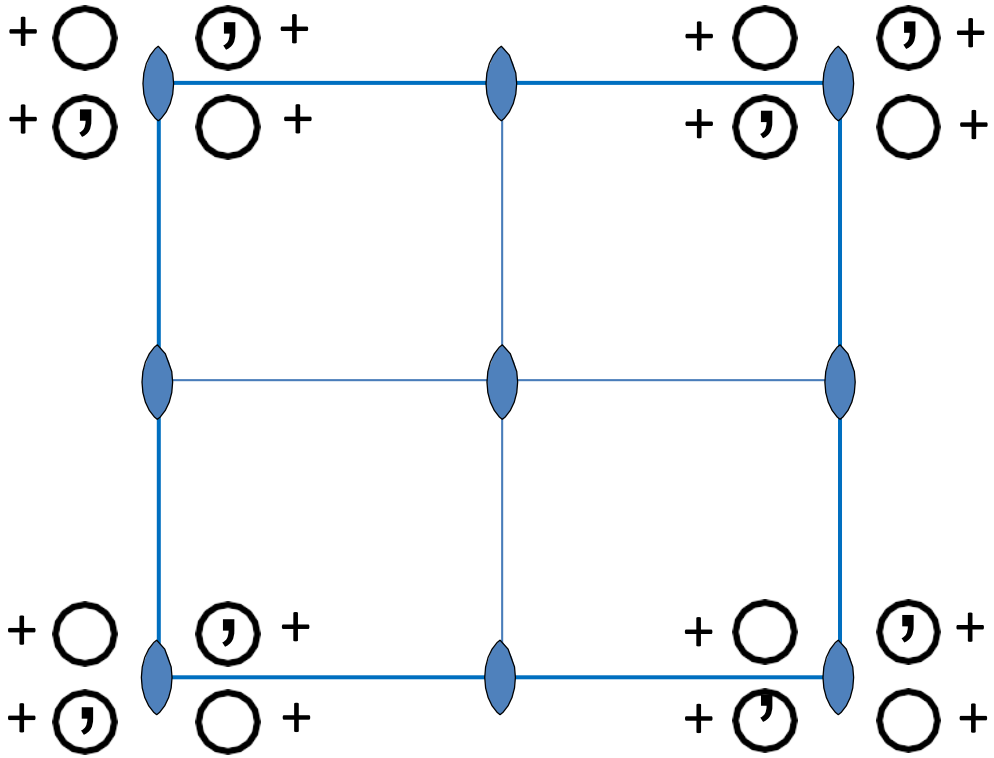
Minimal non-isomorphic supergroups

I [2] $Pnnm$ (47); [2] $Pmmn$ (59); [2] $Pmnm$ (59); [2] $P4mm$ (99); [2] $P4_2mc$ (105); [2] $P\bar{4}2m$ (115)

II [2] $Cmm2$ (35); [2] $Amm2$ (38); [2] $Bmm2$ ($Ammm$, 38); [2] $Imm2$ (44)

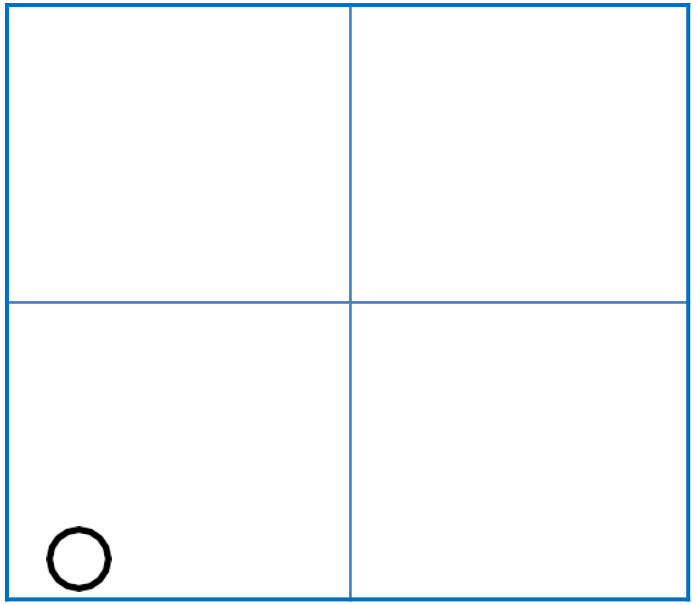
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



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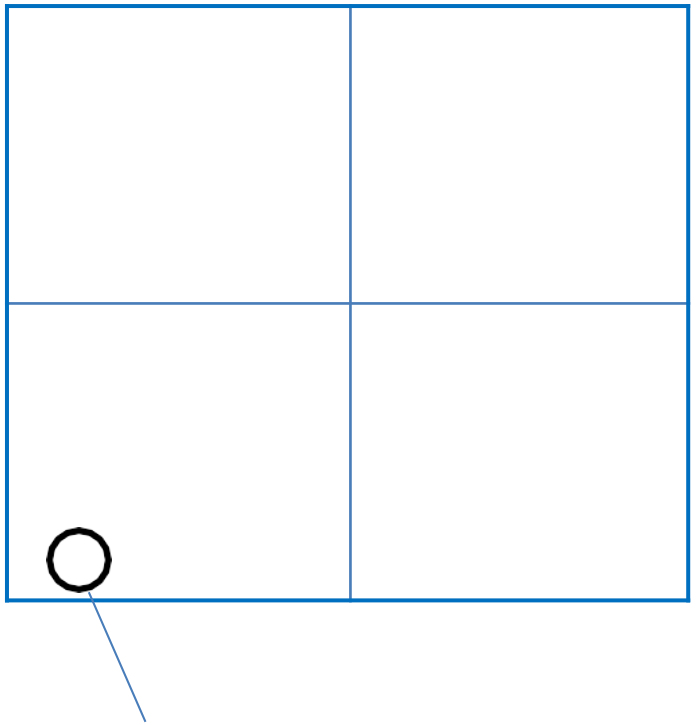
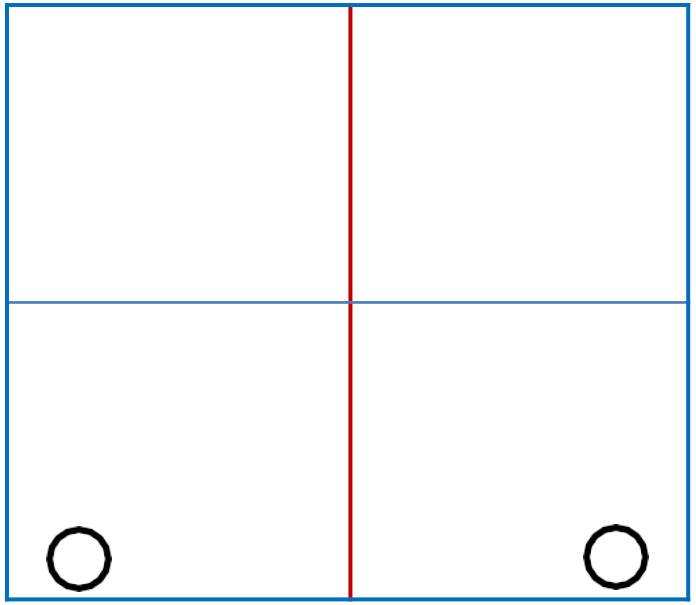
Space group Pmm2 – General Position Diagram



an atom on a general position
(does not sit on a SE)

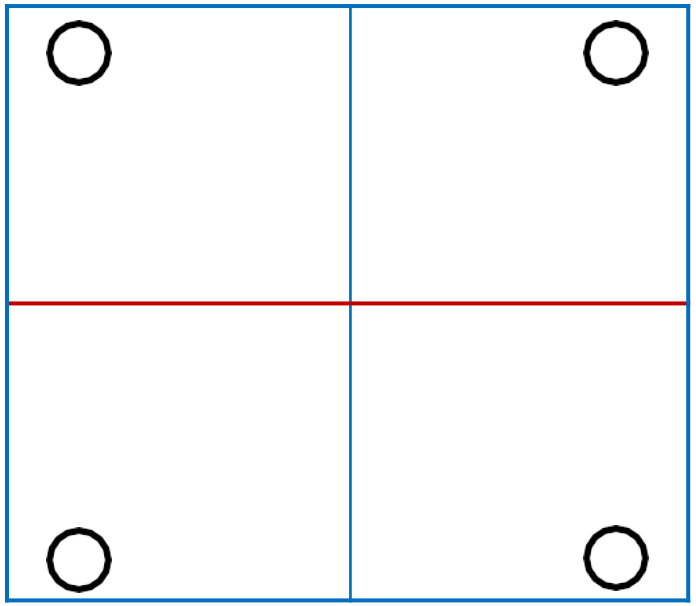
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



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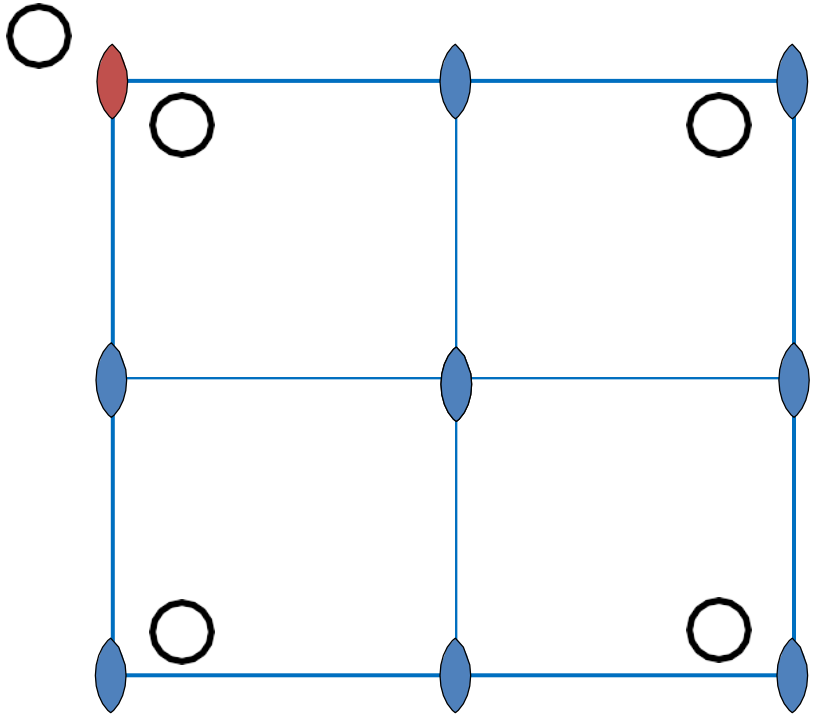
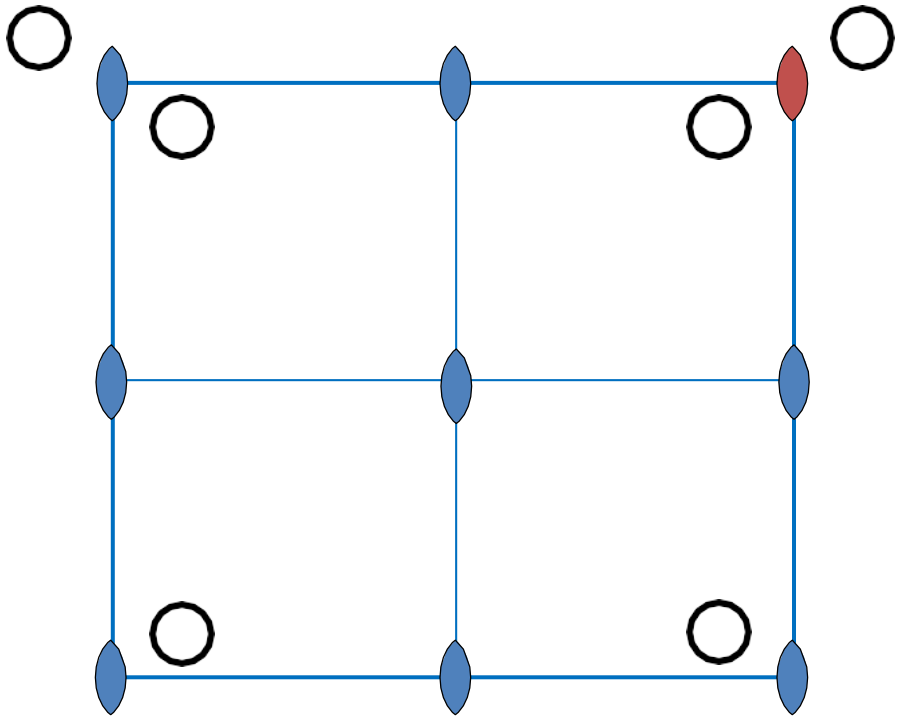
Space group Pmm2 – General Position Diagram



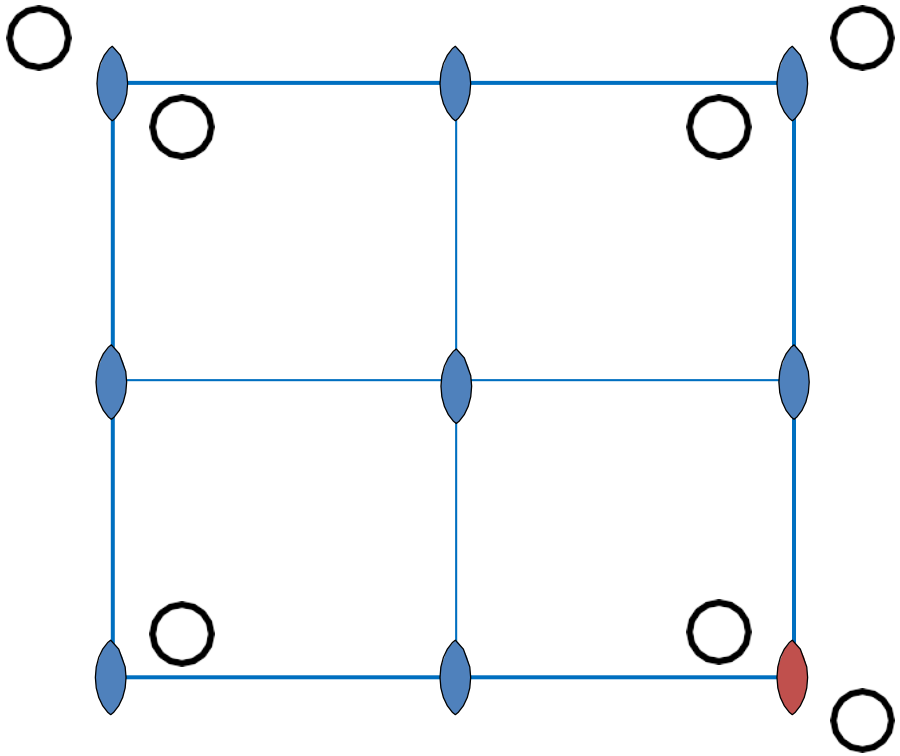
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



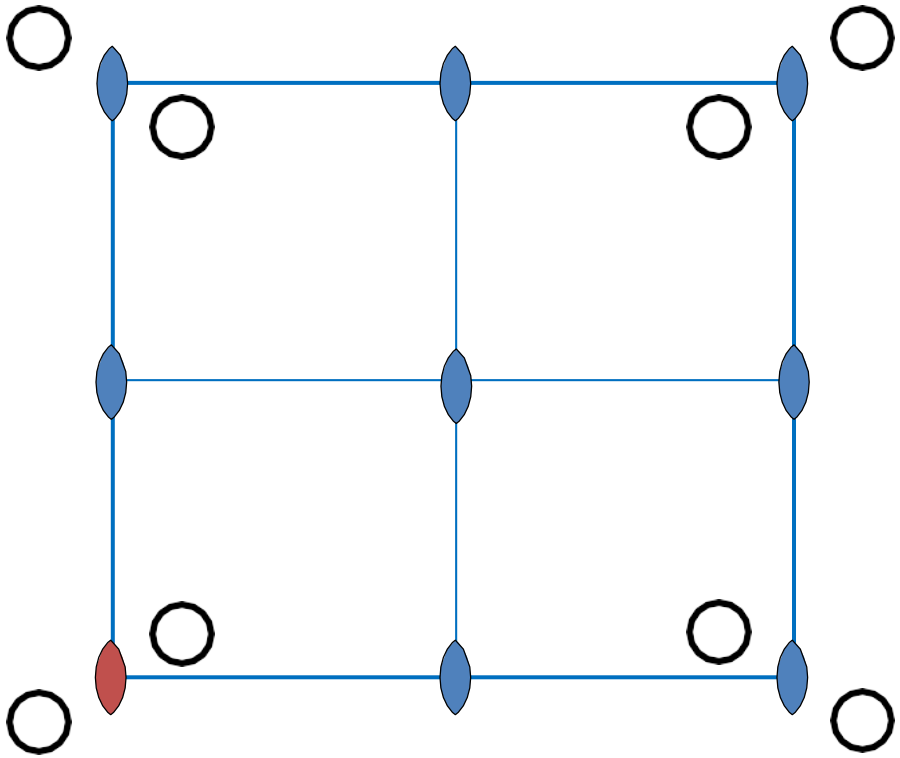
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



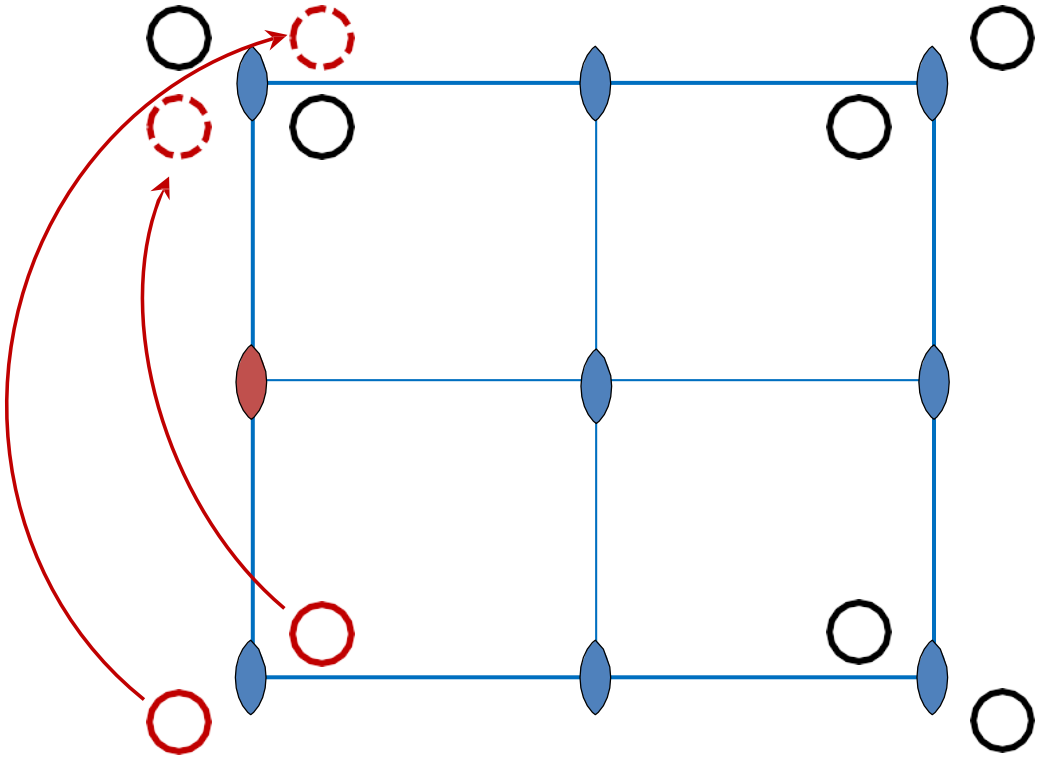
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



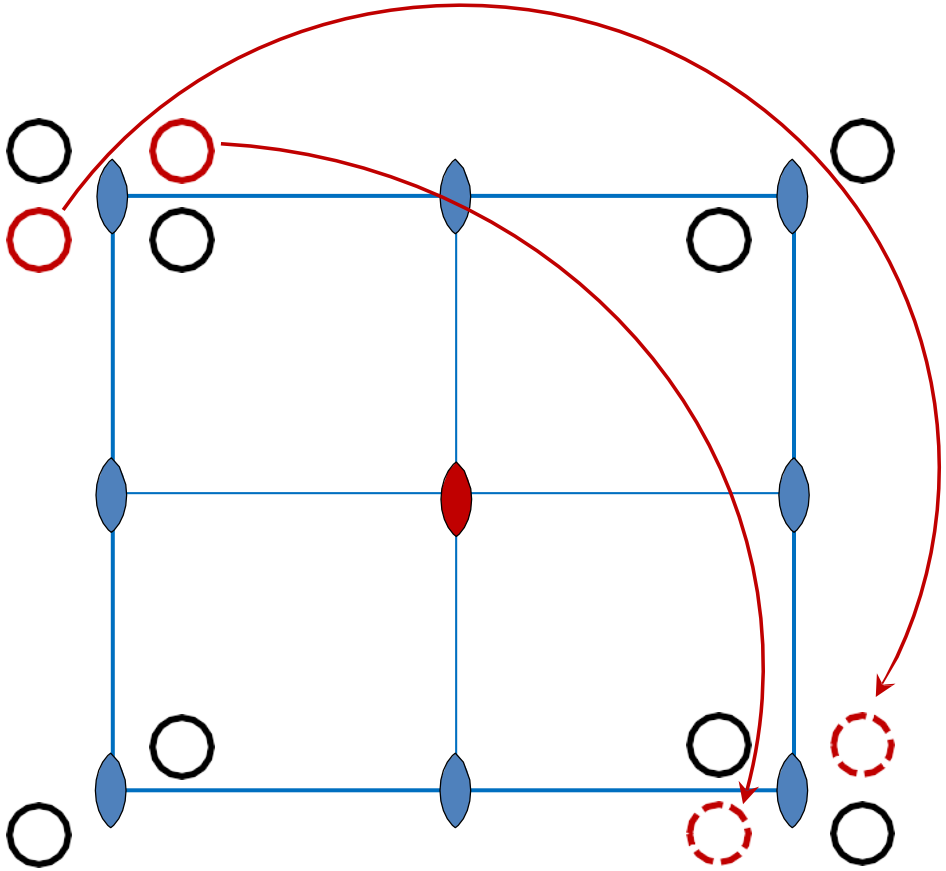
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



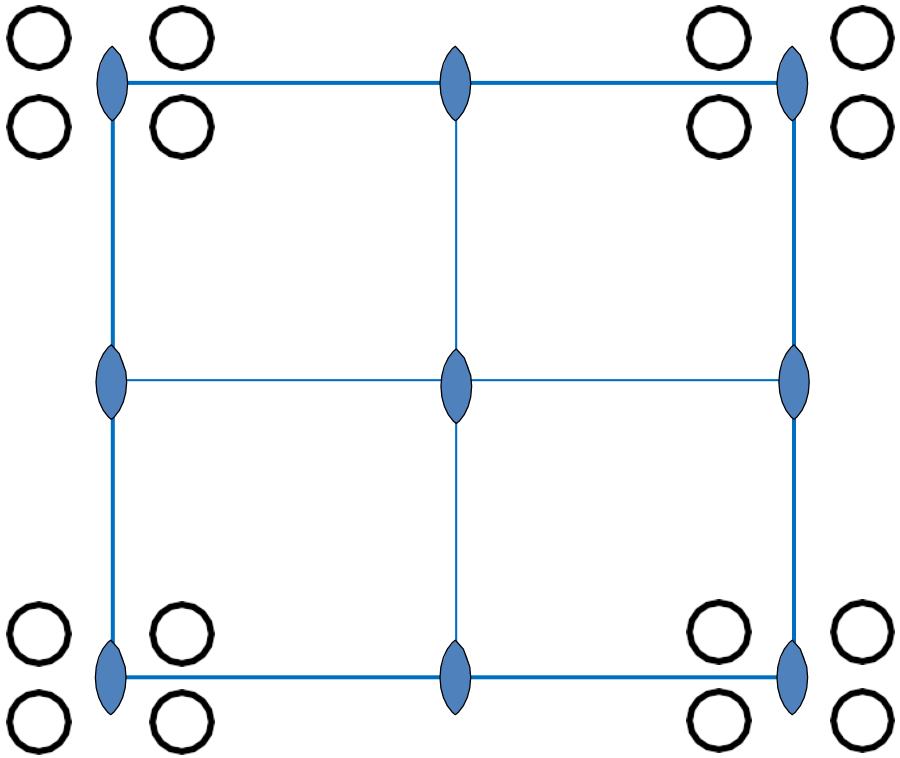
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



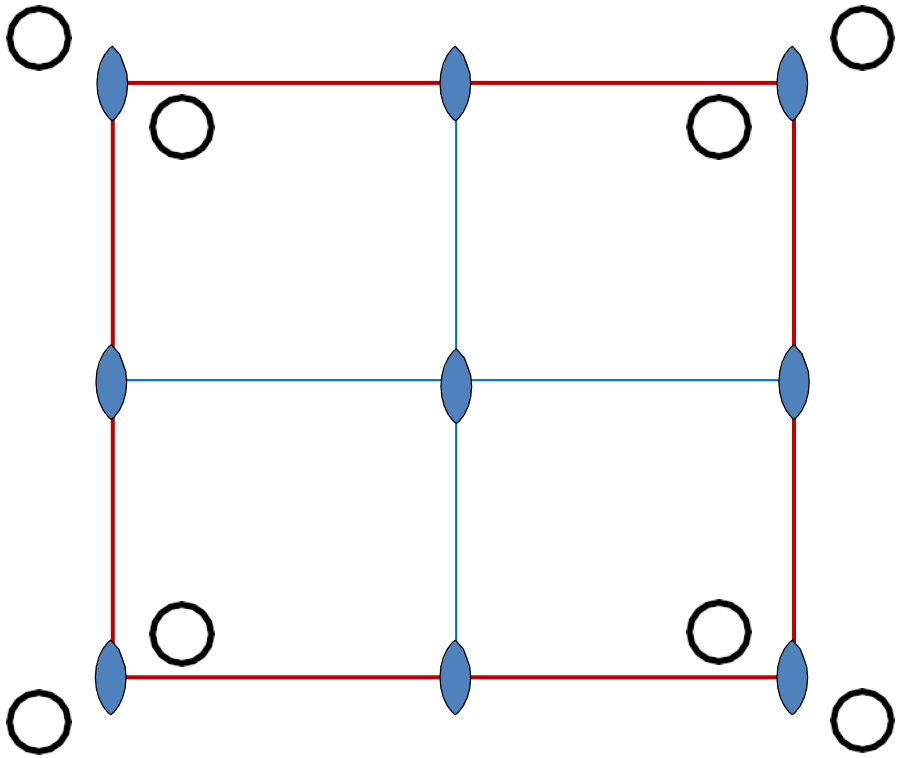
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



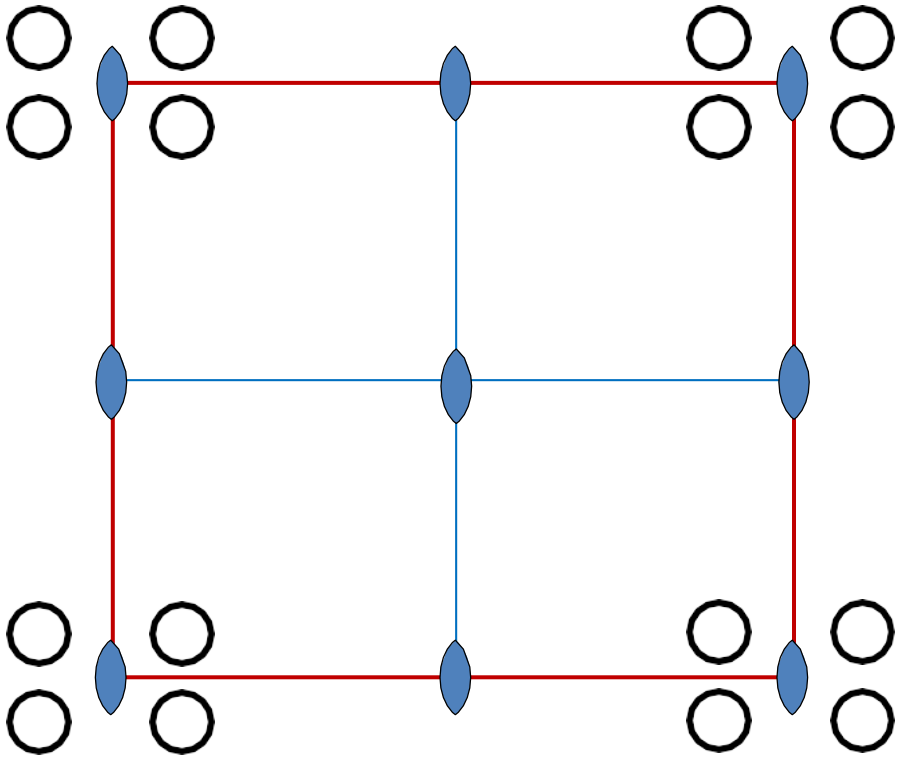
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



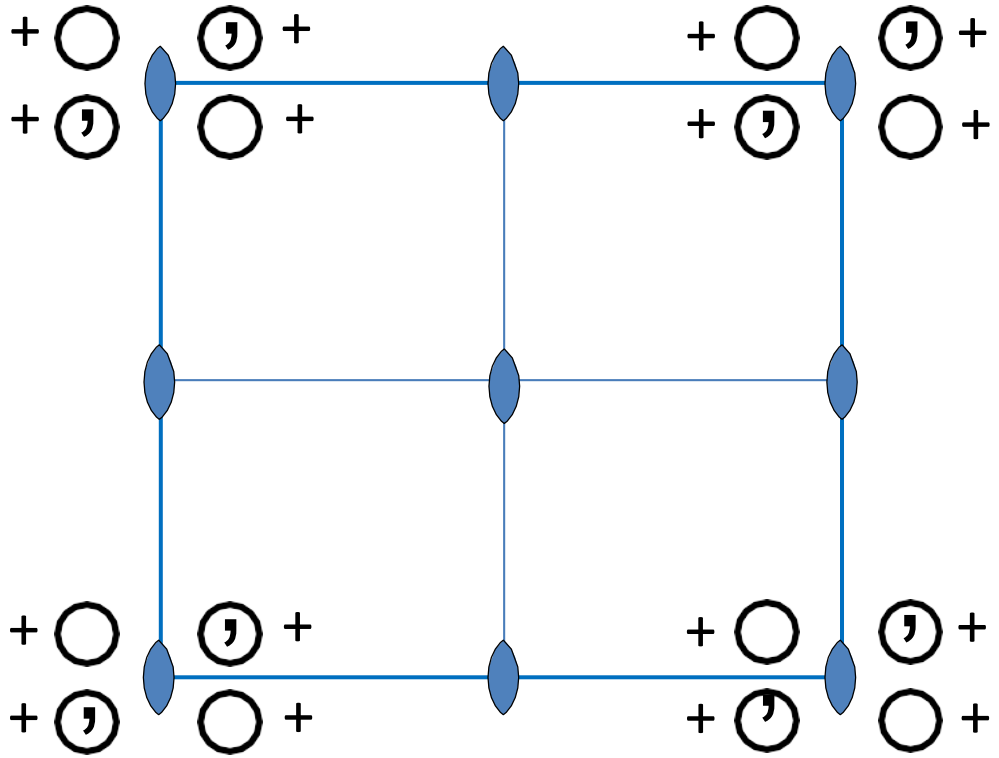
Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



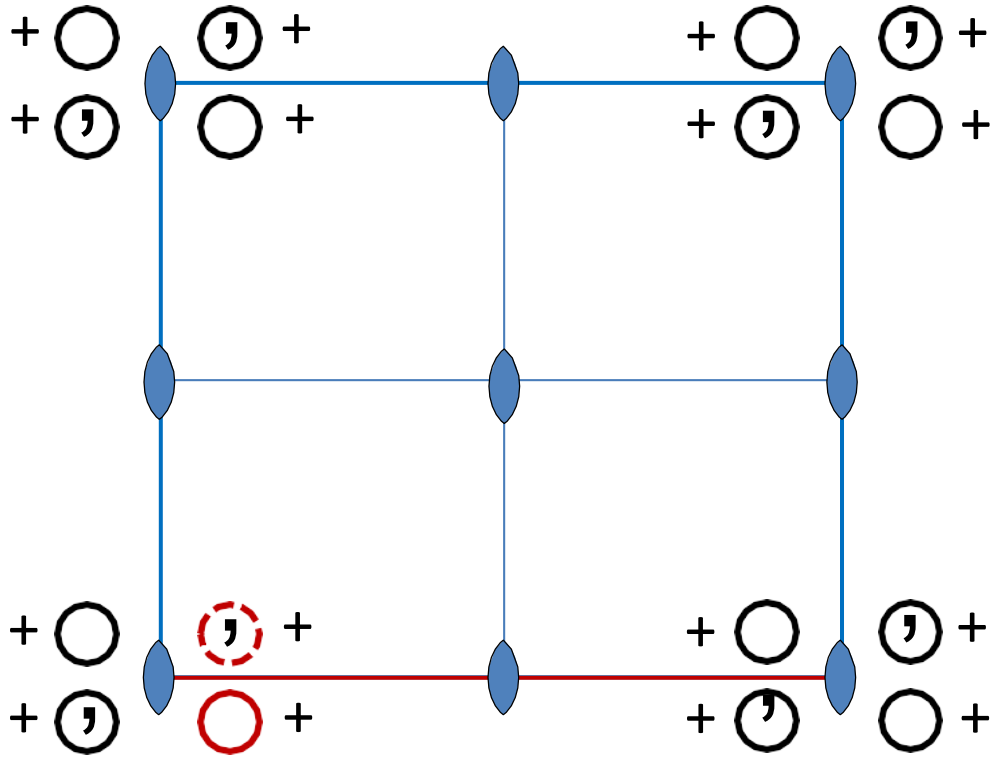
\+

position along the *c*-direction above the projection plane

image and mirror image

Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



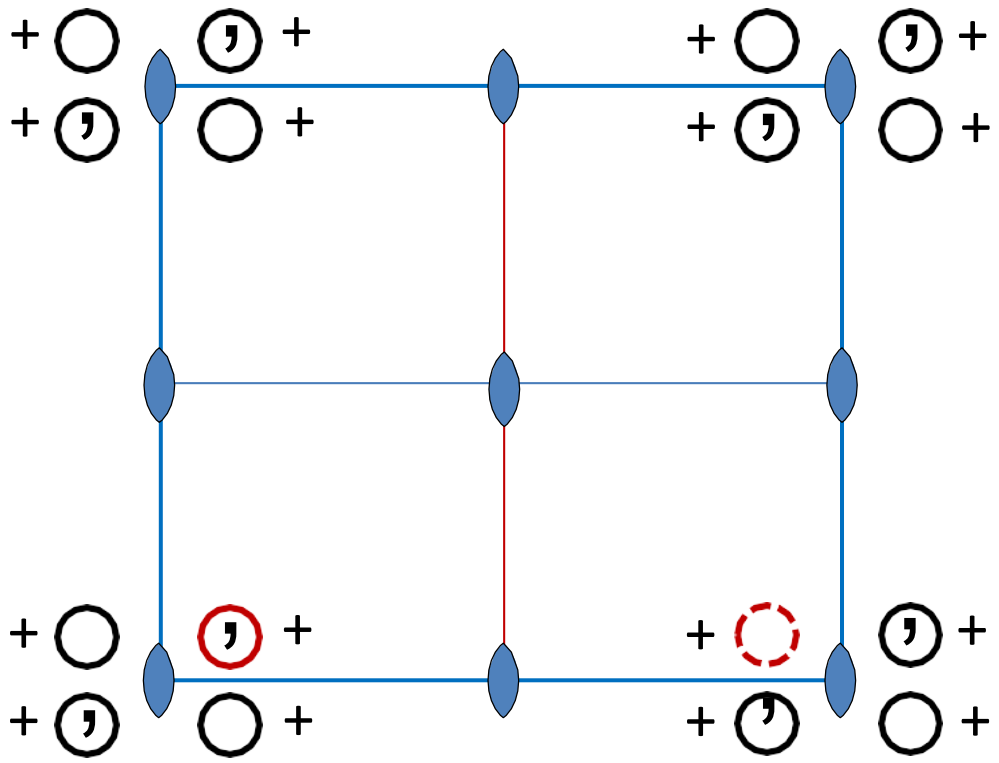
\+

position along the *c*-direction above the projection plane

image and mirror image

Source: Frank Hoffmann

Space group Pmm2 – General Position Diagram



\+

position along the *c*-direction
above the projection plane

image and mirror image
Of chiral object

Source: Frank Hoffmann

230 Space Group

- When talking about crystal structures, people will usually report the *space group* of a crystal
- Space groups are made up from
  - point symmetry (not translational)
  - lattice symmetry (translational)
  - glide and/or screw axes (some translational component)

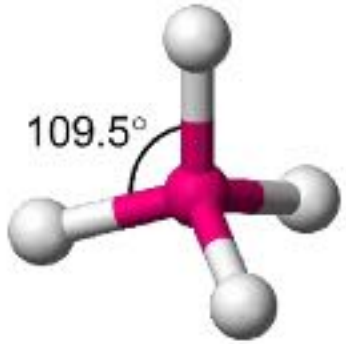
7 crystal systems → **14 Bravais lattices** → **32 point groups** → **230 space groups**

Summary

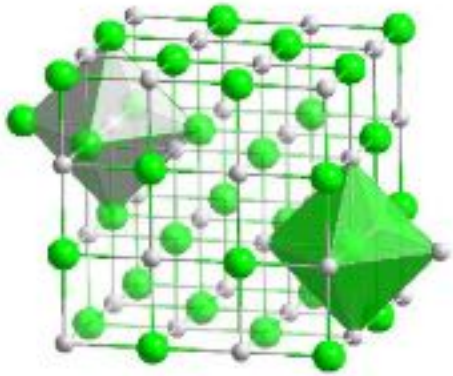
Point Symmetry (3D)	Plane Symmetry (2D)	Space Symmetry (3D)
-	Translation	Translation
Inversion (point mirroring)	Inversion (point mirroring)	Inversion (point mirroring)
Rotation	Rotation	Rotation
Roto-Inversion (rotate, then invert)	-	Roto-Inversion (rotate, then invert)
Reflection	Reflection	Reflection
-	Glide (reflect, then translate, 2D)	Glide (reflect, then translate, 3D)
-		Screw (rotate, then translate)
32 crystal classes	17 plane groups	230 space groups
	5 Bravais lattices	32 crystal classes
		14 Bravais lattices

Source: Frank Hoffmann

Schoenflies vs. Hermann-Mauguin



World of molecules



World of crystals

Symmetry notation system according to
Artur Moritz Schoenflies

Symmetry notation system according to
Carl Hermann und Charles-Victor Mauguin

"Schoenflies symbolism"

"Hermann-Mauguin symbolism"

Source: Frank Hoffmann

Rotoinversions vs. Rotary reflections

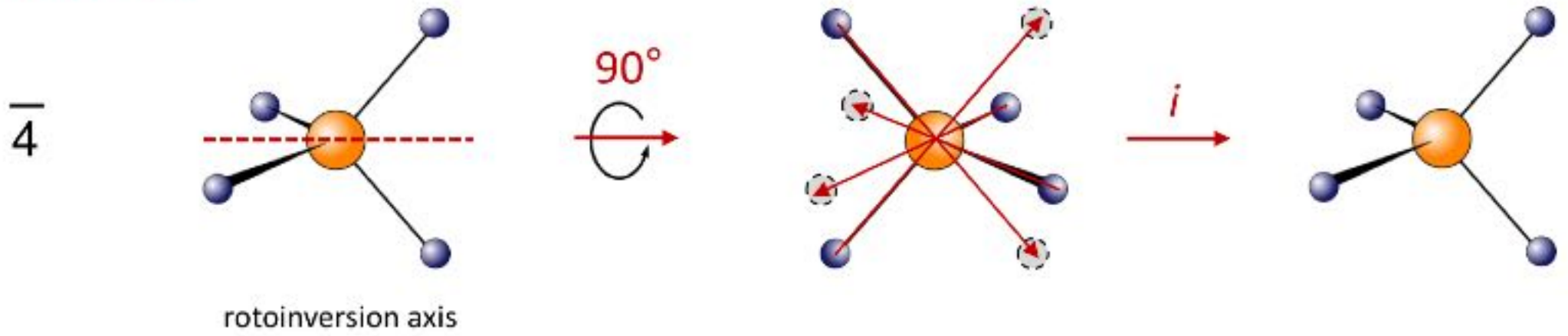
Symmetry elements of macroscopic objects

Schoenflies		Hermann-Mauguin	
Identity	E	Identity	1
Mirror plane	σ	Mirror plane	m
Axis of rotation	C_n	Axis of rotation	n
Center of inversion	i	Center of inversion	$\bar{1}$
Rotation-reflection axis (Improper axis of rotation)	S_n	Rotoinversion axis	$\bar{n}$

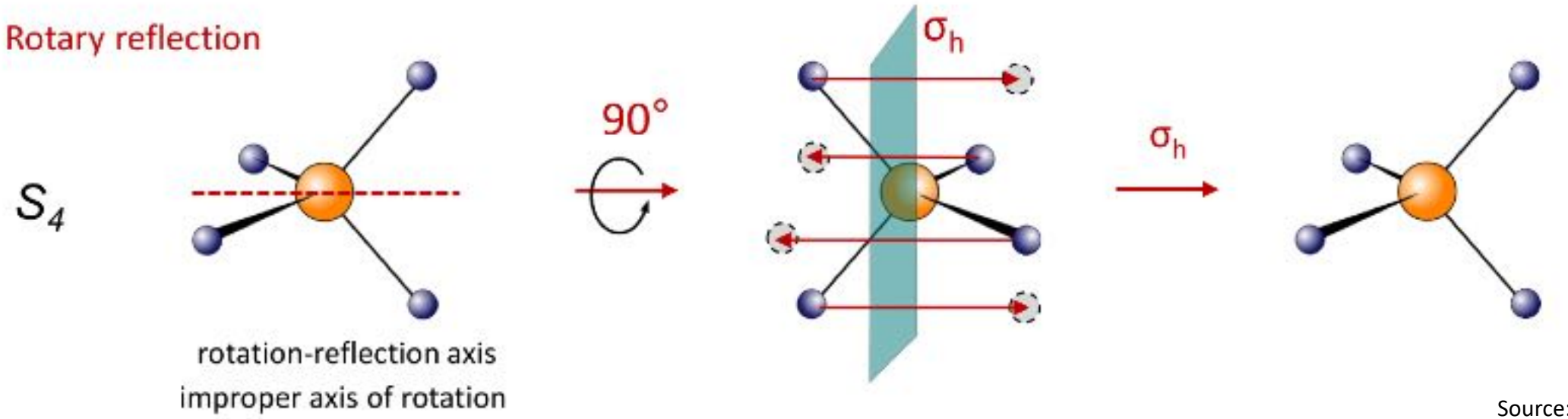
Source: Frank Hoffmann

Roto-inversions vs. Rotary reflections

Rotoinversion



Rotary reflection



Source: Frank Hoffmann

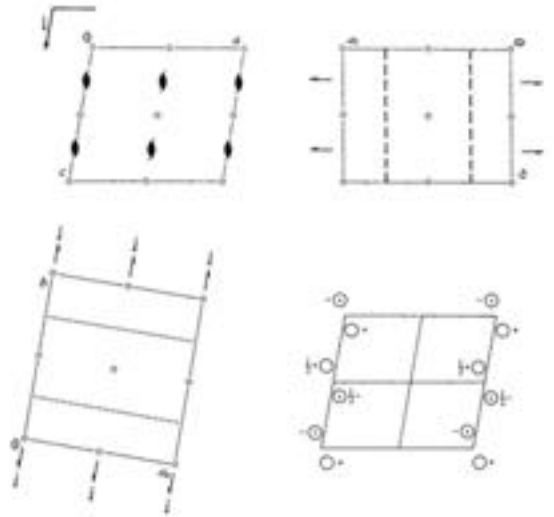
International Tables for Crystallography – Space group P2 1 /c

International Tables for Crystallography (2006). Vol. A. Space group 14, pp. 184–191.

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at 1

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

Symmetry operations

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

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	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\frac{1}{2}-z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\frac{1}{2}-y,z+\frac{1}{2}$	$0kl: l=2n$ $h0l: h=2n$ $hkl: l=2n$
						Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		$hkl: h+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$		$hkl: k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		$hkl: h+l=2n$
2	a	$\bar{1}$	0,0,0	$0,\frac{1}{2},\frac{1}{2}$		$hkl: k+l=2n$

Symmetry of special projections

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

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

Along [010] $p2$ $\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$ 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] $Pnma$ (52); [2] $Pnma$ (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] $Cmcm$ (63)
II	[2] $A12_1/m1$ ($C2/m$, 12); [2] $C12_1/c1$ ($C2/c$, 15); [2] $I12_1/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{a}'=\mathbf{c}$) ($P2_1/m$, 11); [2] $P12_1/c1$ ($\mathbf{b}'=\mathbf{b}$) ($P2_1/c$, 13)

Source: Frank Hoffmann

Space group P2 1 /c – Header

Short symbol $P2_1/c$ Crystal class C_{2h}^5 $2/m$ *Crystal system* Monoclinic

Number No. 14 *Full symbol* $P12_1/c1$ Patterson Symmetry $P12/m1$

UNIQUE AXIS *b*, CELL CHOICE 1

settings

$P2_1/c$ – standard space group

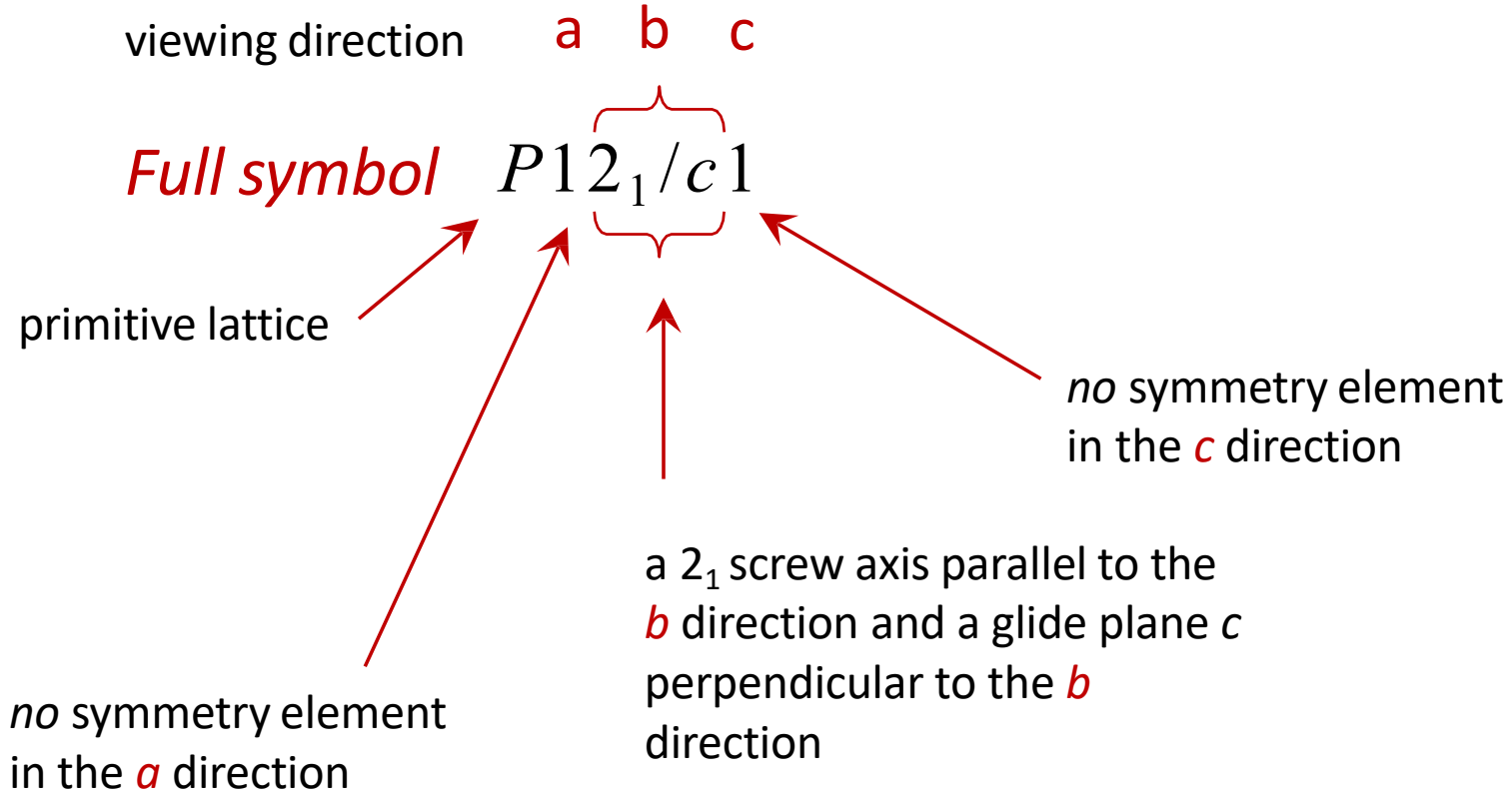
$P2_1/a$

$P2_1/b$ } non-standard space group variants of $P2_1/c$

$P2_1/n$

Source: Frank Hoffmann

Space group P2 1 /c – Header



Source: Frank Hoffmann

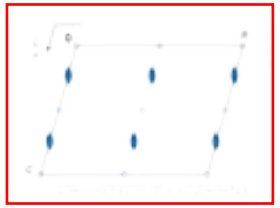
International Tables for Crystallography – Space group P2 1 /c

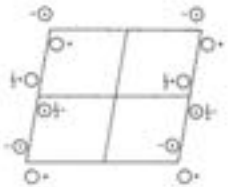
International Tables for Crystallography (2006). Vol. A. Space group 14, pp. 184–191.

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS $\vec{b}$, CELL CHOICE 1





Origin at 1

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

Symmetry operations

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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) $\bar{x},y+\frac{1}{2},\frac{1}{2}-z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\frac{1}{2}-y,z+\frac{1}{2}$	$0kl: l=2n$ $h0l: h=2n$ $hkl: l=2n$
					Special: as above, plus
2 d $\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			$hkl: h+l=2n$
2 c $\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			$hkl: h+l=2n$
2 b $\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl: h+l=2n$
2 a $\bar{1}$	0,0,0	$0,\frac{1}{2},\frac{1}{2}$			$hkl: h+l=2n$

Symmetry of special projections

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

Along [100] $p2_1g$ $\mathbf{a}=\mathbf{b}$ $\mathbf{b}=\mathbf{c}$ 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)

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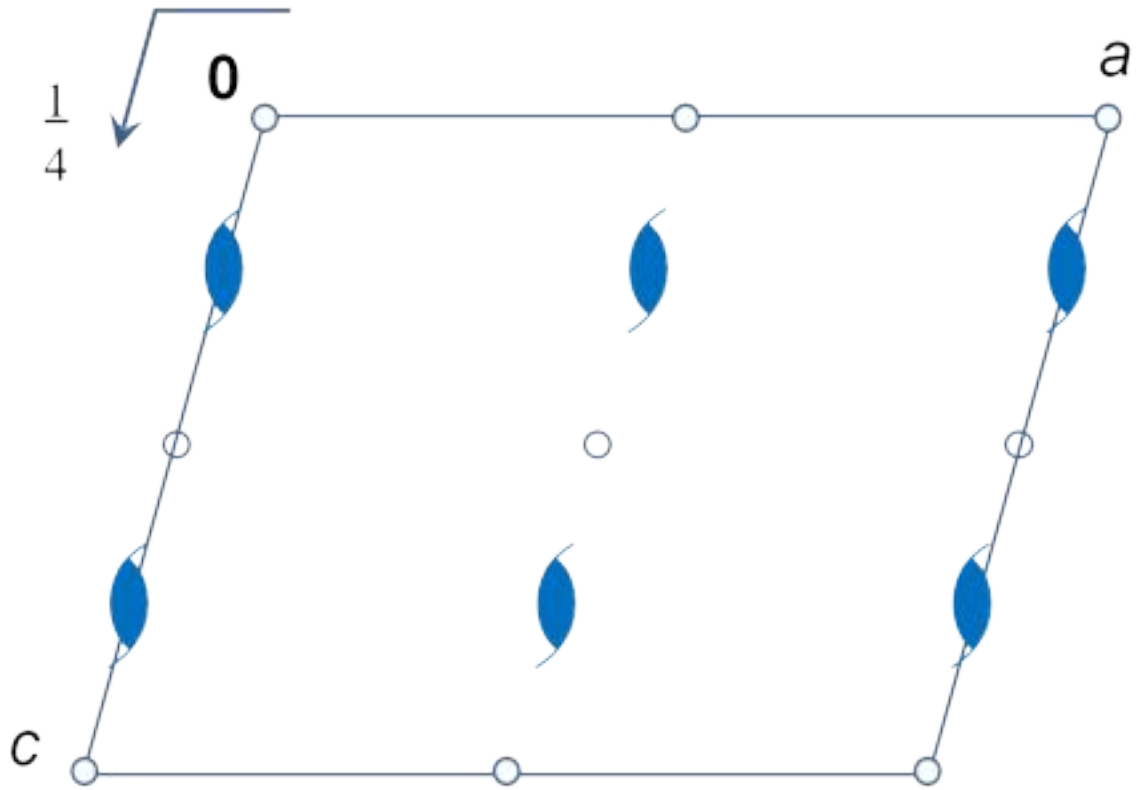
Source: Frank Hoffmann

Diagram of the Symmetry elements – Space group P2 1 /c

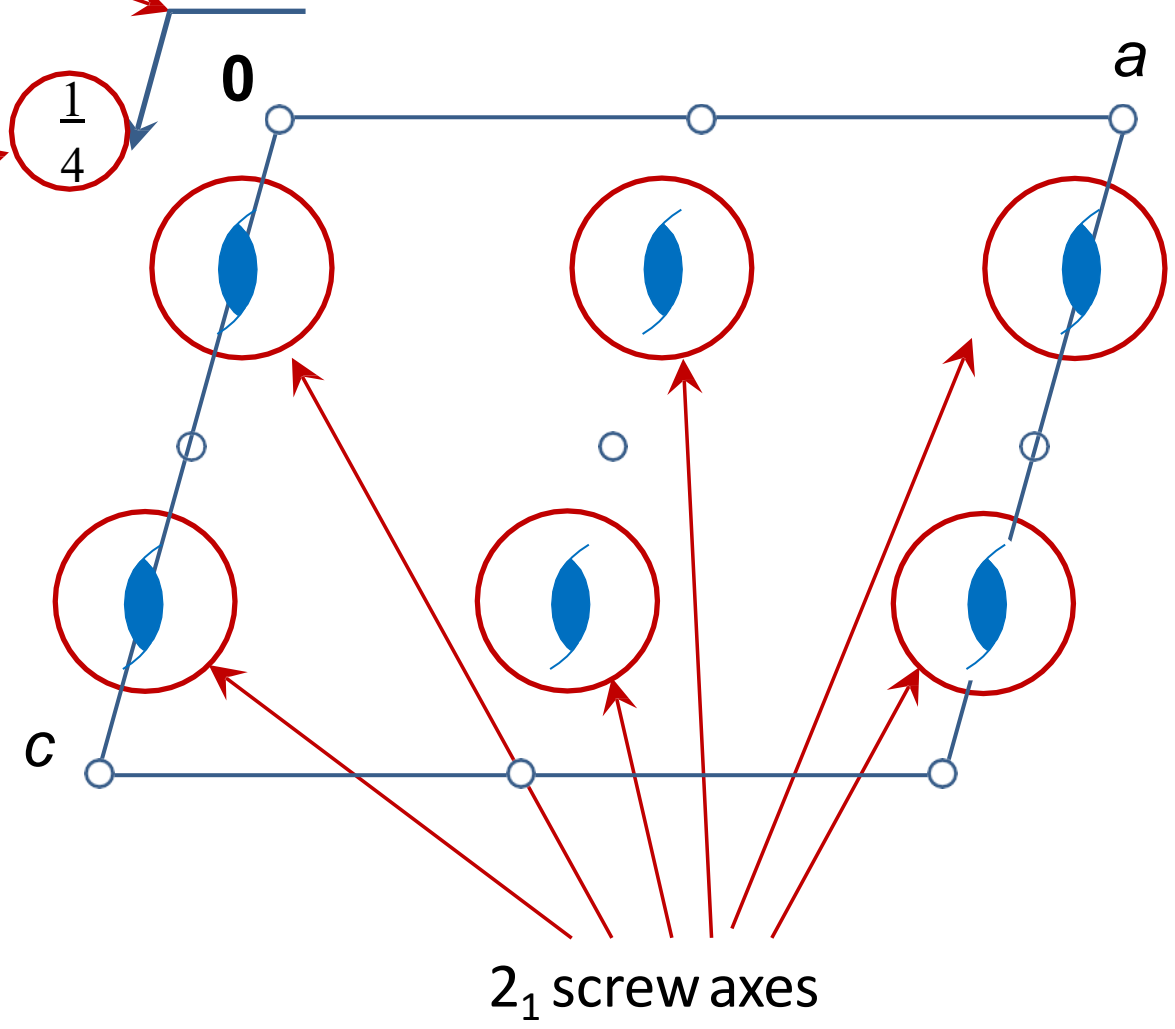


Source: Frank Hoffmann

Diagram of the Symmetry elements – Space group P2 1 /c

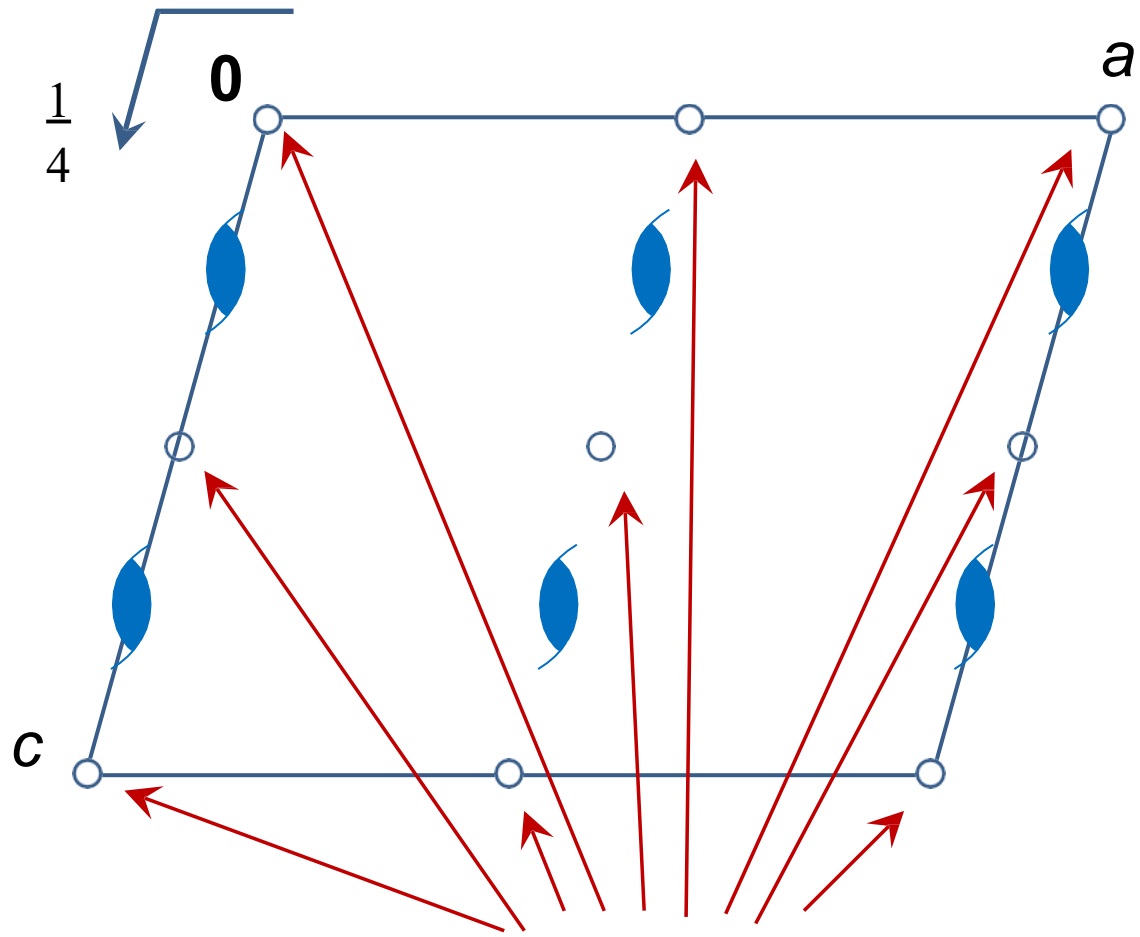
glide plane perpendicular
to the *b* direction with
translation direction *c*

height along
the *b* direction



Source: Frank Hoffmann

Diagram of the Symmetry elements – Space group P2 1 /c



centres of inversion

Source: Frank Hoffmann

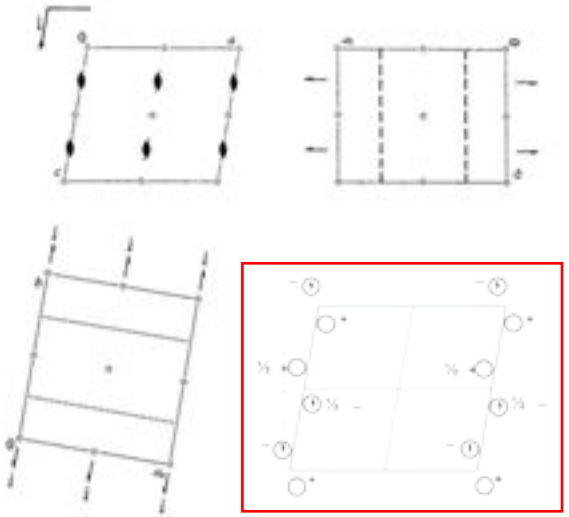
International Tables for Crystallography – Space group P2 1 /c

International Tables for Crystallography (2006). Vol. A. Space group 14, pp. 184–191.

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS $\vec{b}$, CELL CHOICE 1



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						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

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II	[2] $A12_1/m1$ ($C2/m$, 12); [2] $C12_1/c1$ ($C2/c$, 15); [2] $I12_1/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}'=4\mathbf{c}$) ($P2_1/m$, 11); [2] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 13)

Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c

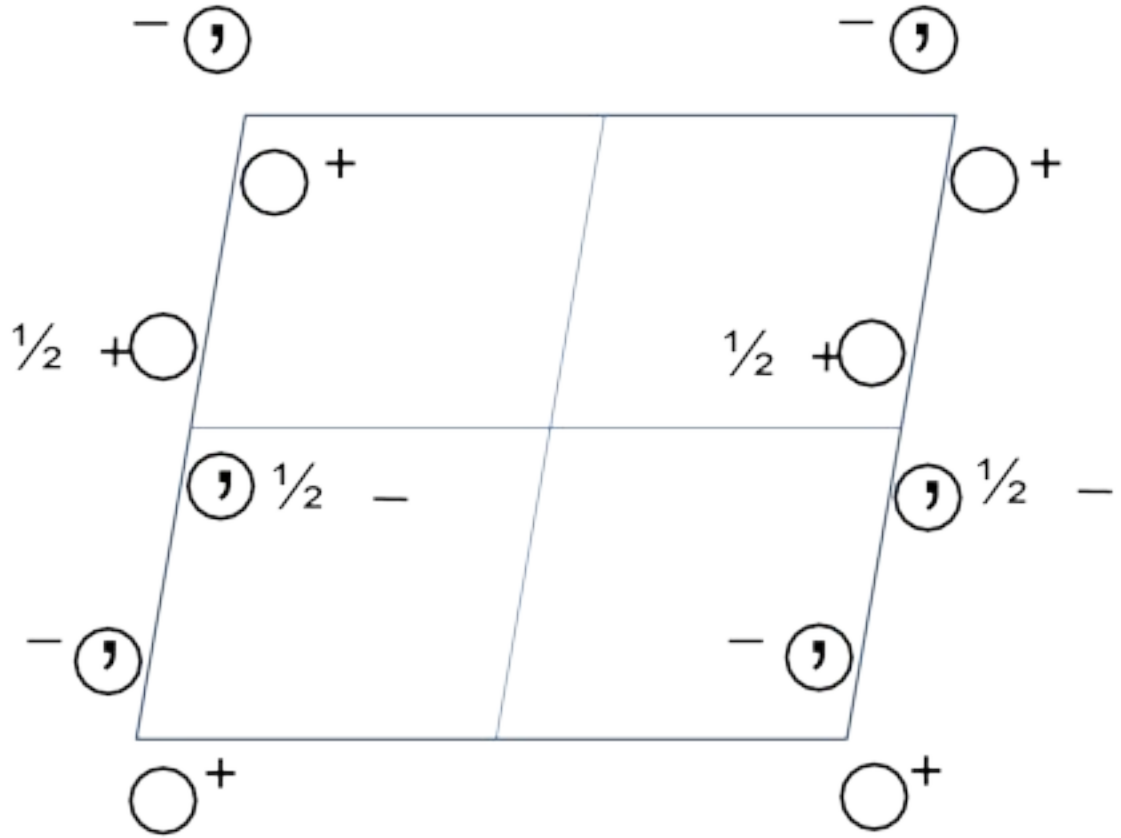


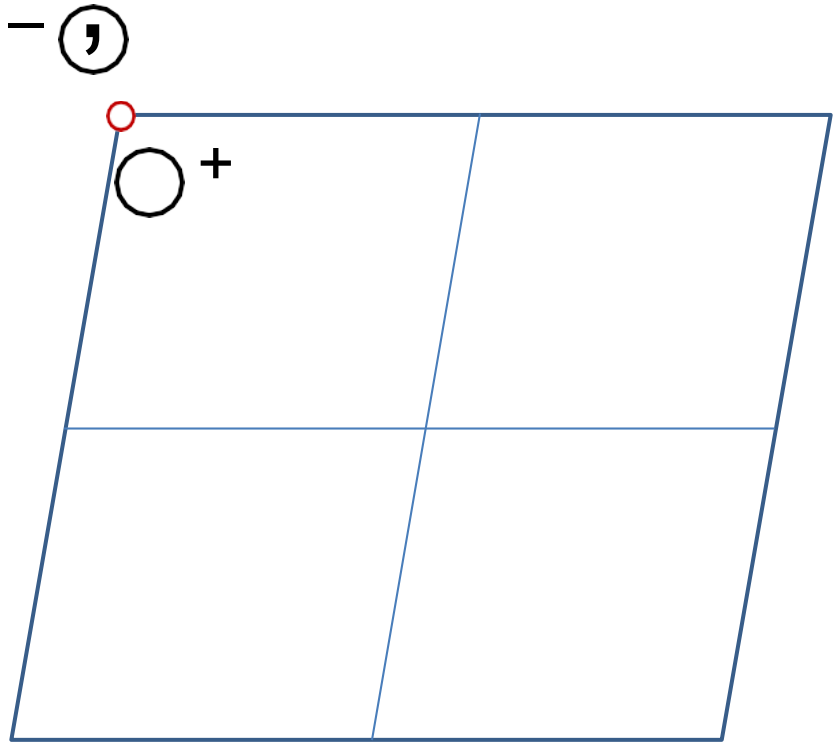
image and mirror image

\+ above the projection plane

– below the projection plane

Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c

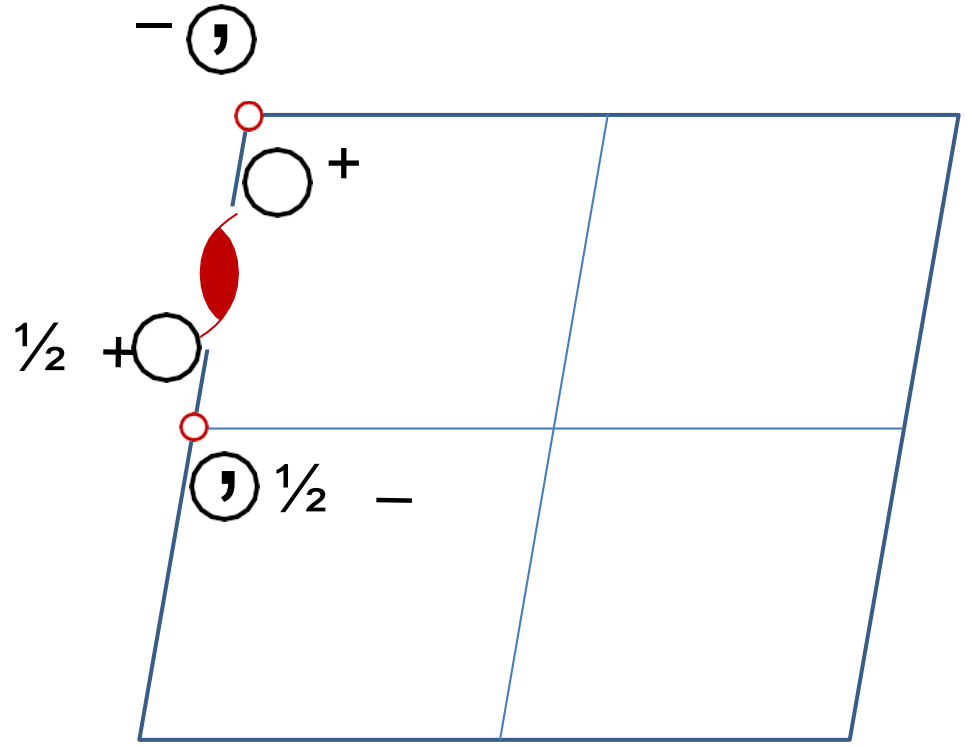


' image and mirror image

\+ – above / below the projection plane

Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c



, ○ image and mirror image

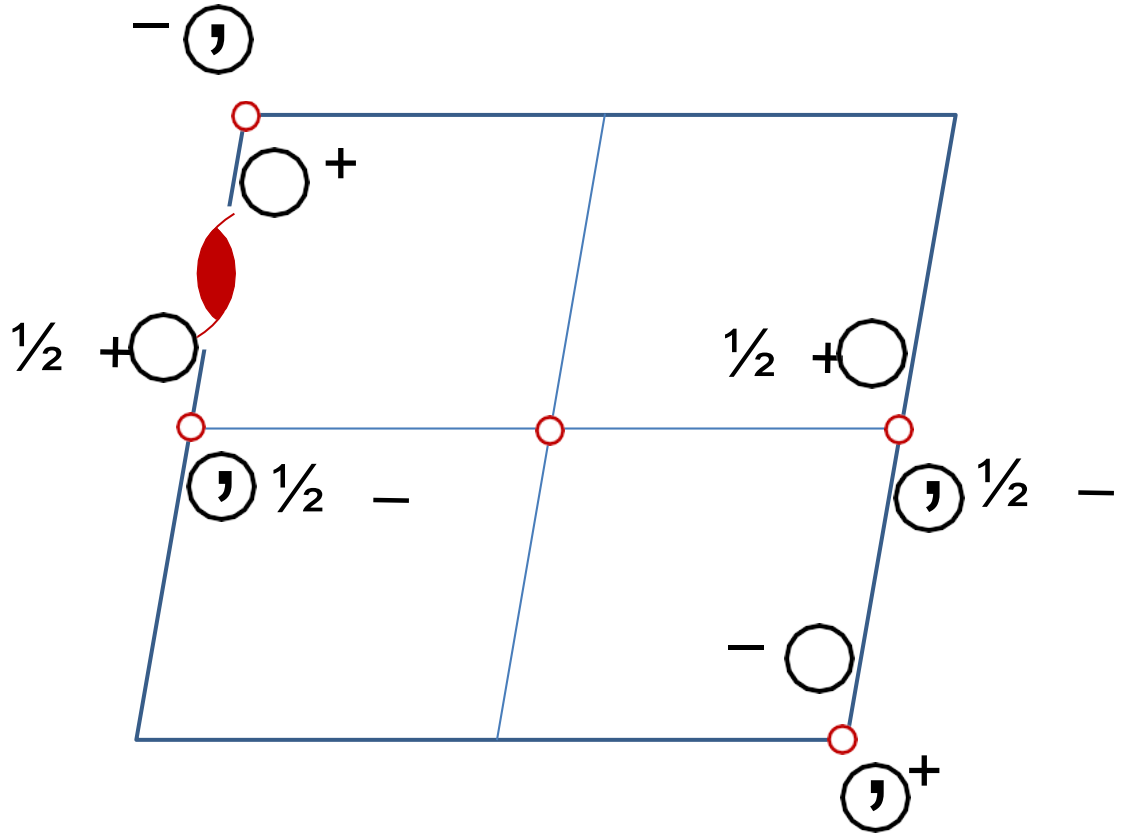
\+ – above / below the projection plane

½ + = ½ + y = y + ½

½ – = ½ – y = -y + ½

Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c



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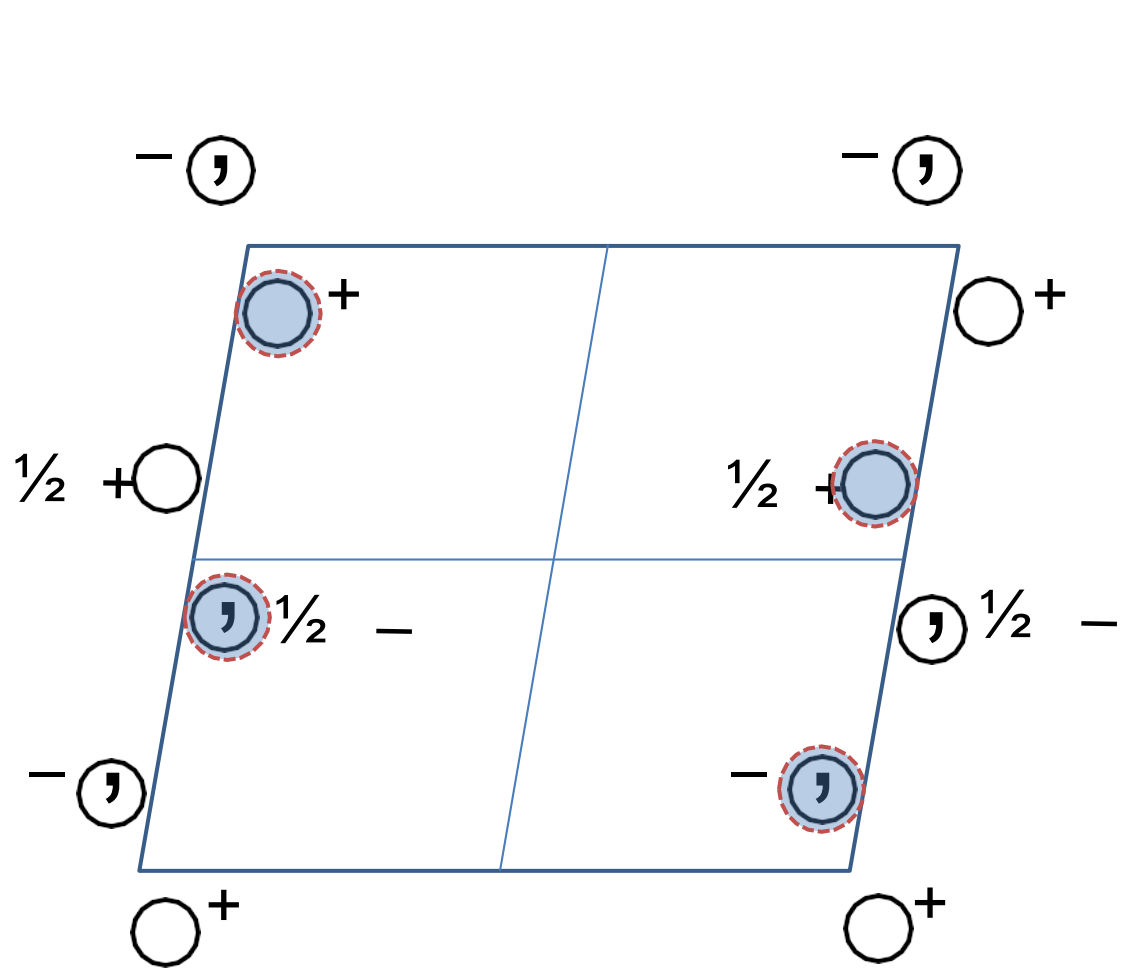
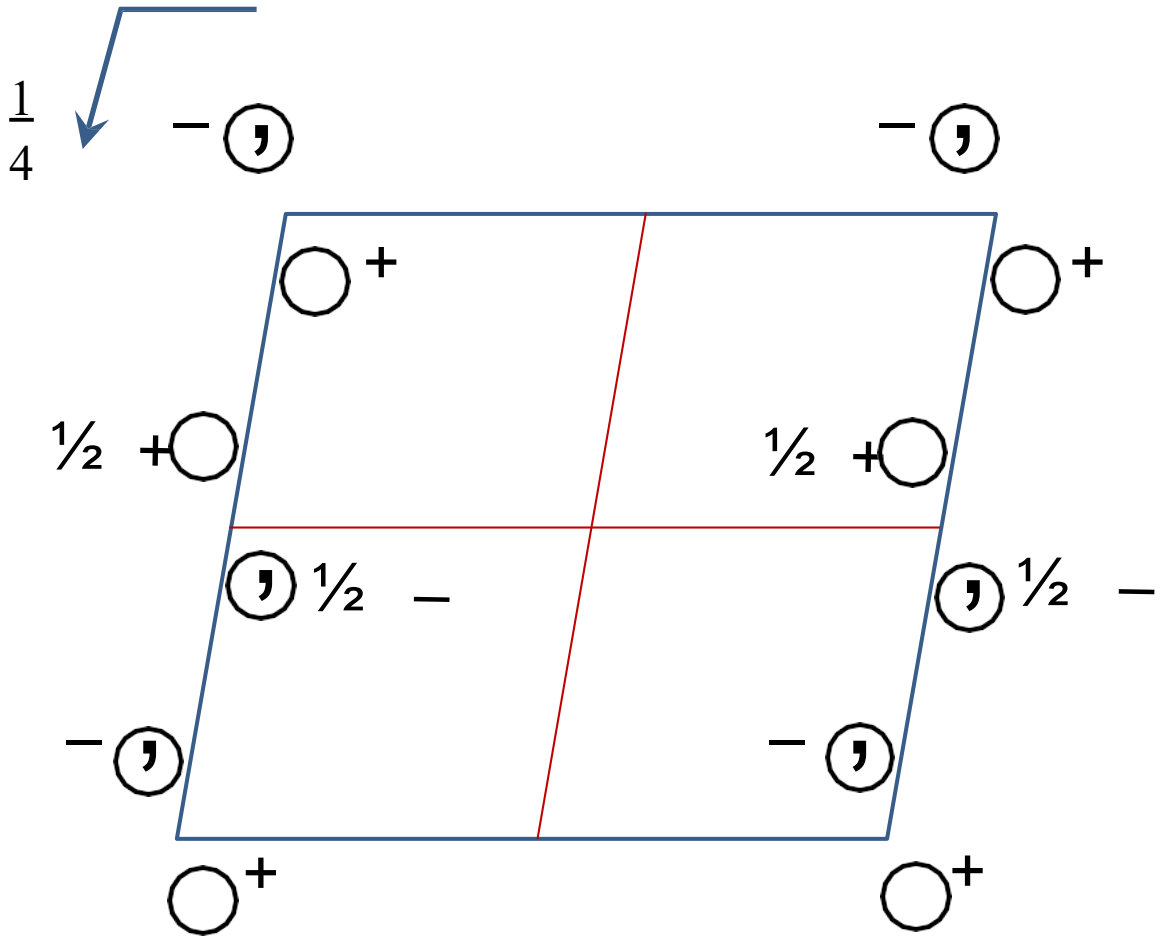
Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c



Source: Frank Hoffmann

General Position Diagram – Space group P2 1 /c

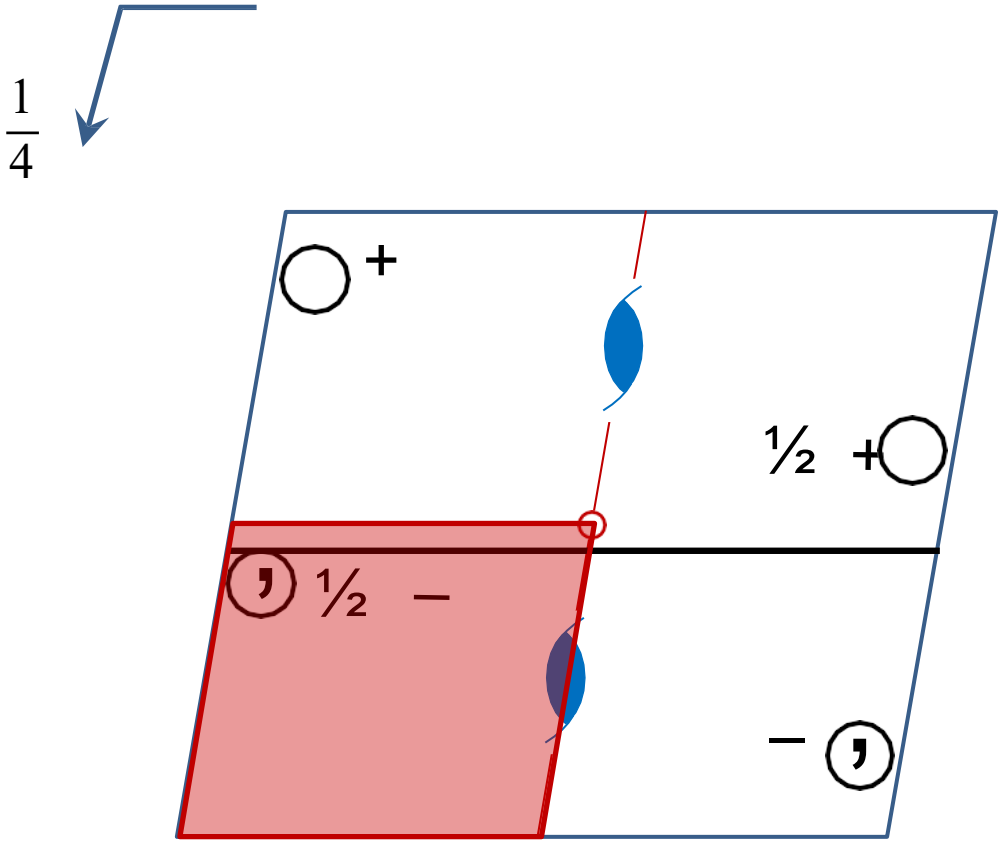


, ○ image and mirror image

\+ − above / below the projection plane

Source: Frank Hoffmann

Asymmetric Unit – Space group P2 1 /c

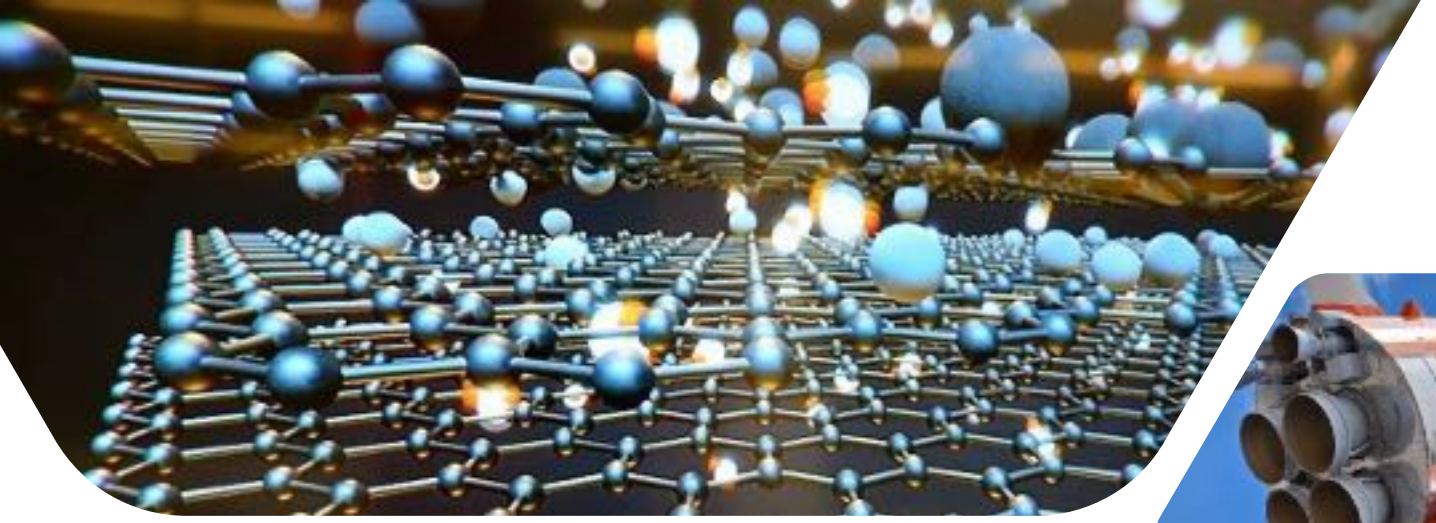


- by pure translations of the unit cell in all 3 spatial directions the whole crystal is build
- however, the *SEs* of the space group act also on atoms *inside* the unit cell, they will be multiplied

→ *asymmetric unit*: is the *set of objects/atoms*, which is *sufficient* to describe all other positions, the complete content of one unit cell, when we apply the SOs of the space group

→ *asymmetric unit*: *must not* have any internal symmetry

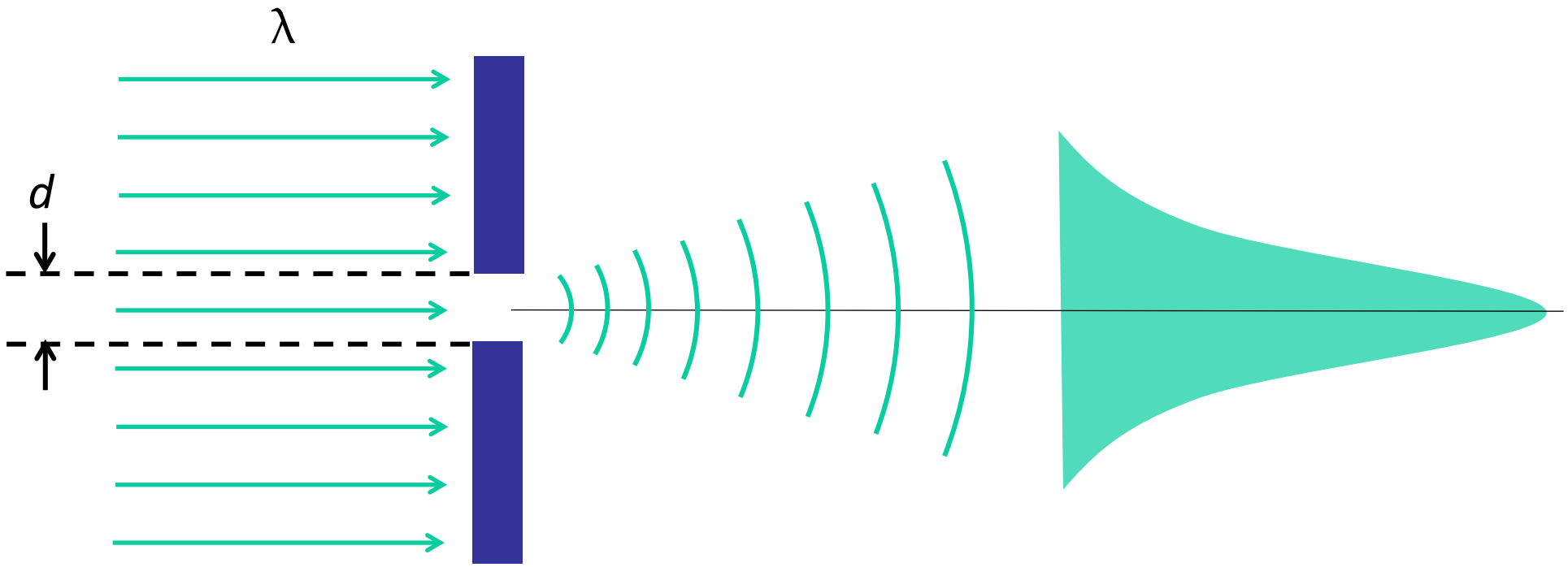
Source: Frank Hoffmann



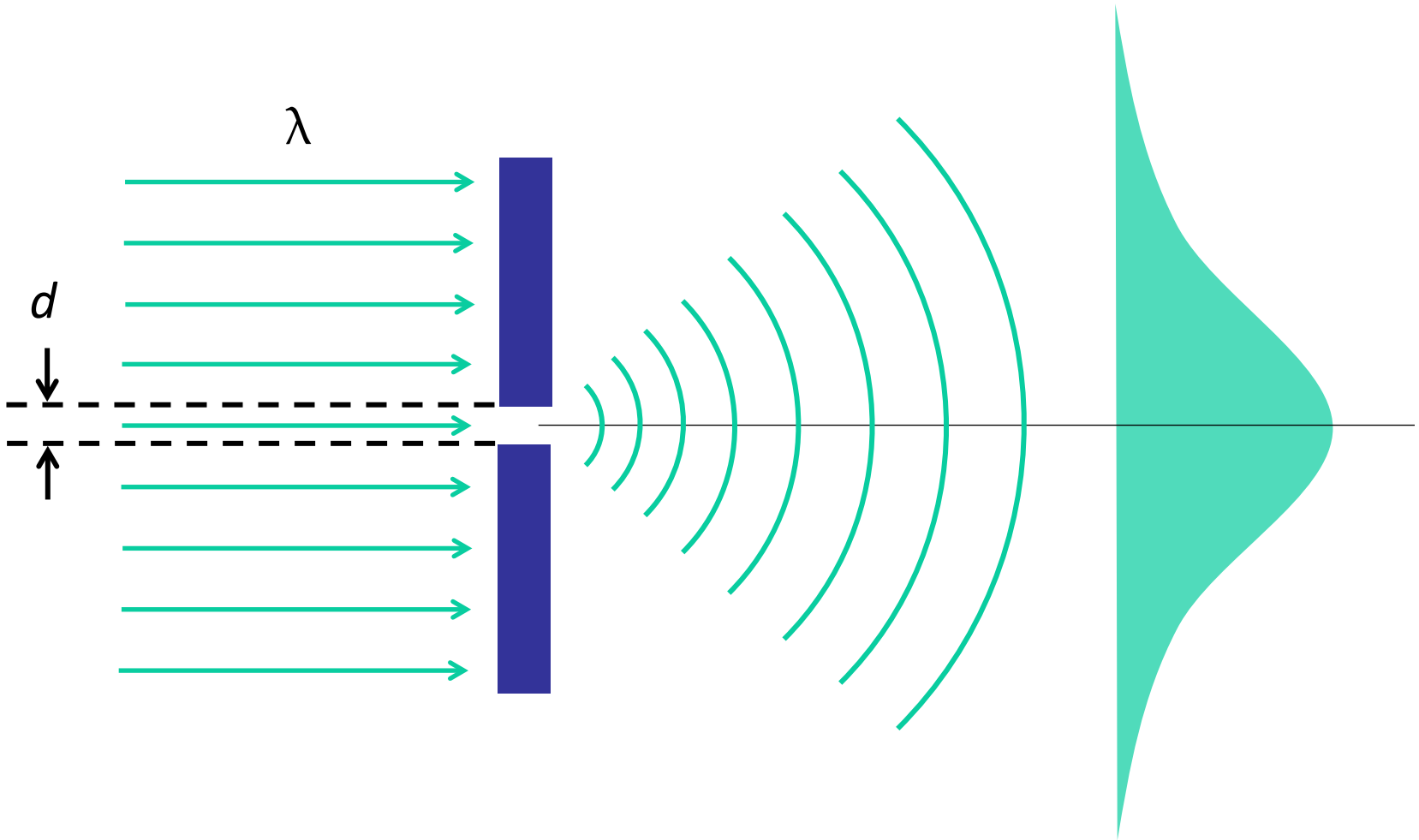
END
Session 1

Single Slit Diffraction

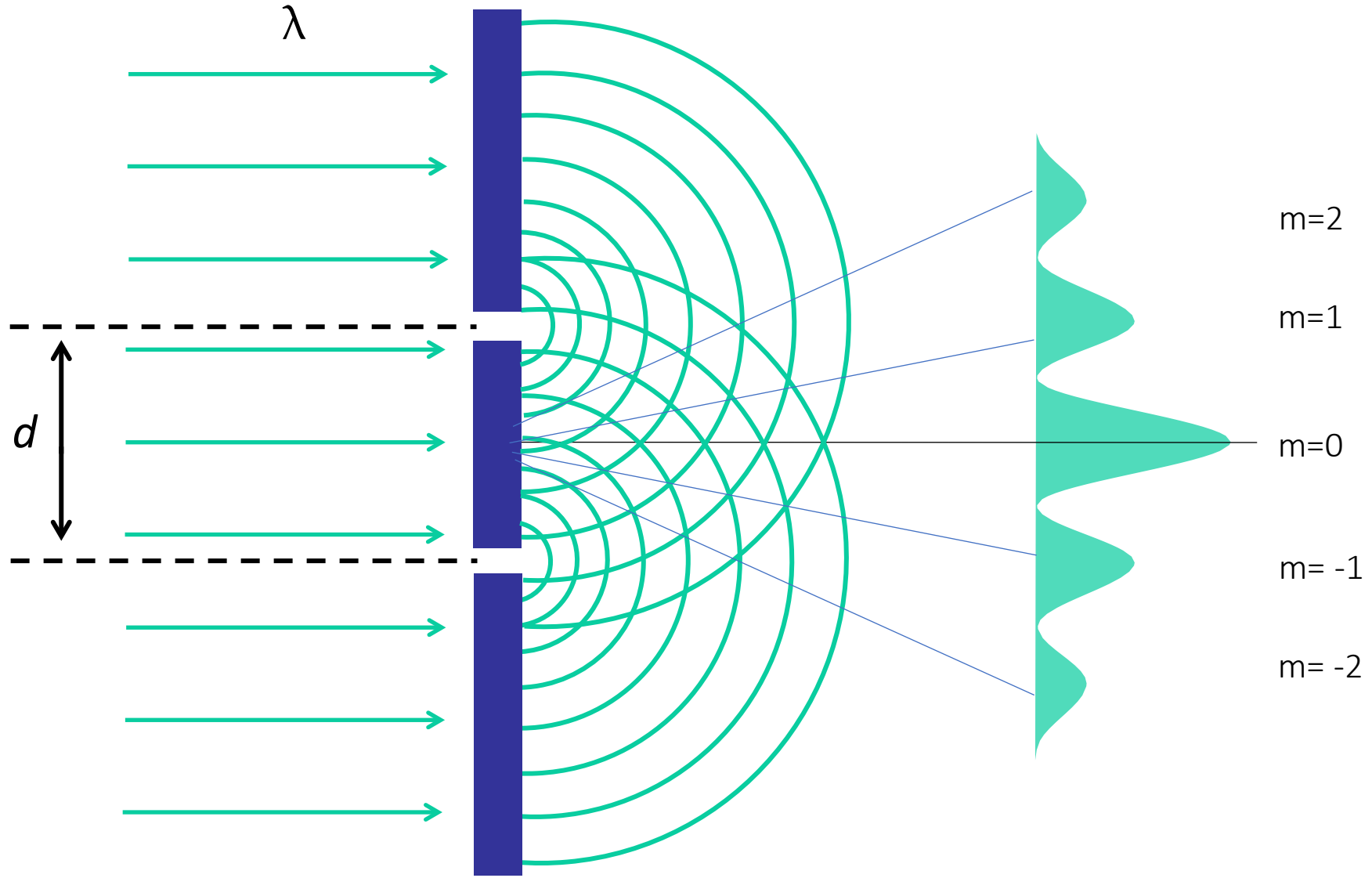
The ‘slit’ scatters light and become a point source



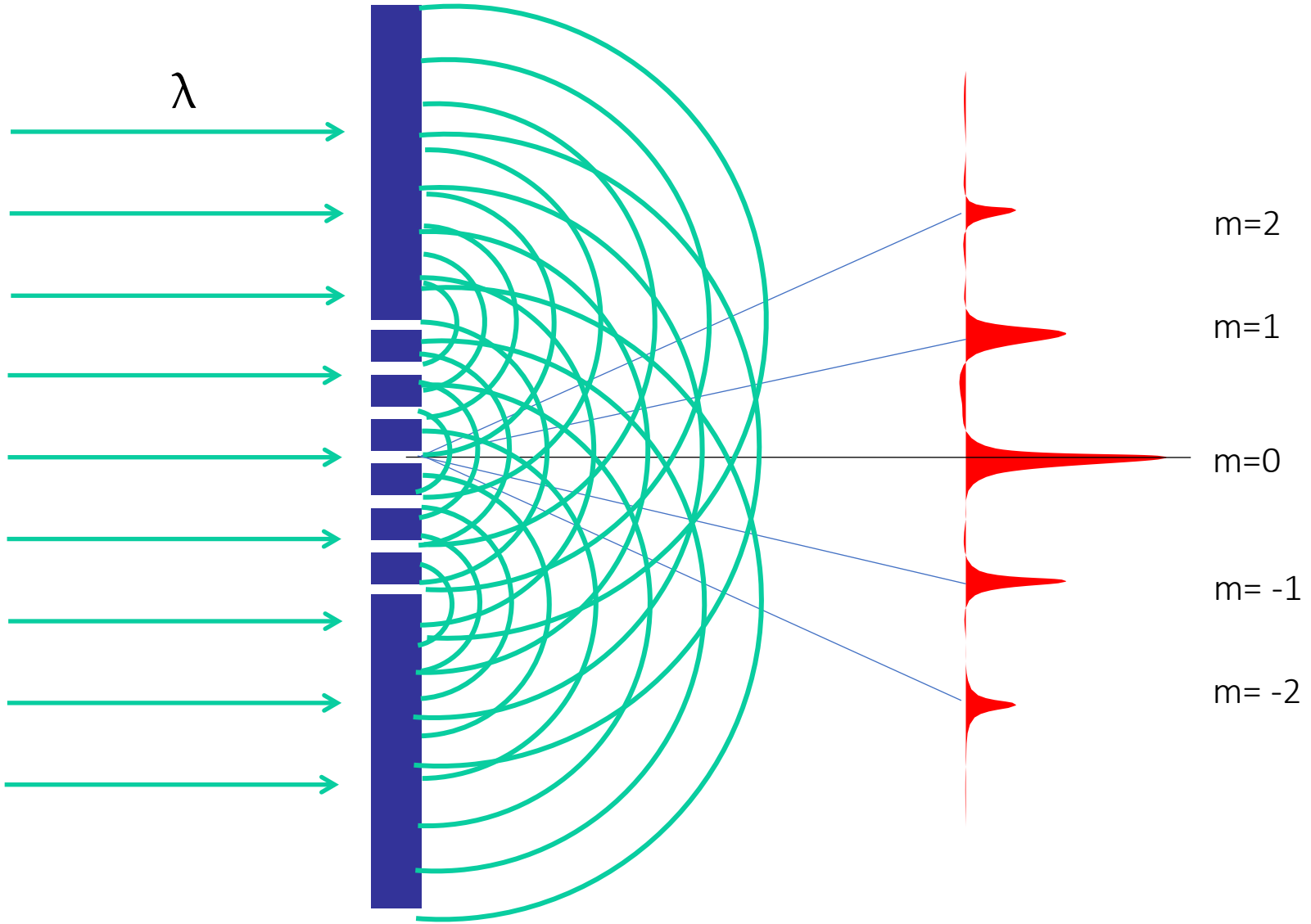
Single Slit Diffraction



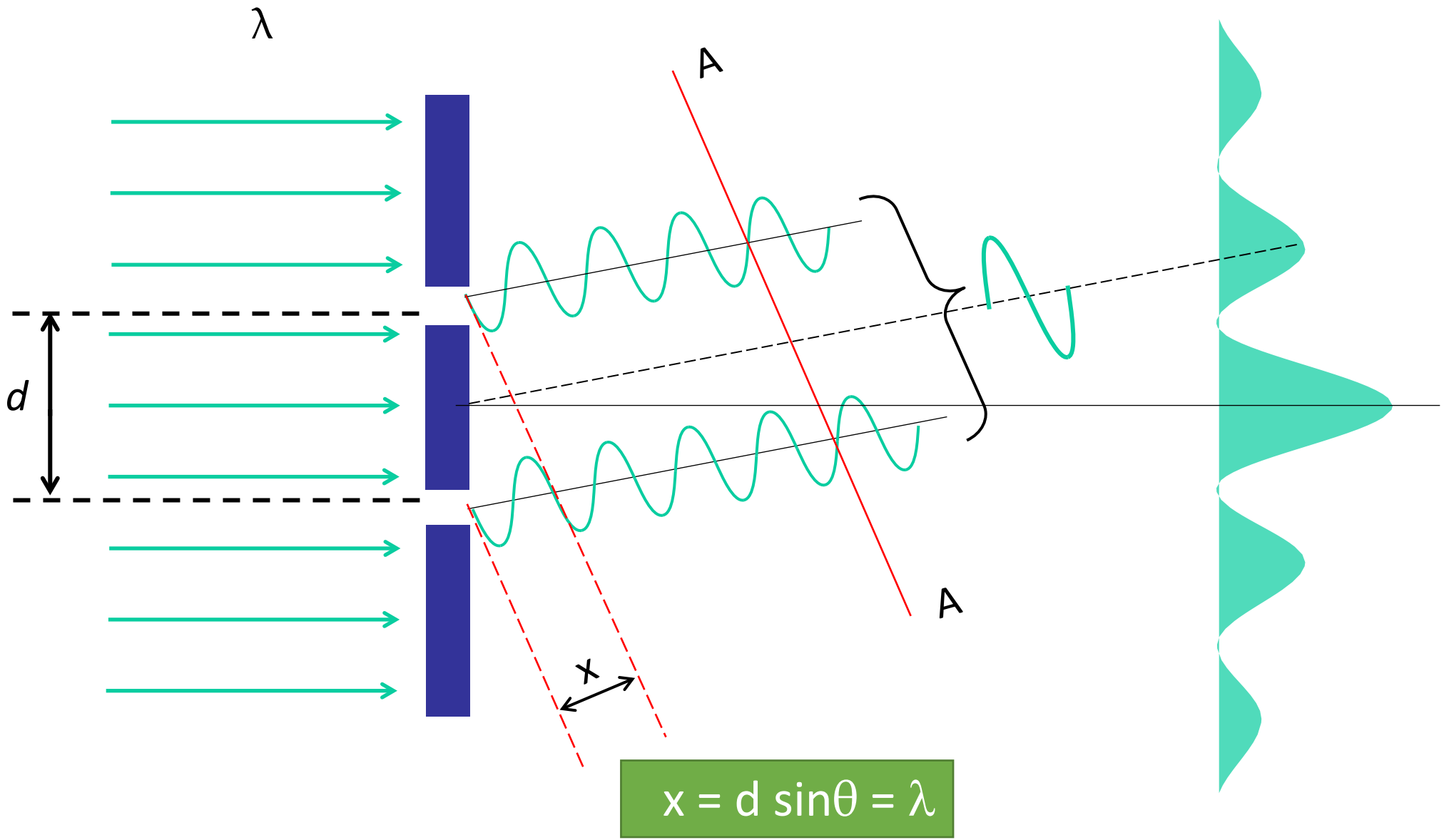
Double Slit Diffraction



Multi Slit Diffraction

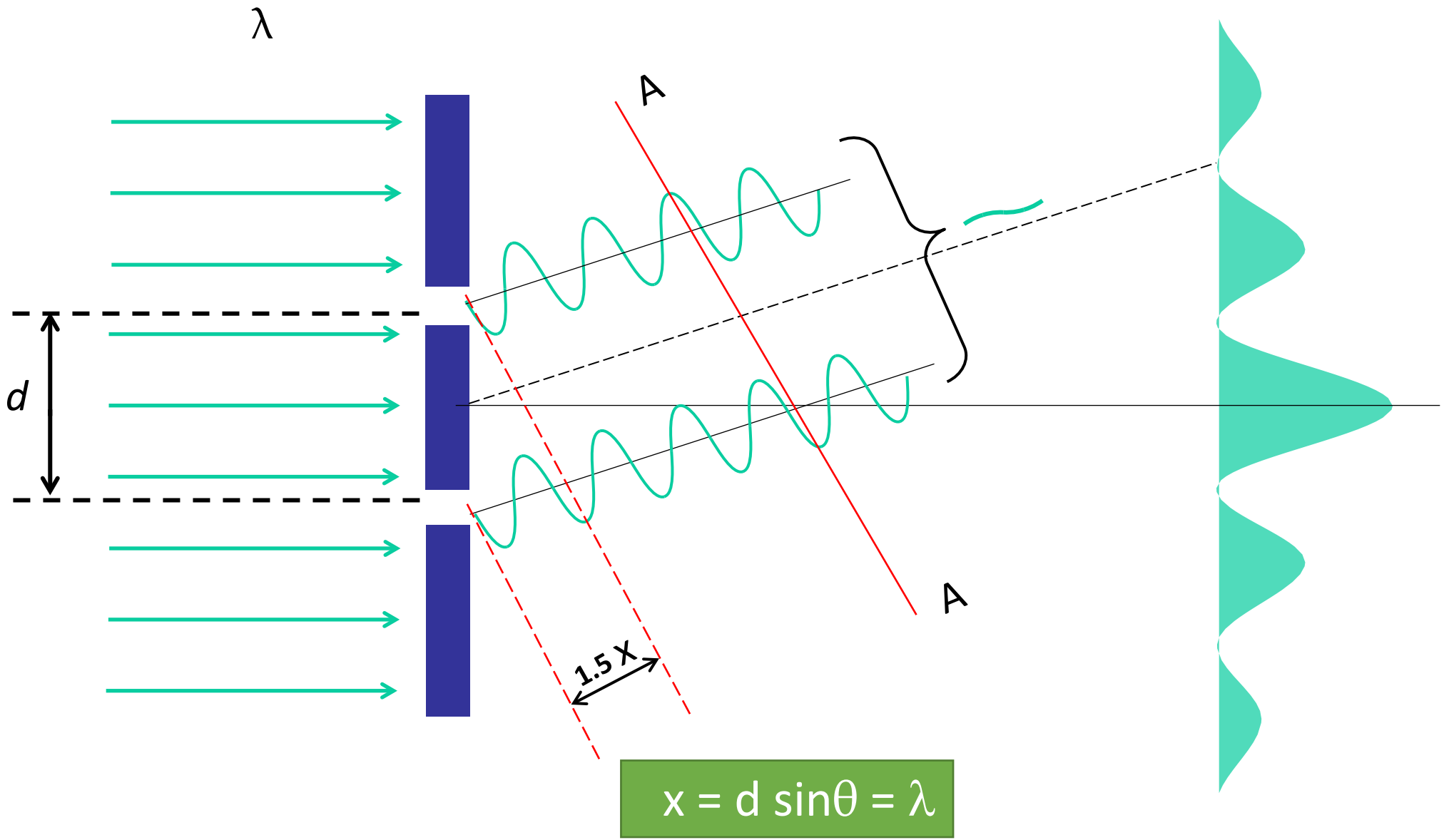


Constructive Interference



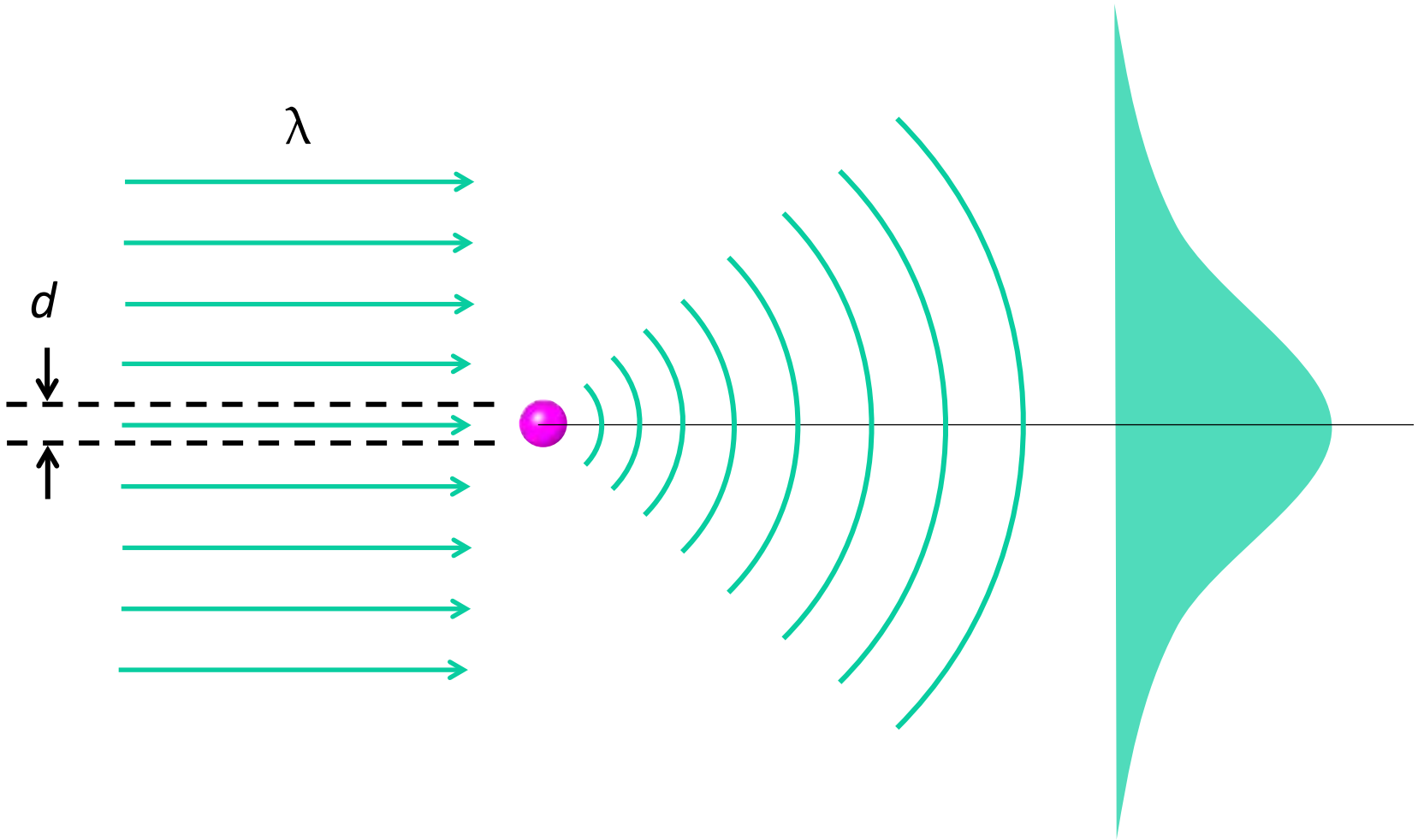
$$x = d \sin\theta = \lambda$$

Destructive Interference

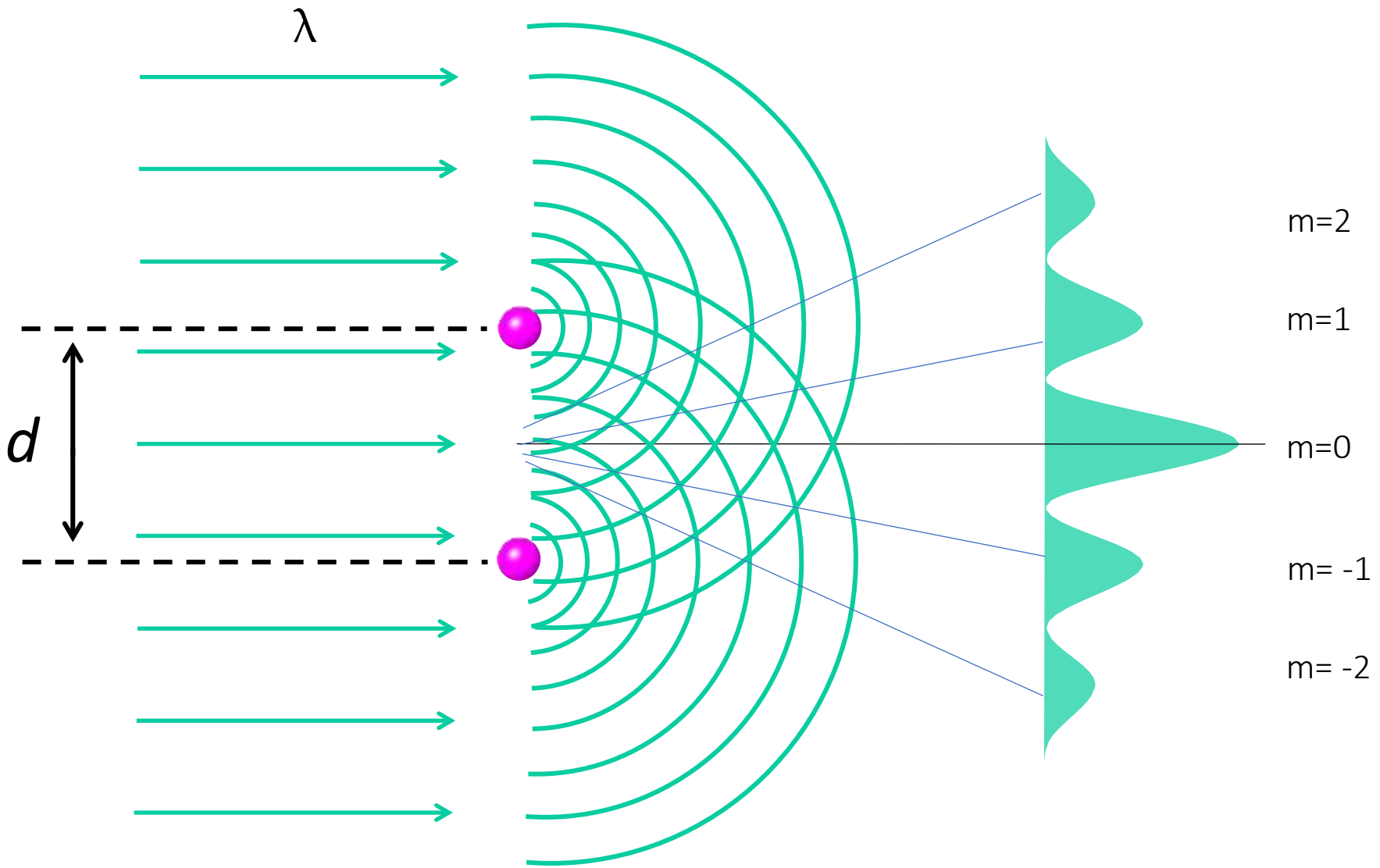


$x = d \sin\theta = \lambda$

Diffraction by One Atom



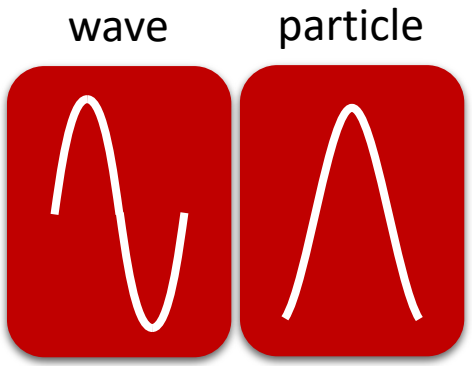
Diffraction by Two Atom



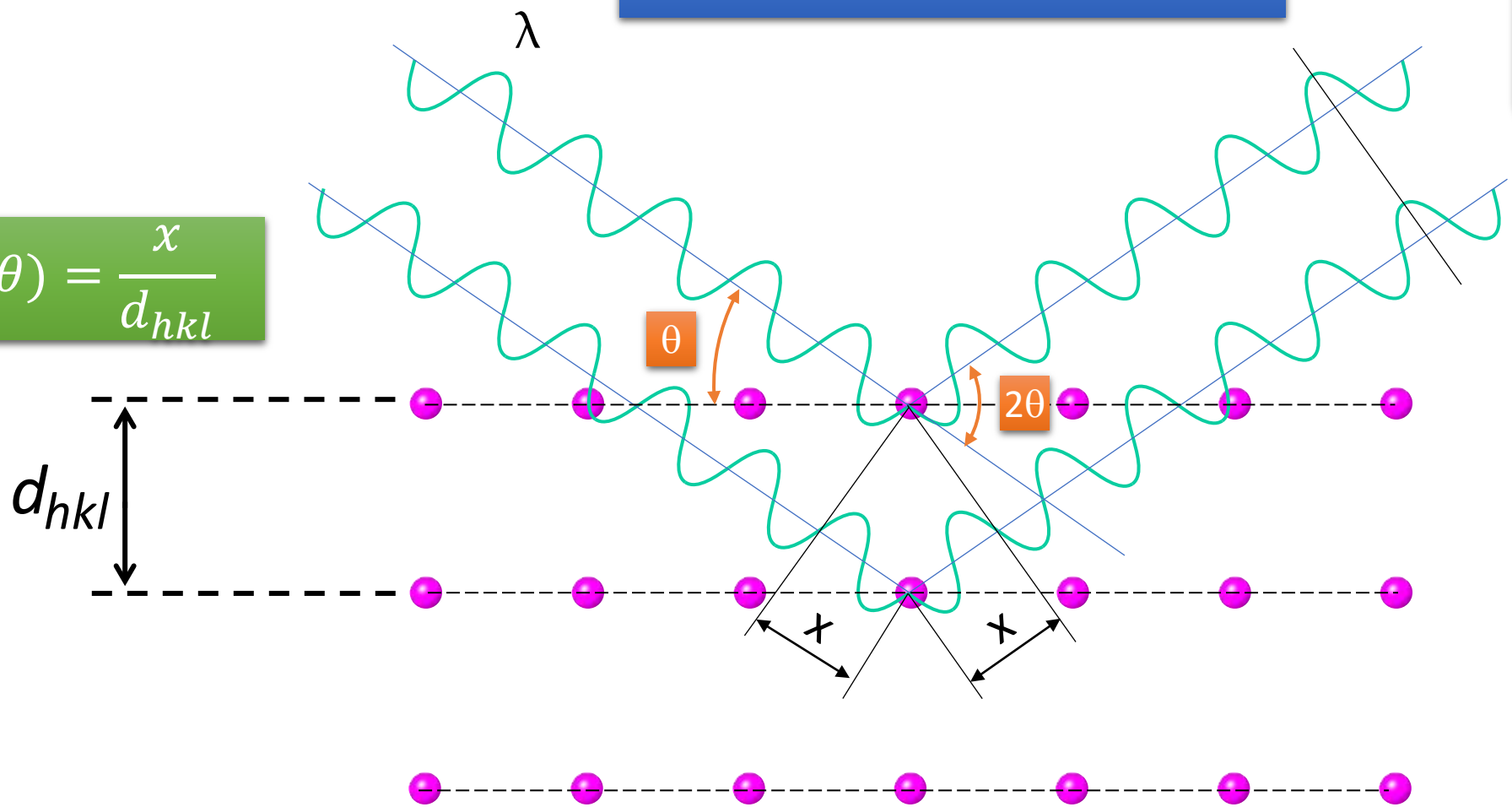
Diffraction by Planes of Atom

- Path difference Δ = 2x => phase shift
- Constructive interference if Δ = nλ
- Criterion for constructive interference:

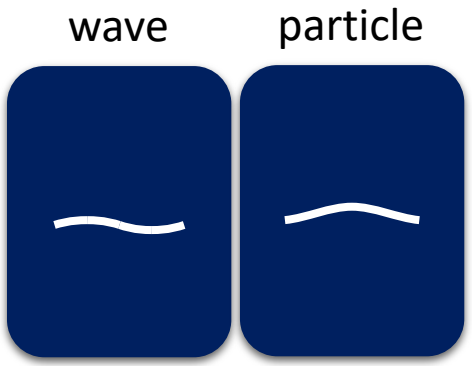
$$\Delta = 2d_{hkl}\sin(\theta) = n\lambda$$

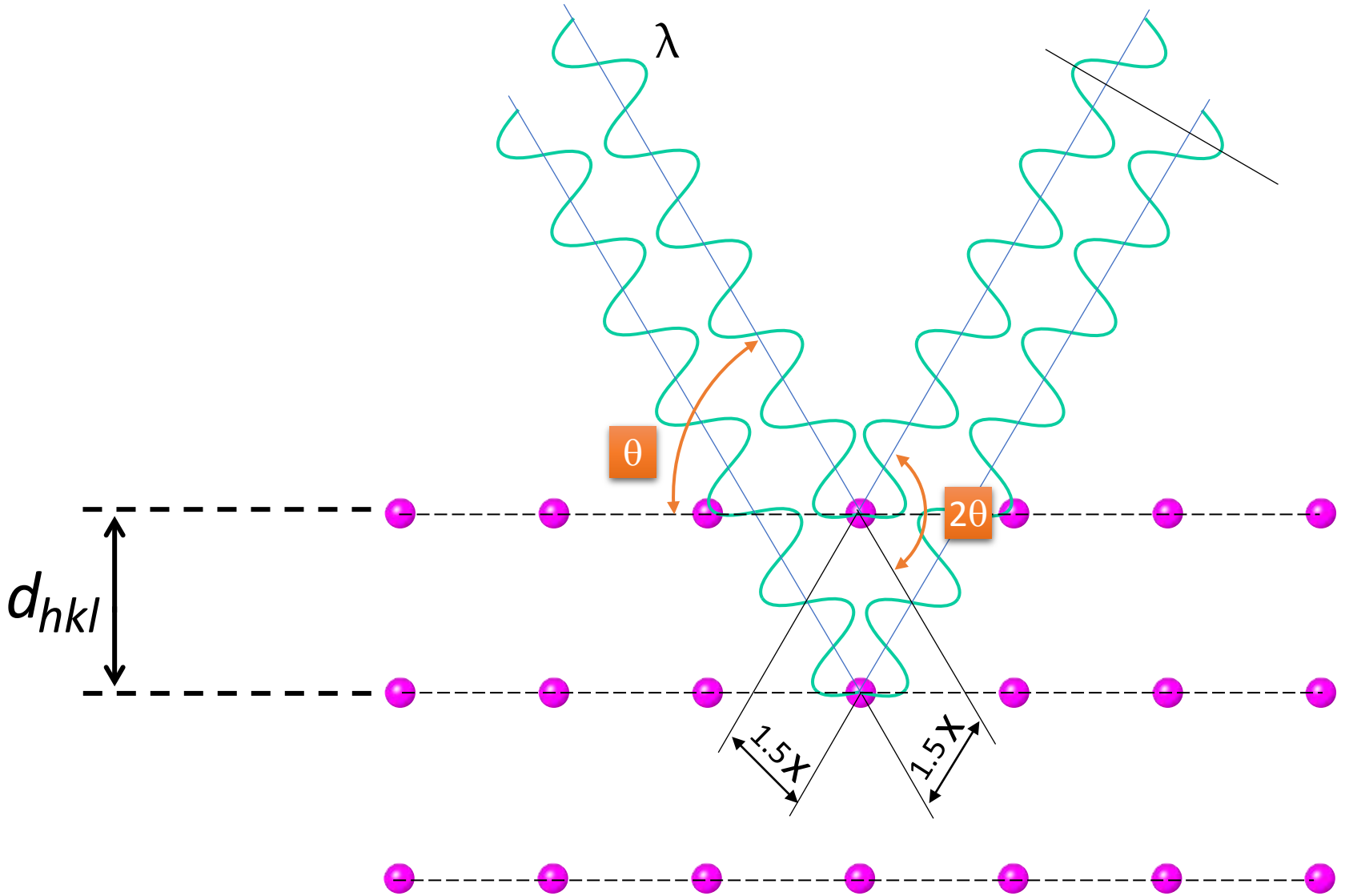


$$\sin(\theta) = \frac{x}{d_{hkl}}$$

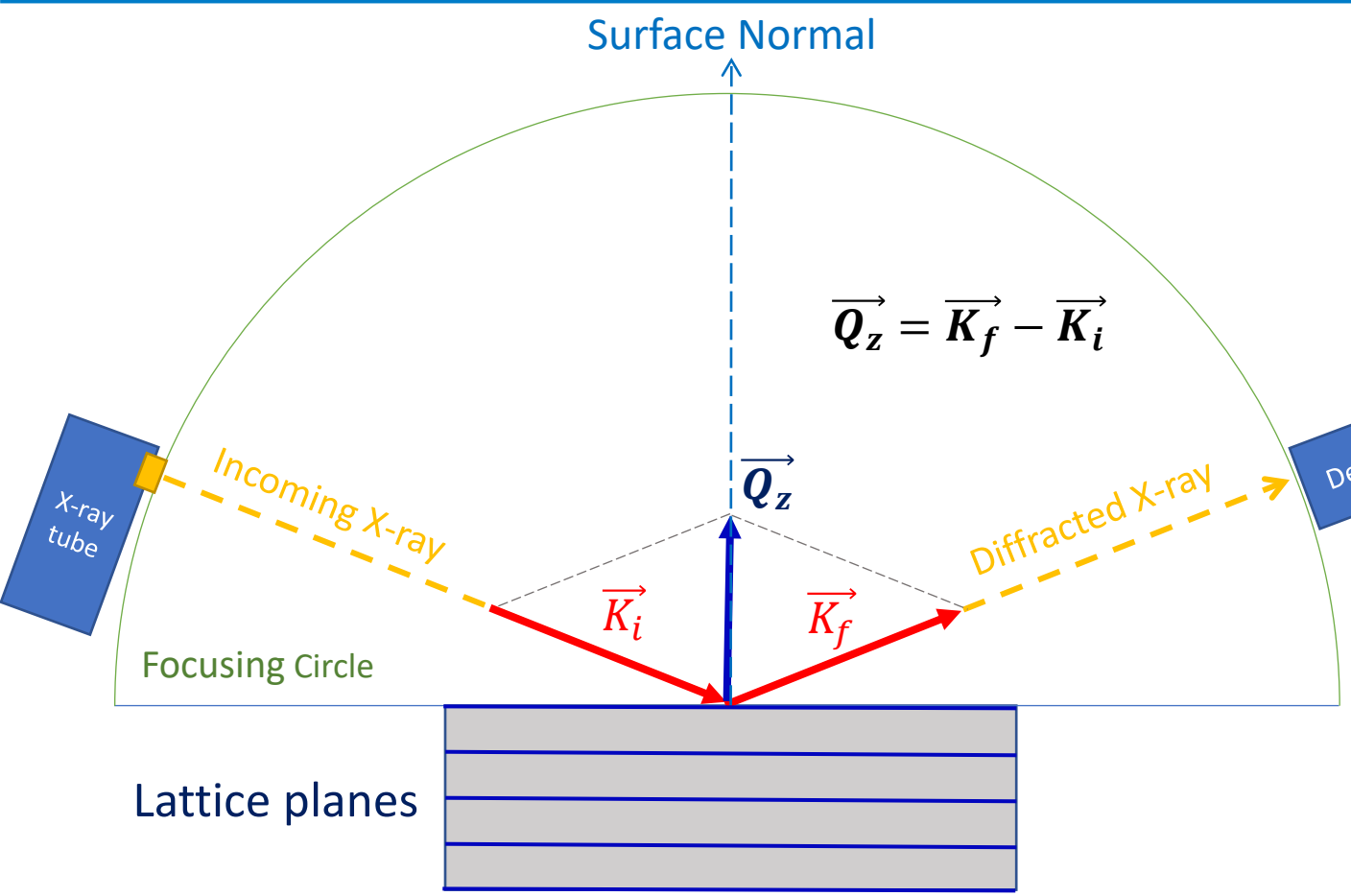


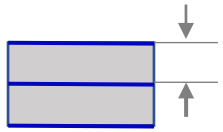
Diffraction by Planes of Atom



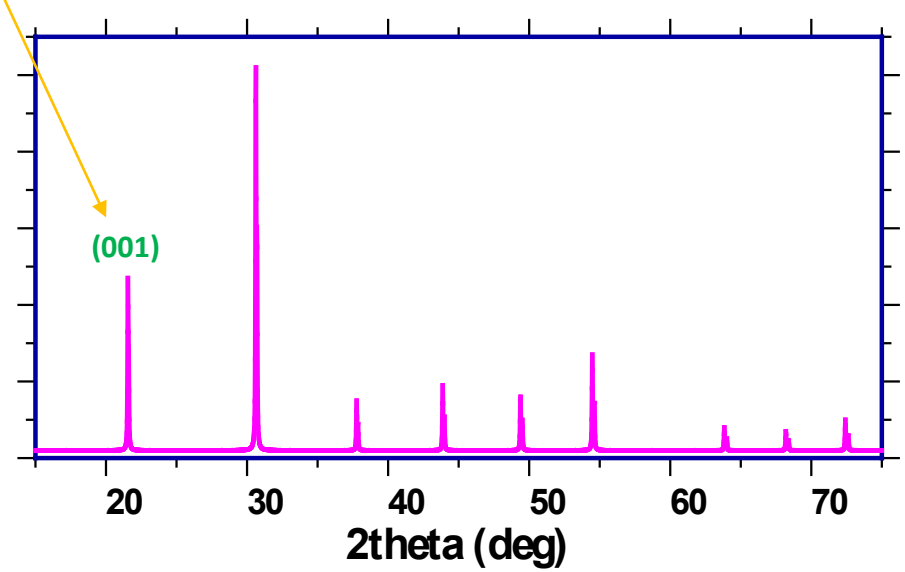


Bragg-Brentano Geometry



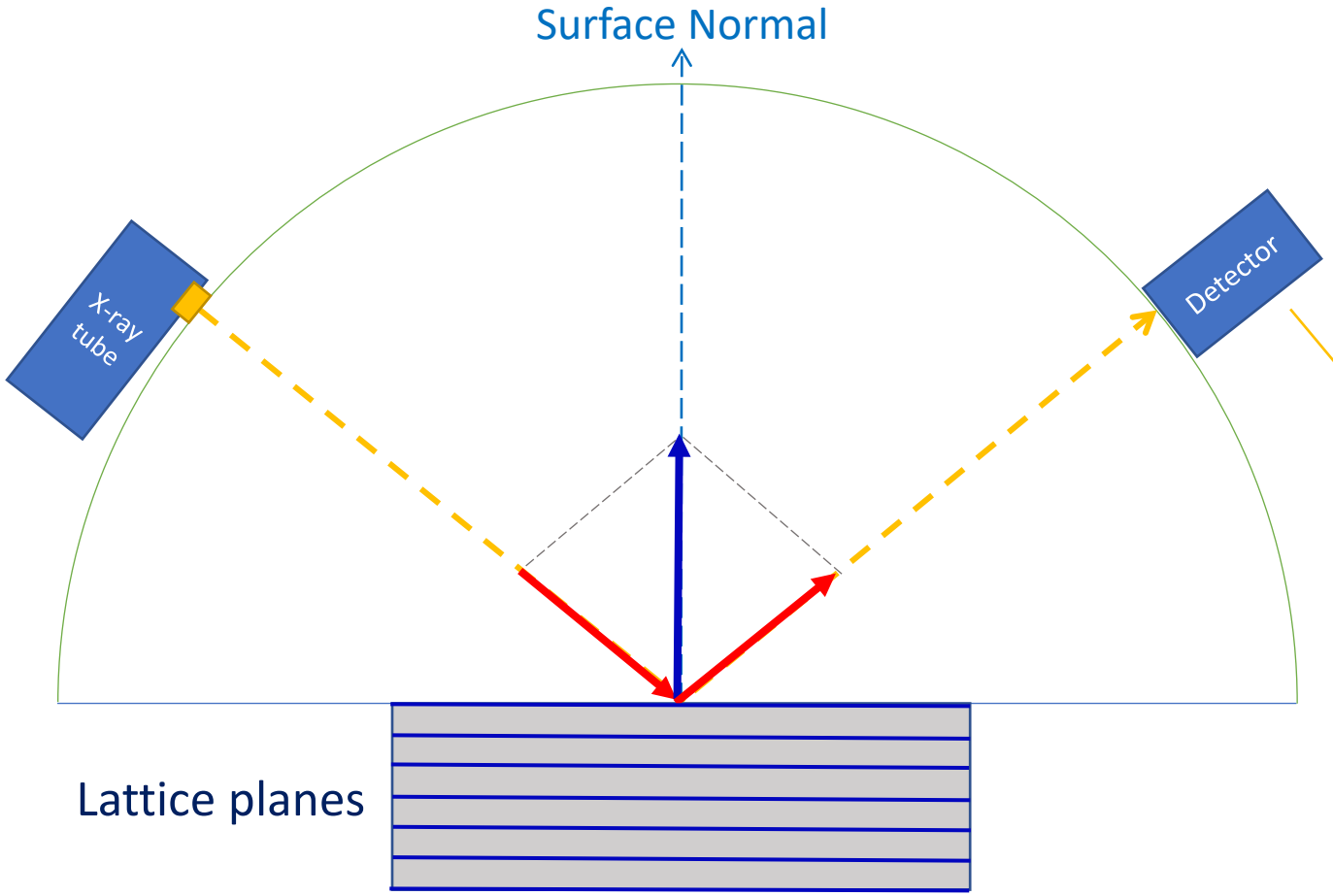


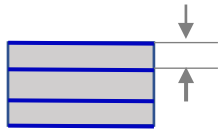
Large d

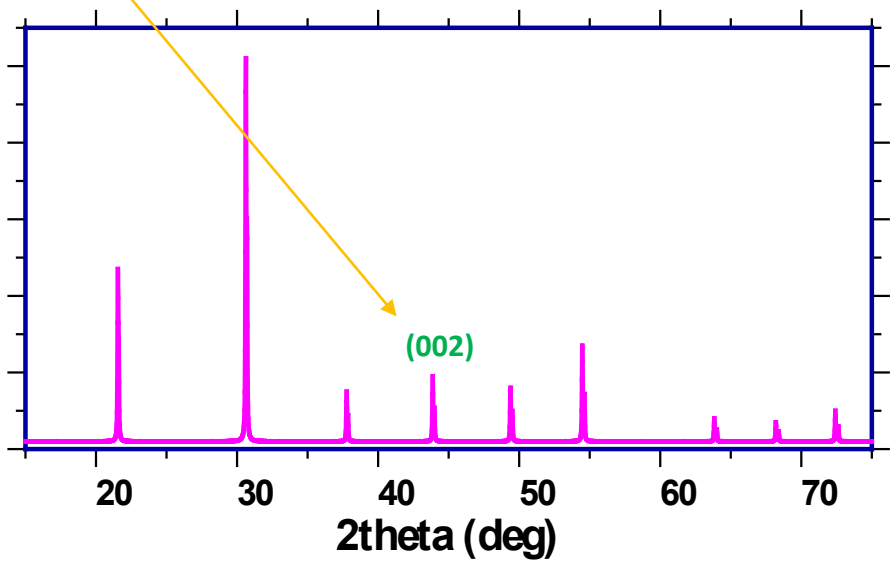


Bragg's law: $n\lambda = 2\boldsymbol{d}_{hkl}.sin\boldsymbol{\theta}$

Bragg-Brentano Geometry

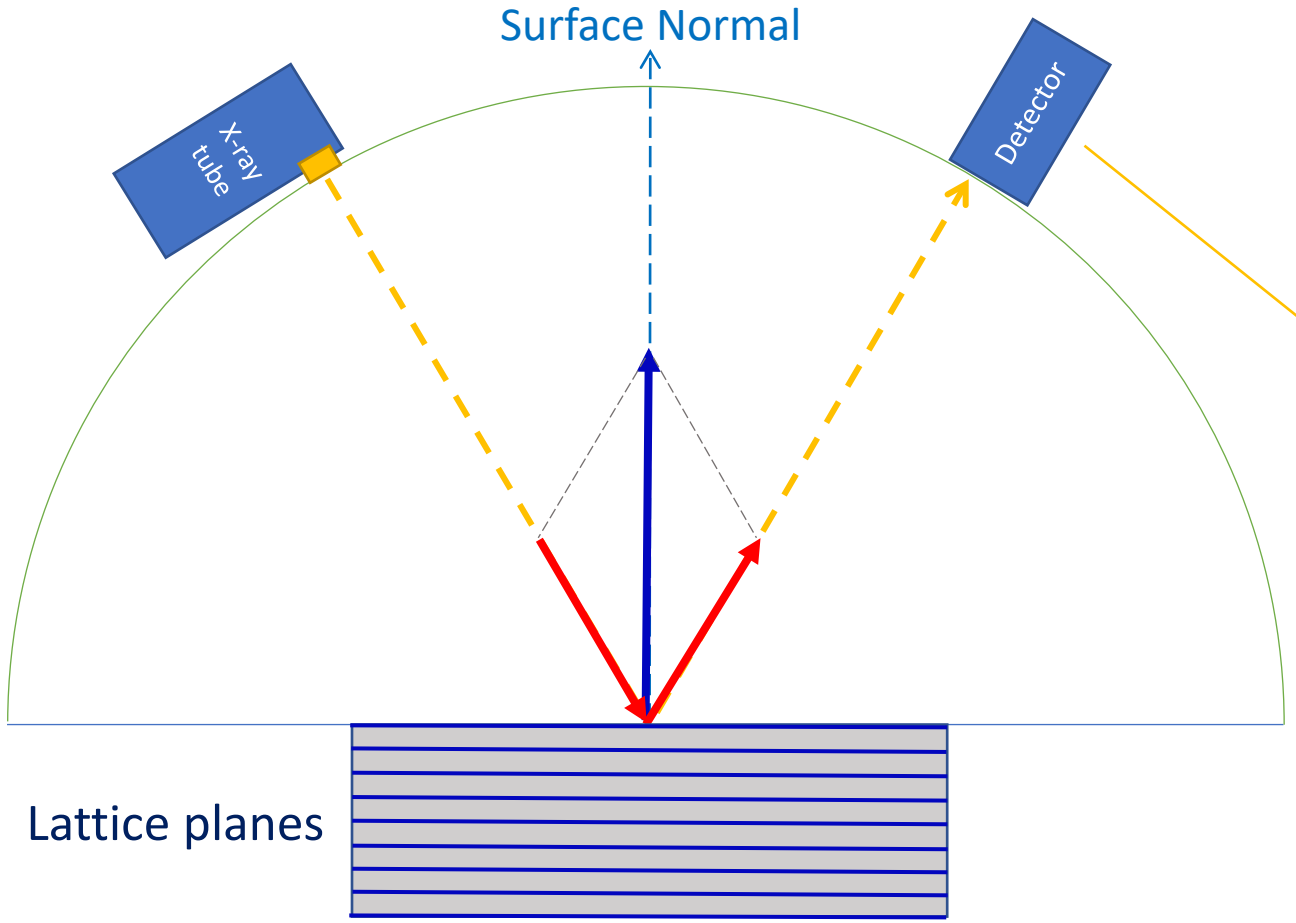


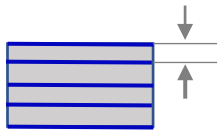


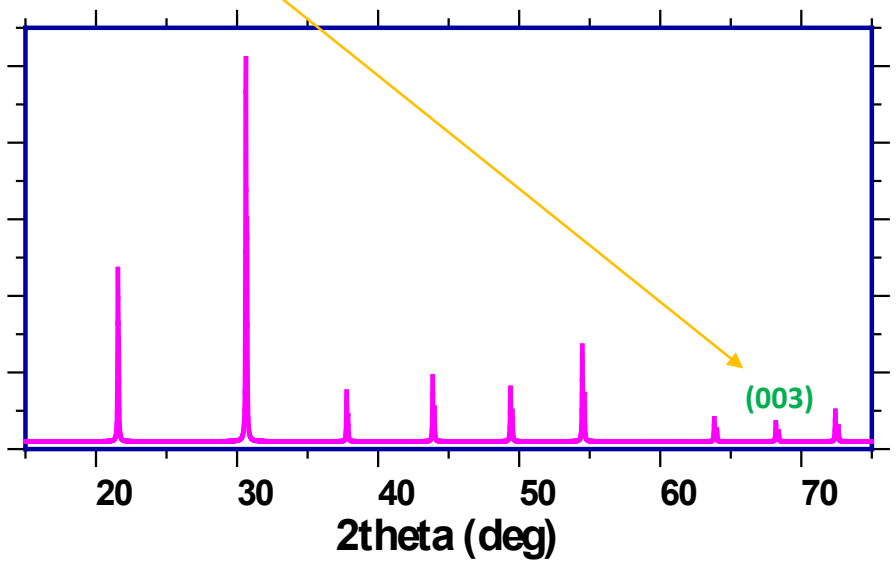


Bragg's law: $n\lambda = 2\boldsymbol{d}_{hkl}.sin\boldsymbol{\theta}$

Bragg-Brentano Geometry

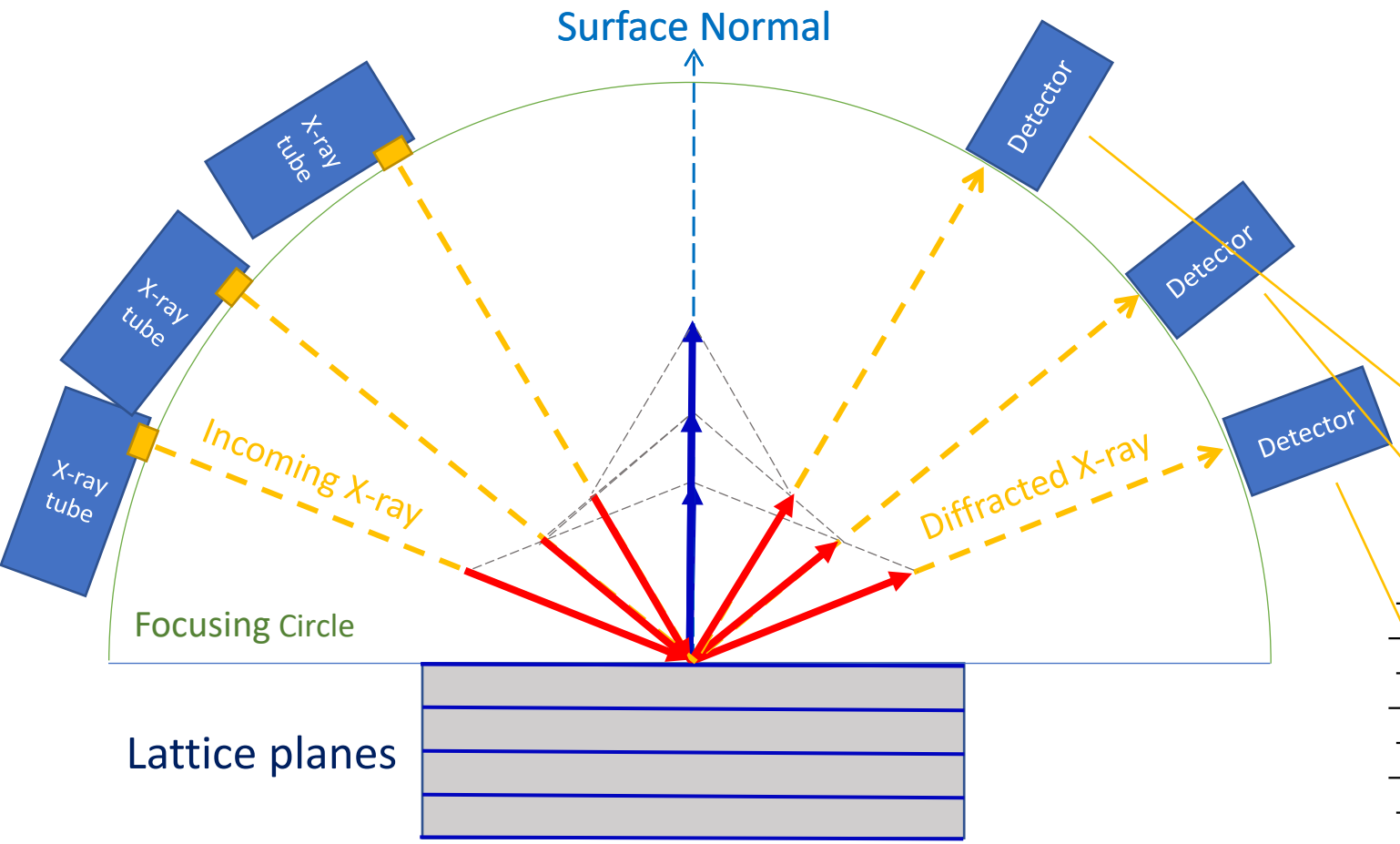


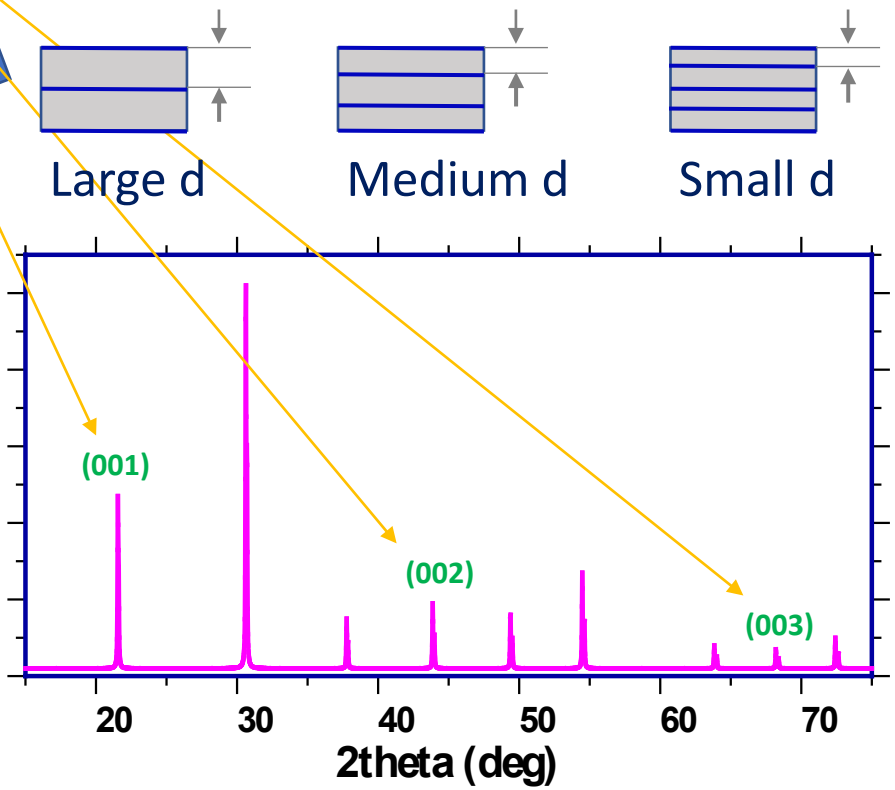




Bragg's law: $n\lambda = 2\boldsymbol{d}_{hkl}.sin\boldsymbol{\theta}$

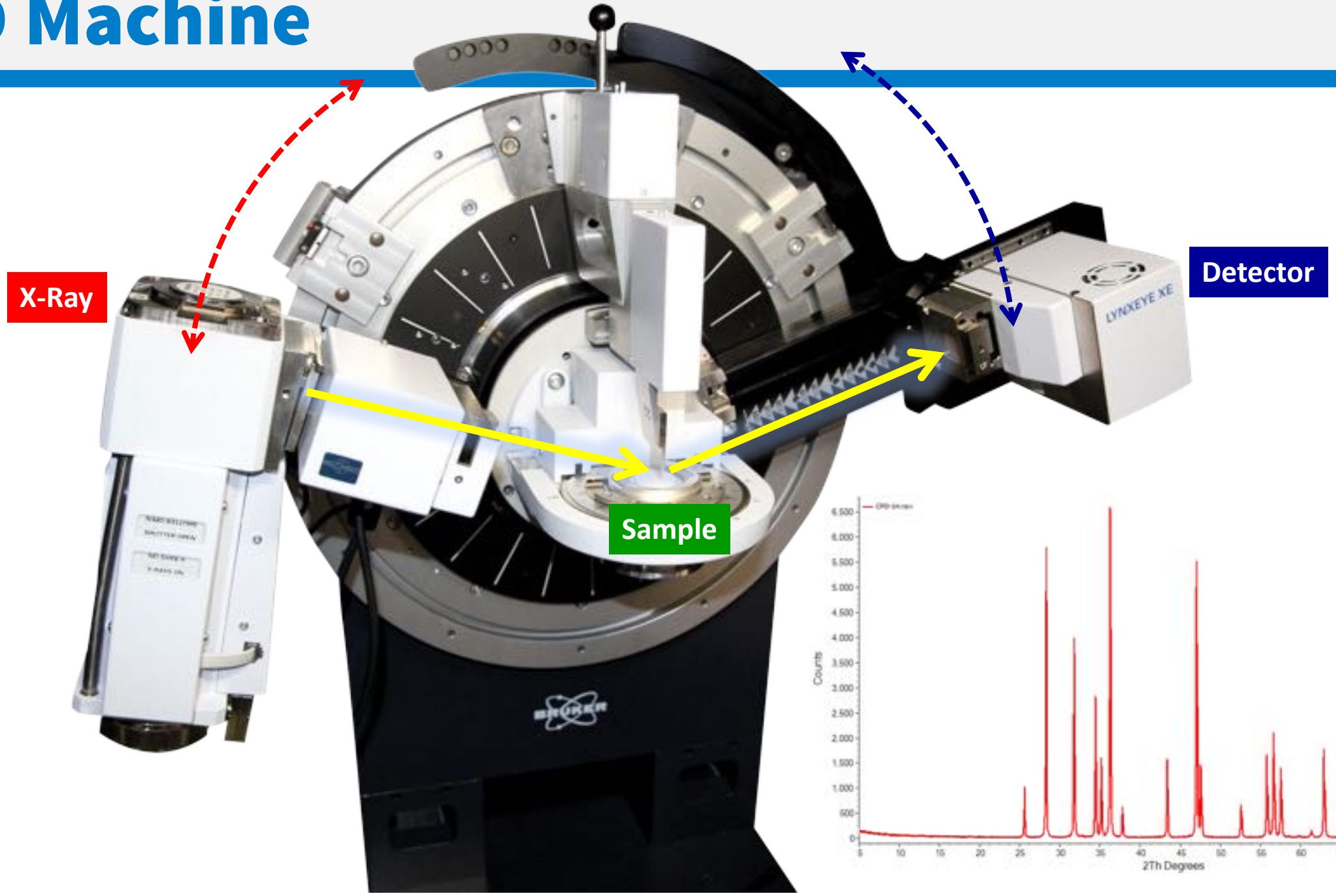
Bragg-Brentano Geometry



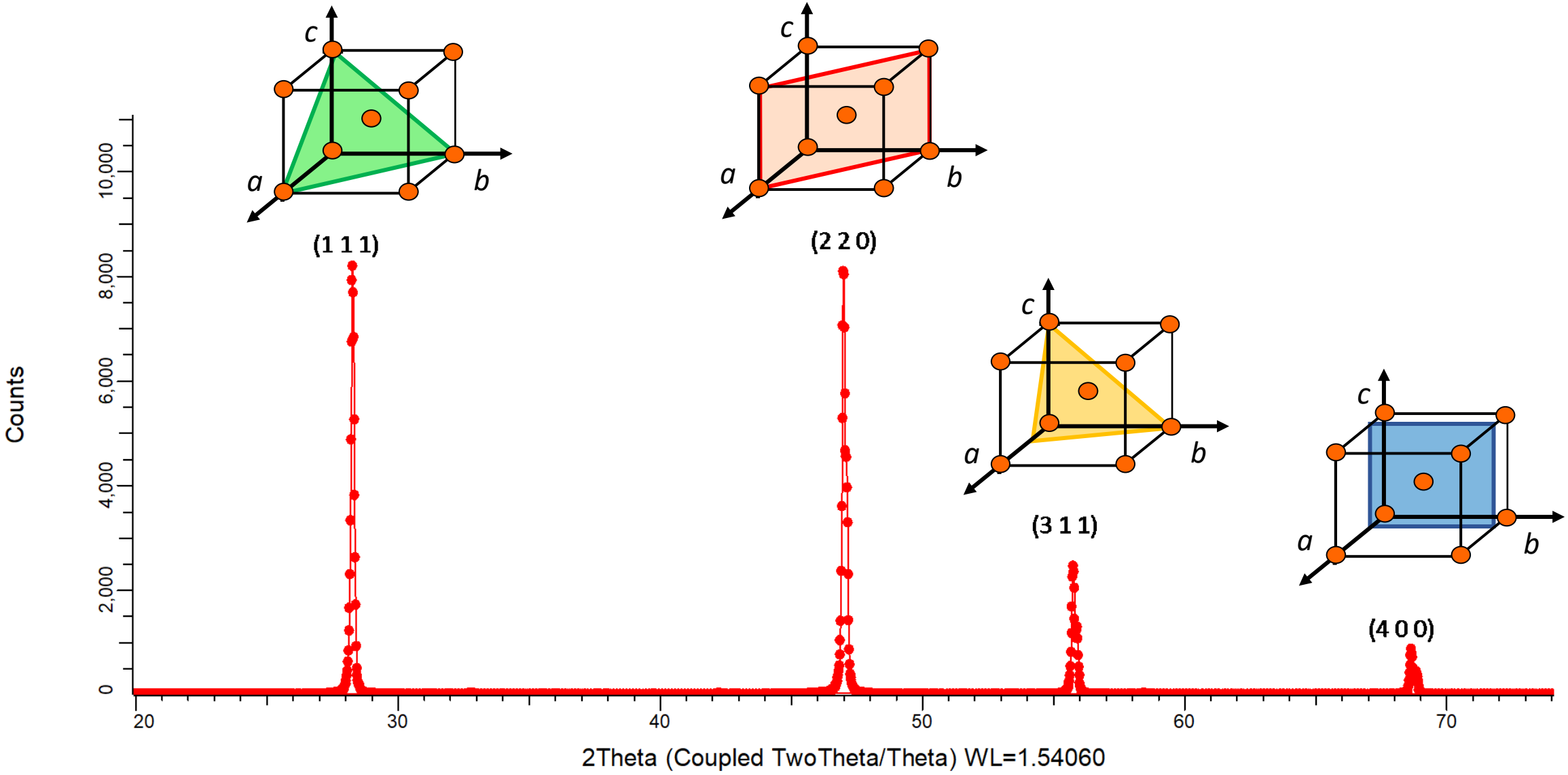


Bragg's law: $n\lambda = 2\boldsymbol{d}_{hkl}.sin\boldsymbol{\theta}$

XRD Machine



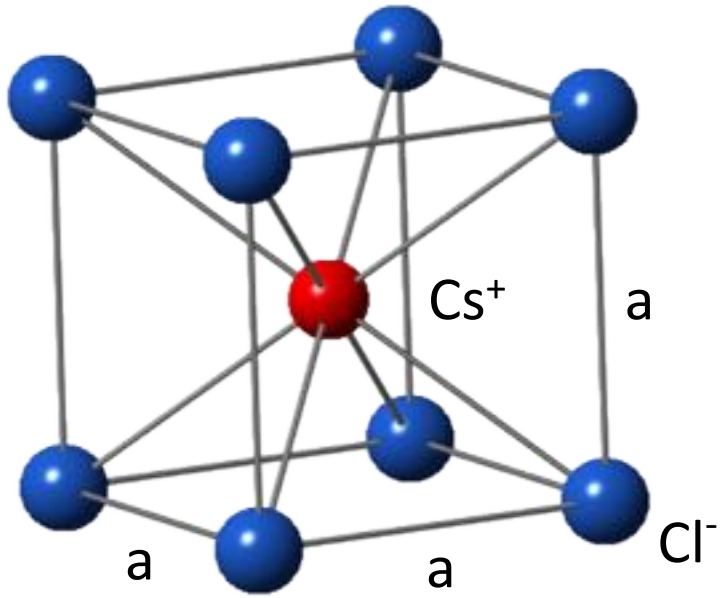
Powder Diffraction Pattern



Reflection Position and Intensity

What influences the peak position and intensity of Bragg reflections?

Example: **CsCl**



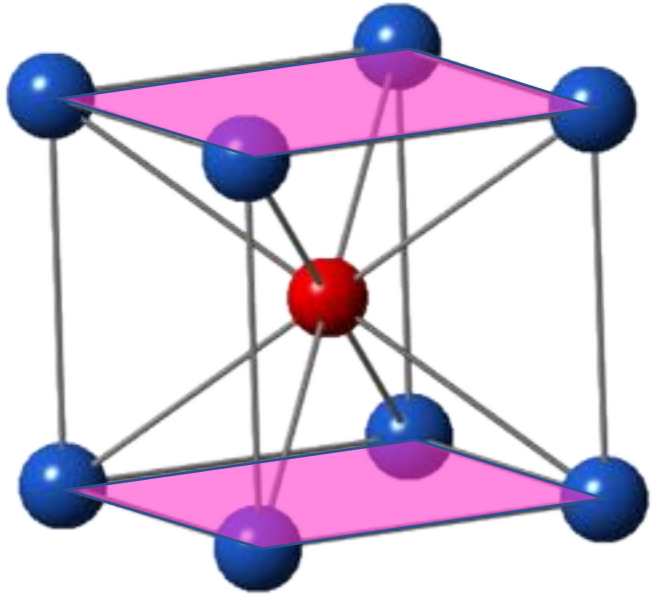
Reflection Position and Intensity

Real crystal structure CsCl **a** = 4.11Å, **λ**=1.54Å

Calculate: $d_{(hkl)}$ and θ_{hkl} for the following (hkl)

hkl	d	θ	2θ	I
(001)				
(011)				
(111)				
(002)				

(001) Reflection

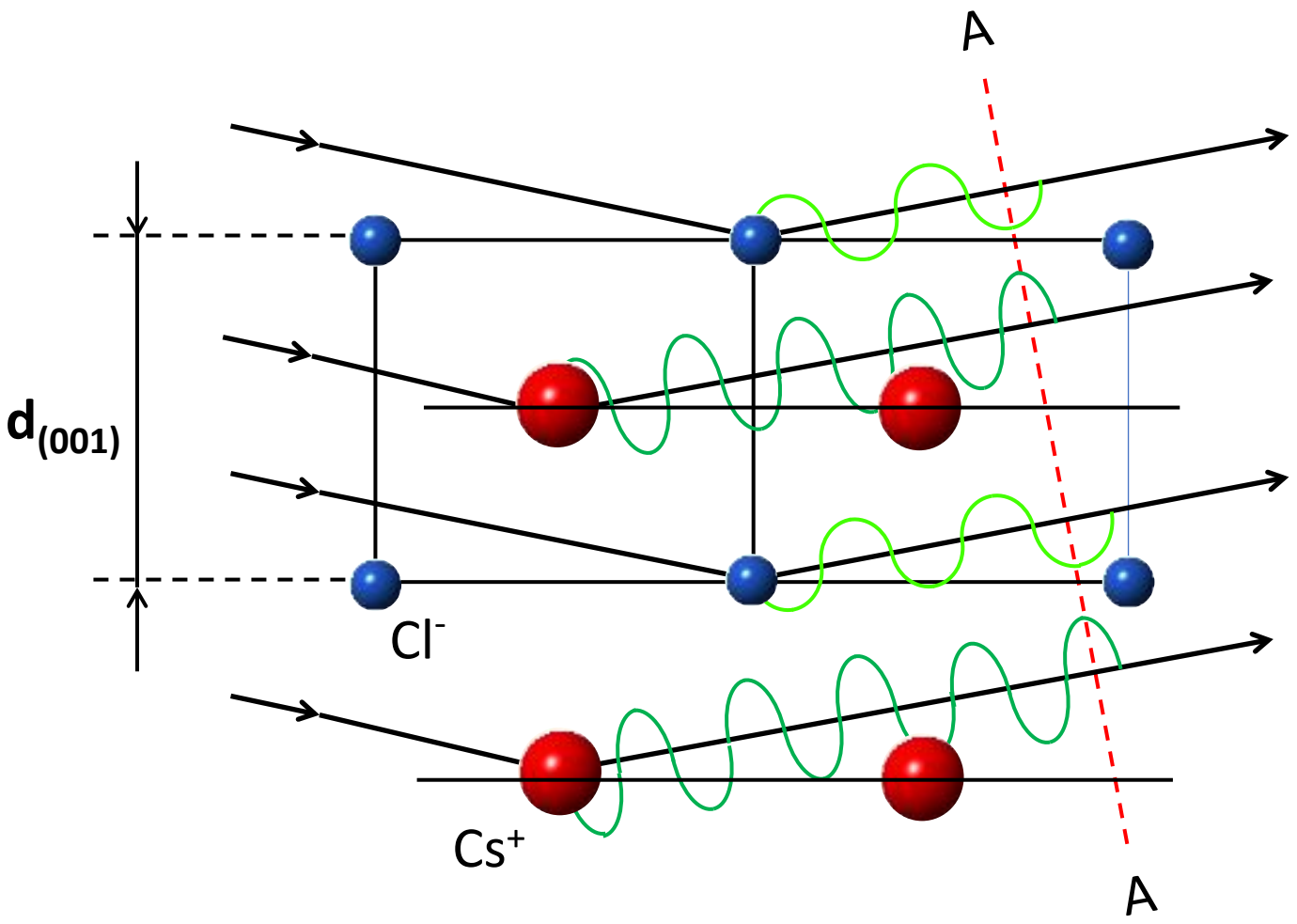


$$d_{(001)} = a = 4.11\ \text{Å}$$

Re-call Bragg equation: $\lambda = 2d \sin\theta$

$$\theta = \sin^{-1}\left(\frac{\lambda}{2d}\right) = \sin^{-1}\left(\frac{1.54}{4.11}\right) = 10.80°$$

(001) Reflection



(001) Reflection

The diagram shows the (001) planes scattering in phase

- The reflecting power of atoms (normally called the atomic scattering factor) is related to the number of electrons in the atom

  Cs^+ = 54 electrons

  Cl^- = 18 electrons

  - the reflected beam from Cs^+ atoms has an amplitude 3x larger than the beam from Cl^- atoms

(001) Reflection

Look at the wavefront A - A of the reflected beam.

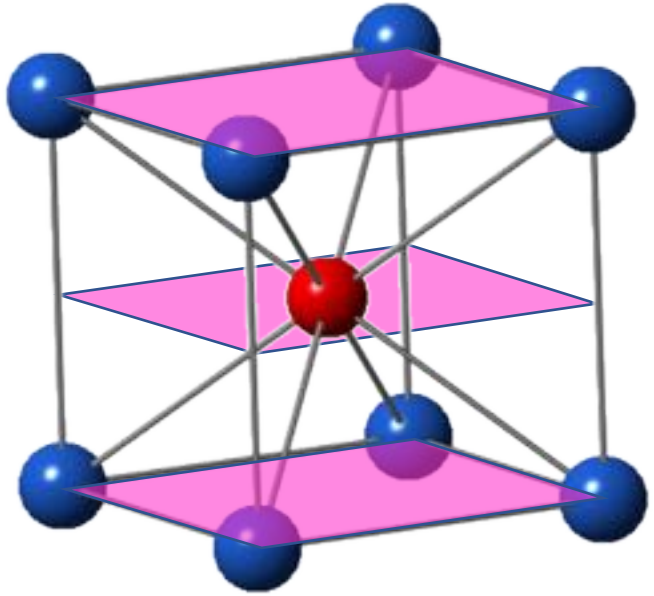
- Beams from Cl^- atoms (on planes d_{100} apart) are in phase.
- Beams from Cs^+ atoms (also on planes d_{100} apart) are in phase.

But, since Cs^+ planes are exactly half-way between Cl^- planes, beams from Cs^+ and Cl^- planes are exactly out of phase.

- Amplitude of diffracted beam $\propto y(54 - 18) = y(36)$

  (y is some constant)
- Intensity = $I_{001} \propto y^2 (36)^2 = 1296y^2$ (Weak reflection)

(002) Reflection

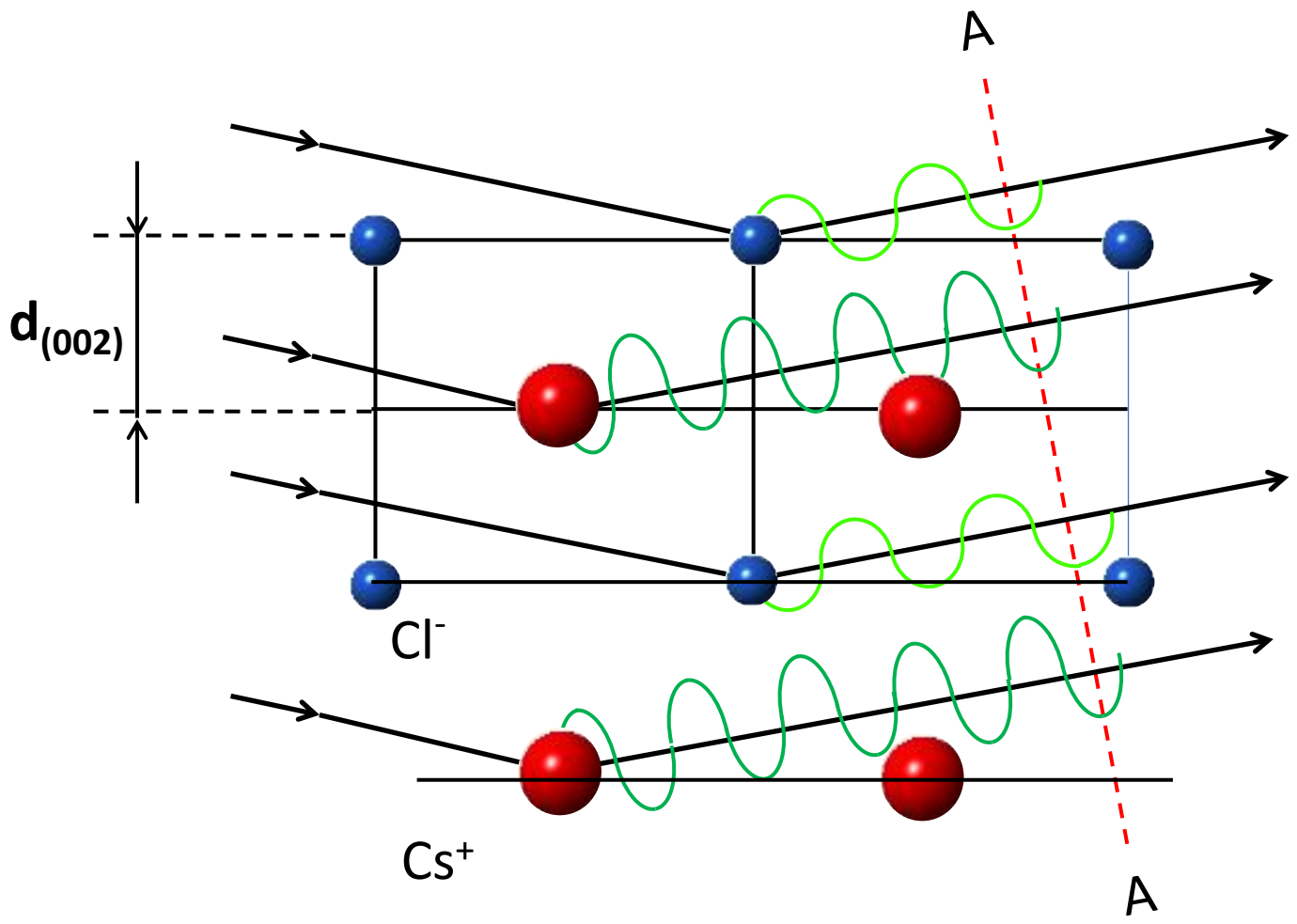


$$d_{(002)} = \frac{a}{2} = \frac{4.11}{2} = 2.055\ \text{Å} \qquad \theta = 22.07°$$

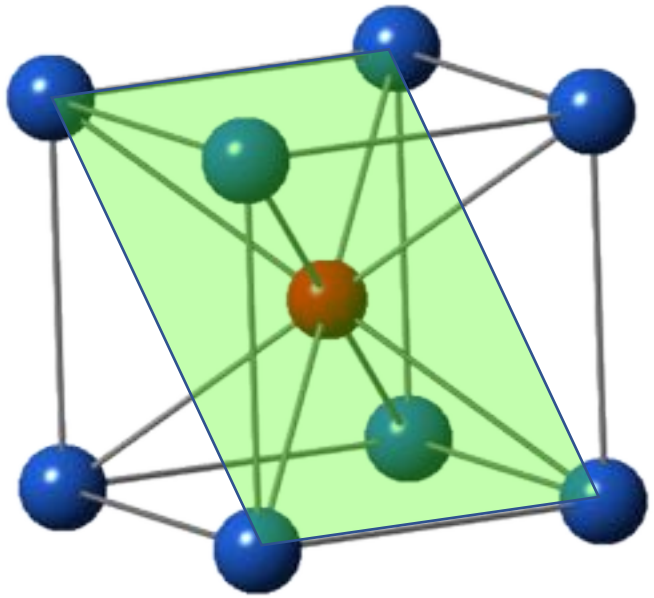
This time all atoms scatter in-phase.

- Amplitude of diffracted beam $\propto$ y (54 + 18) = y(72)
- Intensity of diffracted beam $I_{(002)} \propto y^2 \times 72^2 = 5184y^2$ (Strong reflection)

(002) Reflection



(002) Reflection

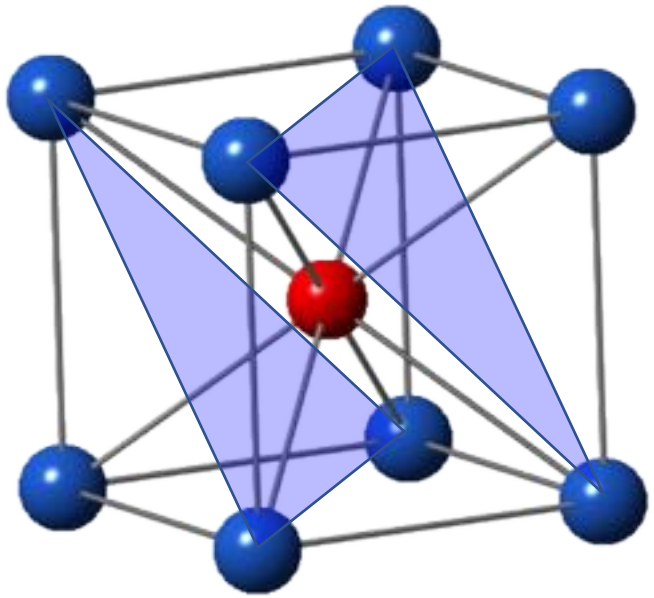


Cs^+ and Cl^- ions all lie in the (011) planes
Cs^+ and Cl^- scatter in phase

$$d_{(011)} = \frac{a}{\sqrt{2}} = \frac{4.11}{\sqrt{2}} = 2.91\ \text{Å} \qquad \theta = 15.34°$$

$$I_{(011)} \propto y^2(54 + 18)^2 = 5184y^2$$ (Strong reflection)

(111) Reflection



Cl^- ions lie in (111) planes and d(111) apart. Cl^- ions scatter in phase

Cs^+ ions lie mid-way between Cl^- planes. Cl^+ ions scatter out of phase

$$d_{(111)} = \frac{a}{\sqrt{3}} = \frac{4.11}{\sqrt{3}} = 2.373\ \text{Å} \qquad \theta = 18.94°$$

$$I_{(111)} \propto y^2(54-18)^2 = 1296y^2$$ (Weak reflection)

Reflections

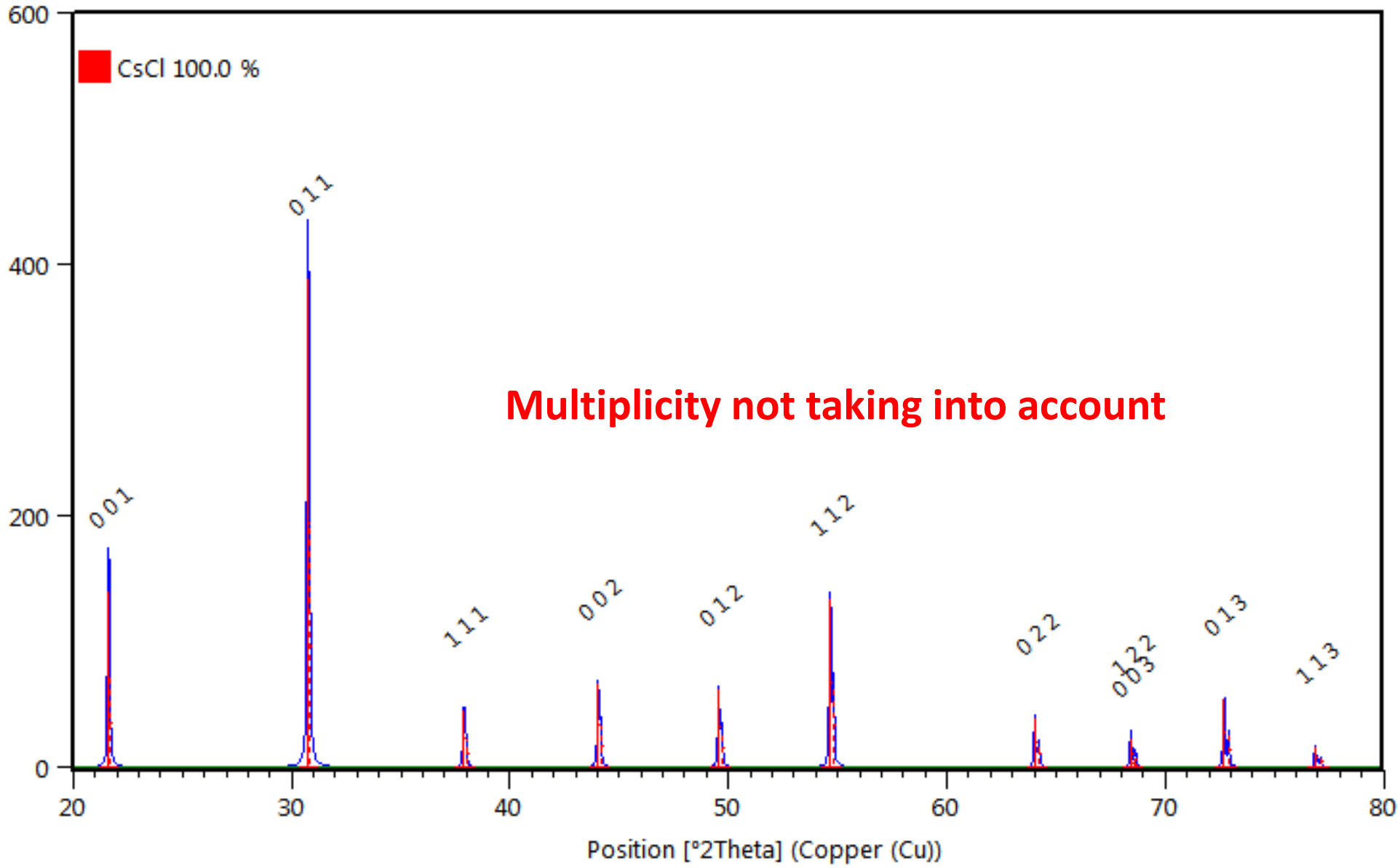
To summarize:

hkl	d	θ	**2θ**	**I**	remark
100	4.11	10.84	21.60	1296	Weak
110	2.91	15.34	30.69	5184	Strong
111	2.373	18.94	37.88	1296	Weak
200	2.055	22.07	44.01	5184	Strong

from lattice + **from 'building block'**

Crystal Structure

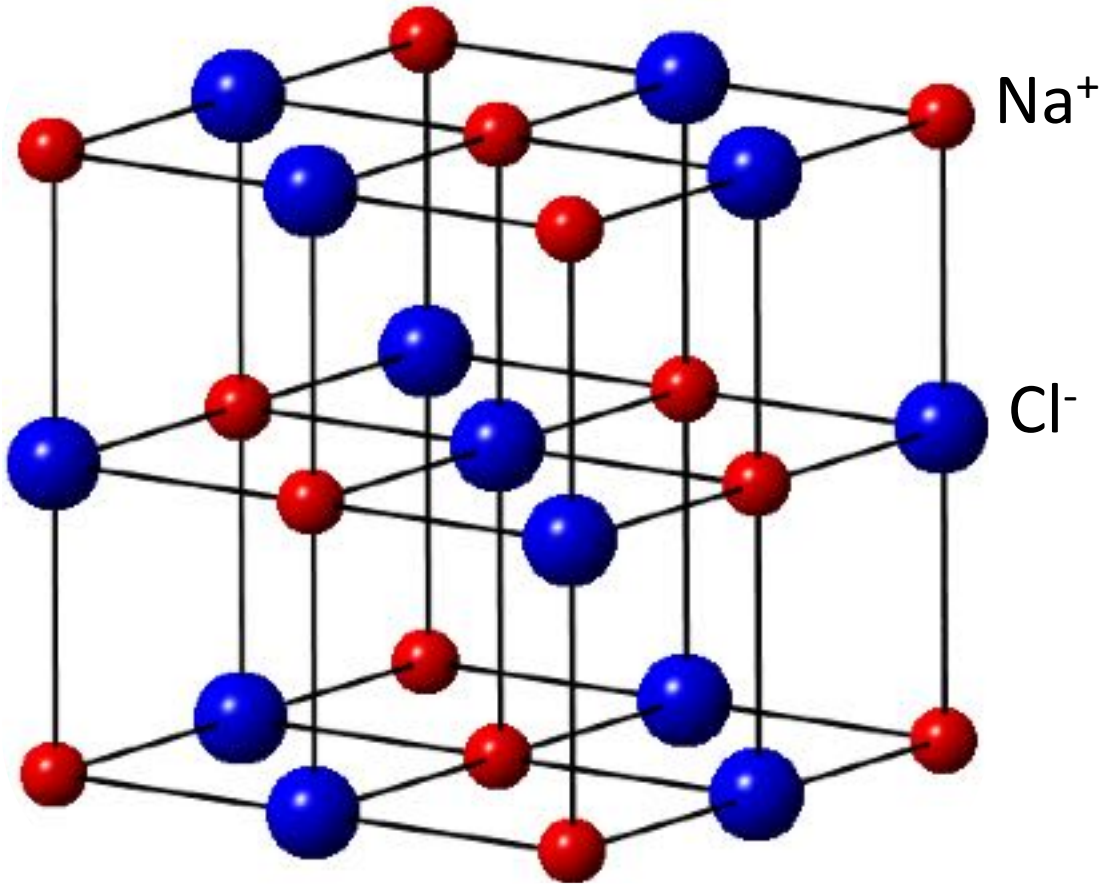
CsCl Diffraction Pattern



Multiplicity not taking into account

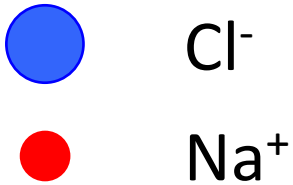
A (not quite so) Simple Crystal Structure

NaCl - Sodium Chloride

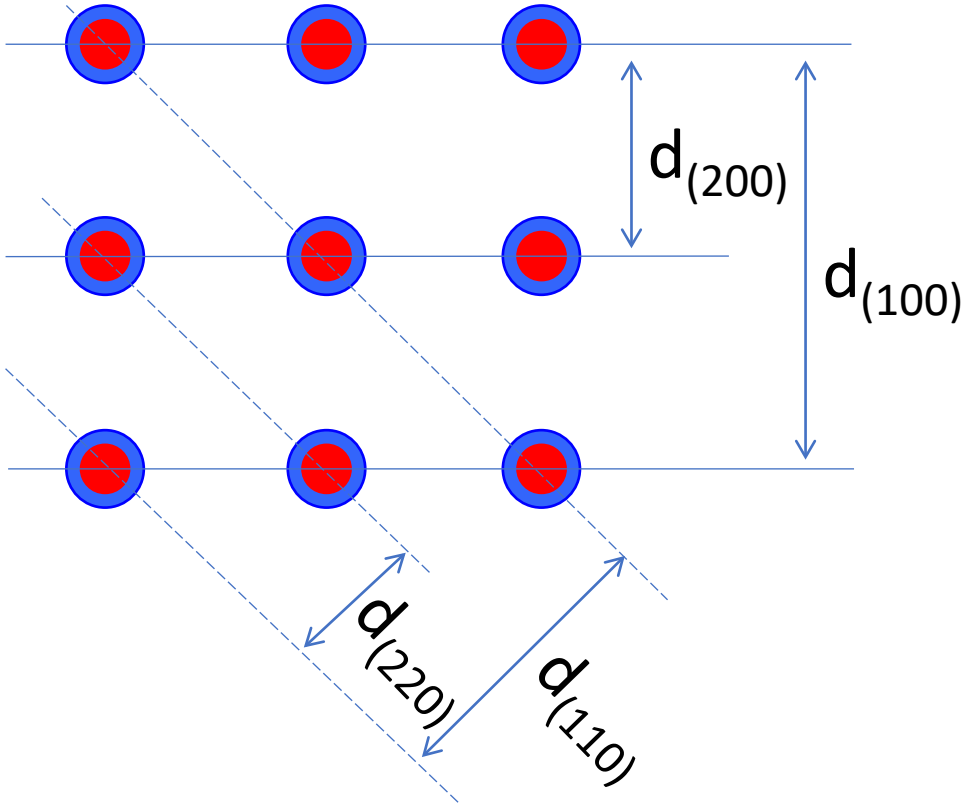


Reflections

NaCl (FCC)

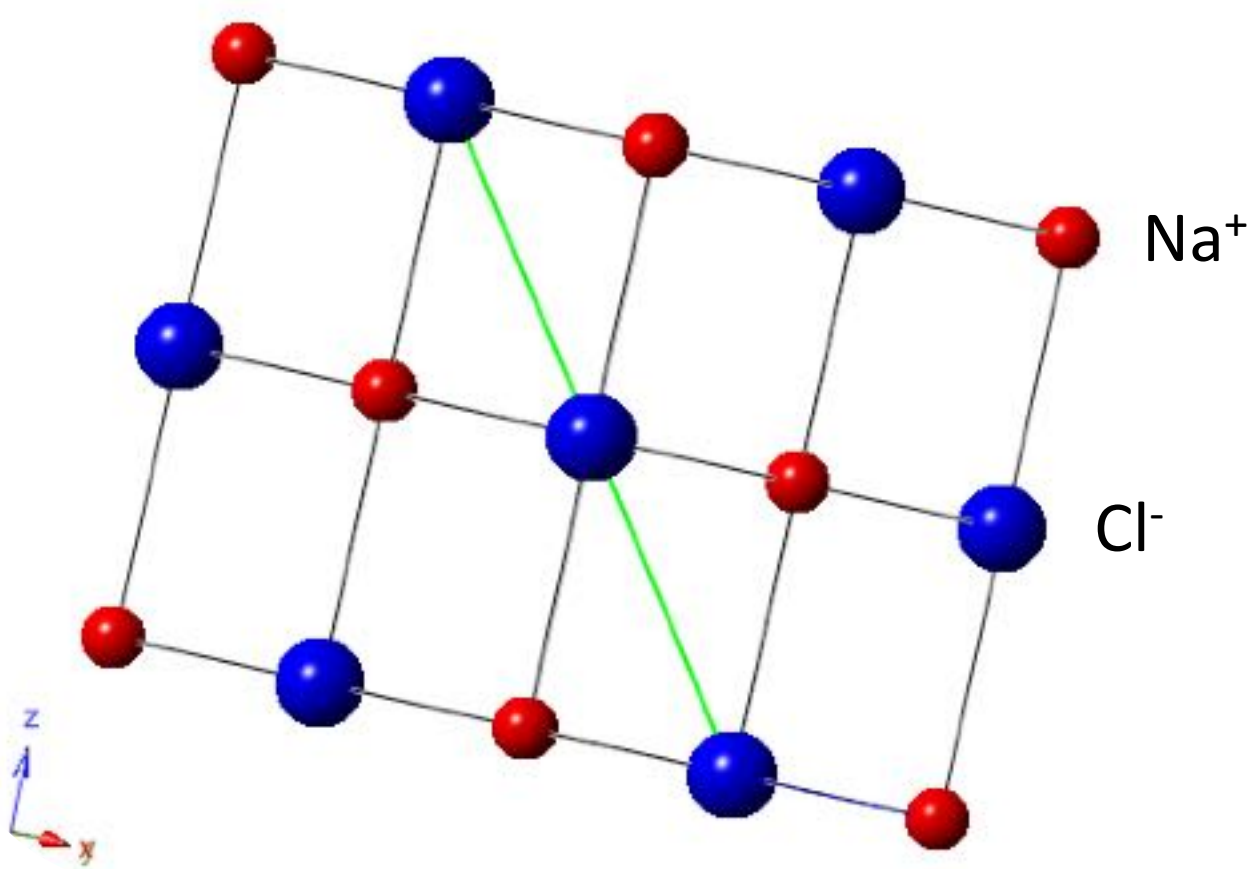


Top View



- (100) absent completely
- (200) strong
- (110) absent completely
- (220) strong

(111) reflection



(111) reflection

Cl^- atoms lie in (111)planes
Na^+ atoms lie in between

$I \propto A^2(18\text{-}8)^2 = 100\ A^2$

} **Scatter out of phase**

= (111) is quite weak

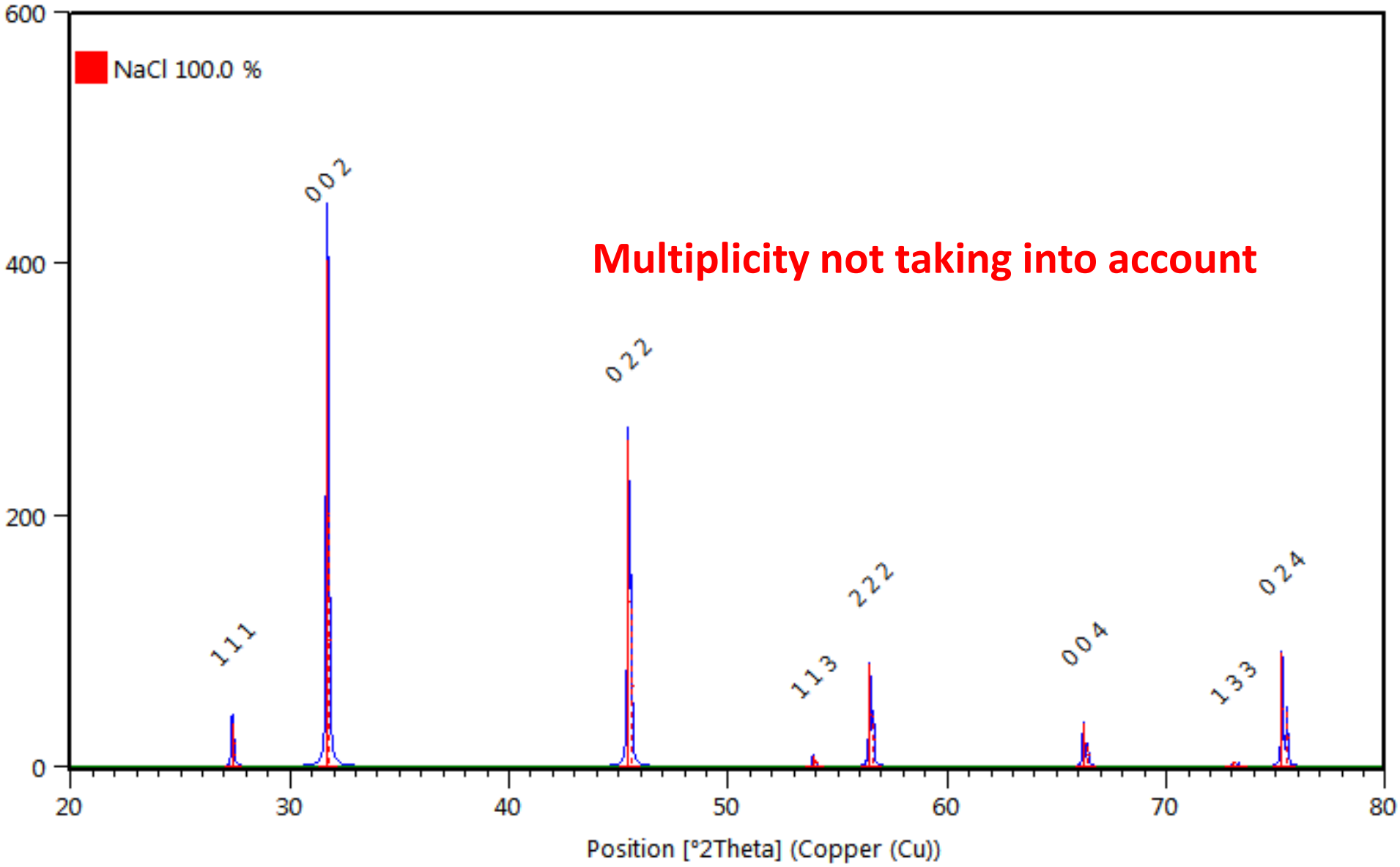
Cl^- atoms lie in (222)planes
Na^+ atoms lie in (222)planes

$I \propto A^2\ (18+8)^2 = 262\ A^2$

} **Scatter in phase**

= (222) is quite strong

NaCl Diffraction Pattern



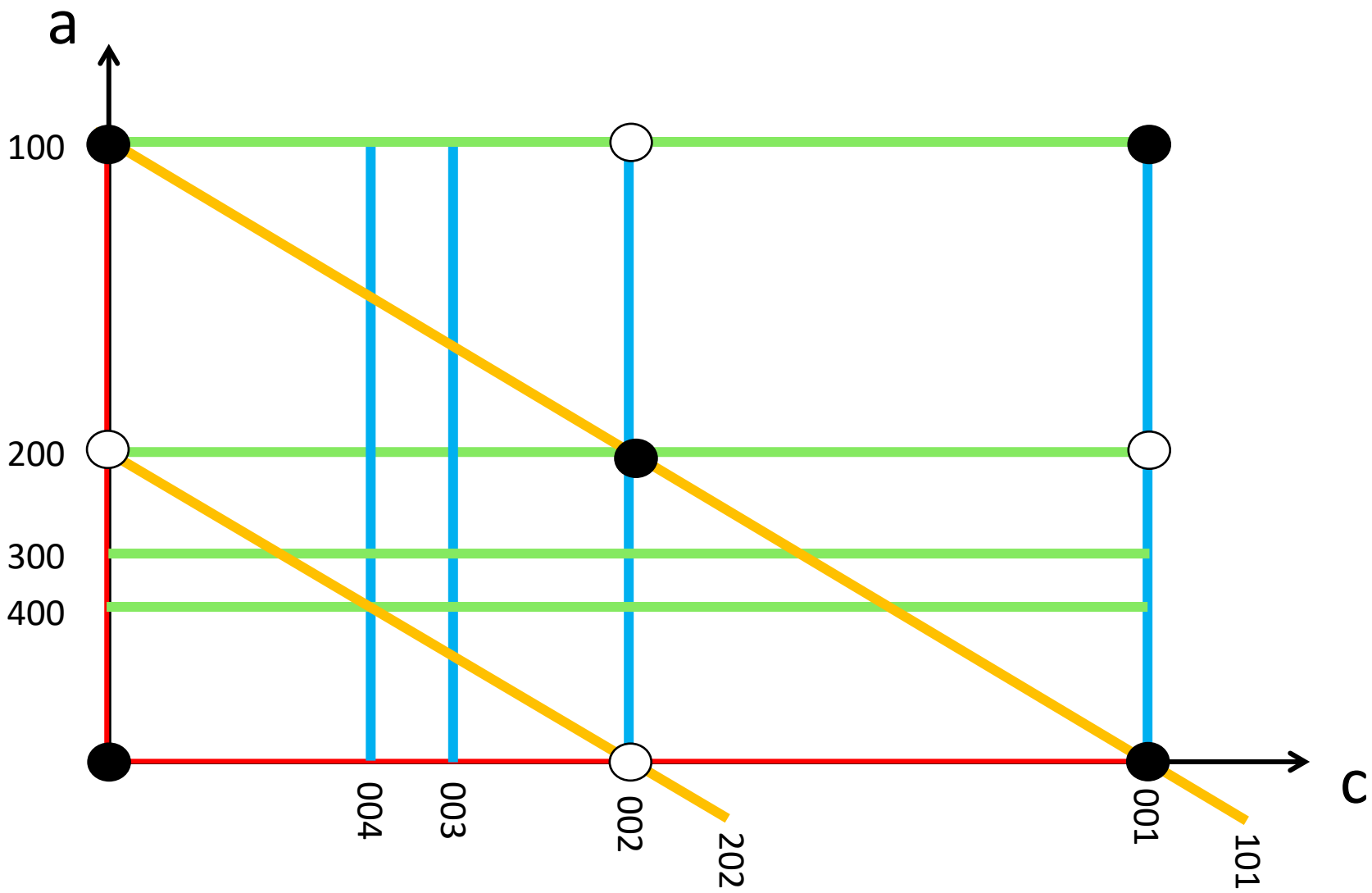
Summary

The diffraction pattern is like a finger print of the crystal structure:

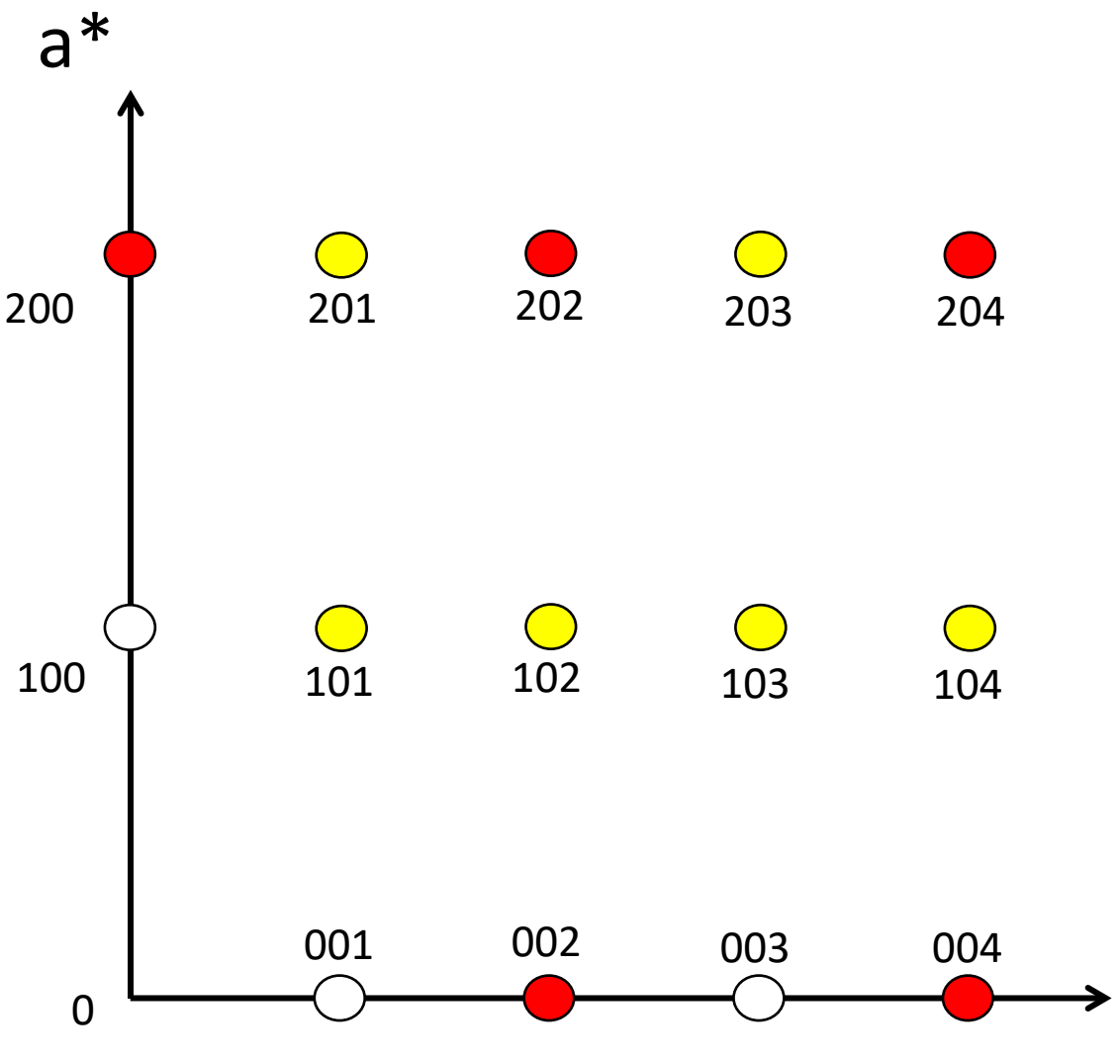
➔ d values reflect the unit cell parameters (grid)

➔ intensities reflect the atoms/molecules (building blocks)

Real Space



Reciprocal Space



$$\lambda = 2d_{hkl}sin\theta$$

$$d^*_{hkl} = 1/d_{hkl}$$

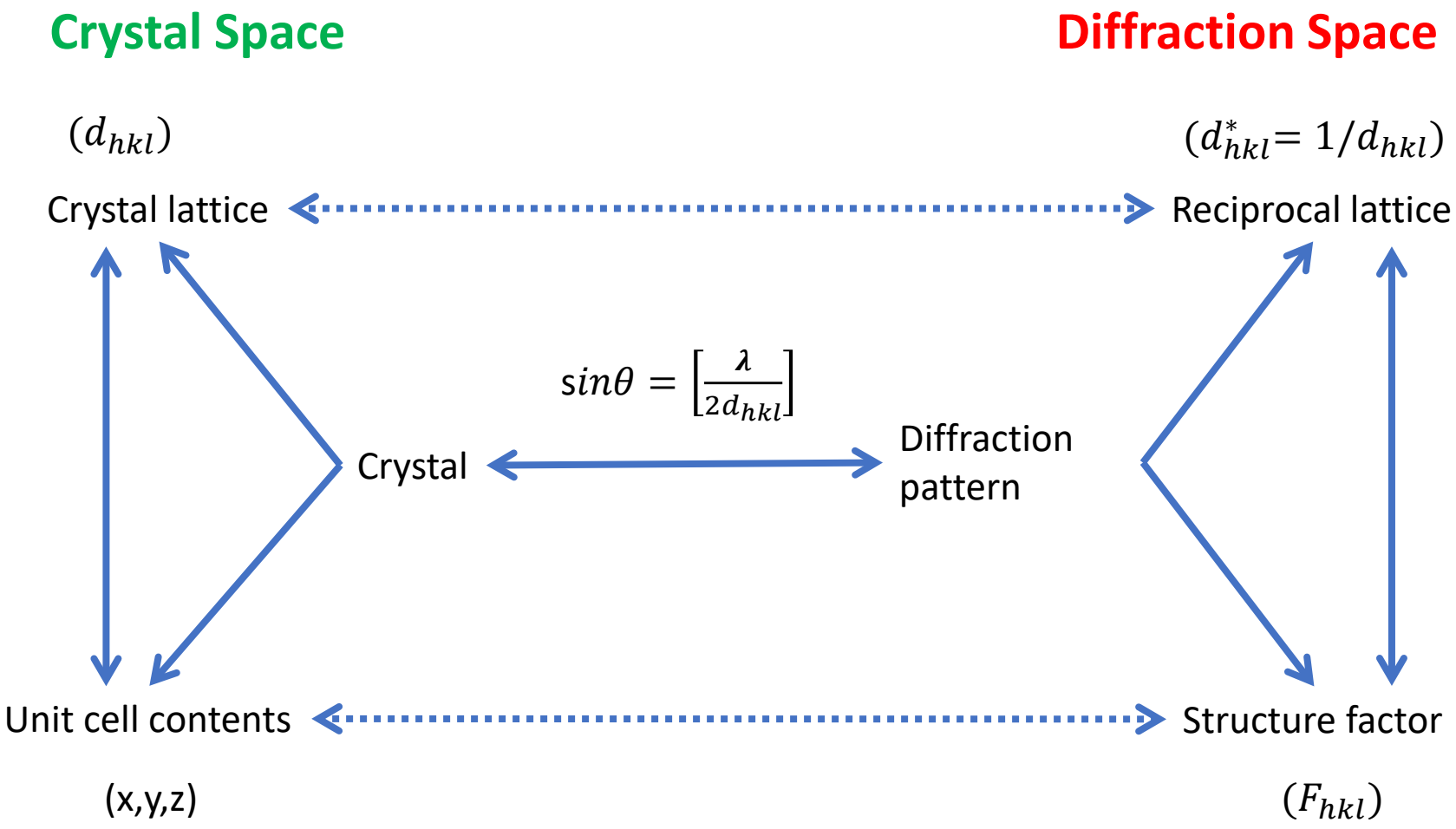
h0l = 2*n*
h+*l* = 2*n*

Systematic presence

Weak reflection

Systematic absence

Real Space and Reciprocal Space



Crystal System Reciprocal Space

Orthorhombic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Tetragonal

$$\frac{1}{d_{hkl}^2} = \left[h^2 + k^2 + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$$

Cubic

$$\frac{1}{d_{hkl}^2} = (h^2 + k^2 + l^2)\frac{1}{a^2}$$

Monoclinic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2\sin^2\gamma} + \frac{k^2}{b^2\sin^2\gamma} - \frac{2hk\cos\gamma}{ab\sin^2\gamma} + \frac{l^2}{c^2}$$

Hexagonal

$$\frac{1}{d_{hkl}^2} = \left[\frac{4}{3}(h^2 + k^2 + hk) + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$$

Triclinic

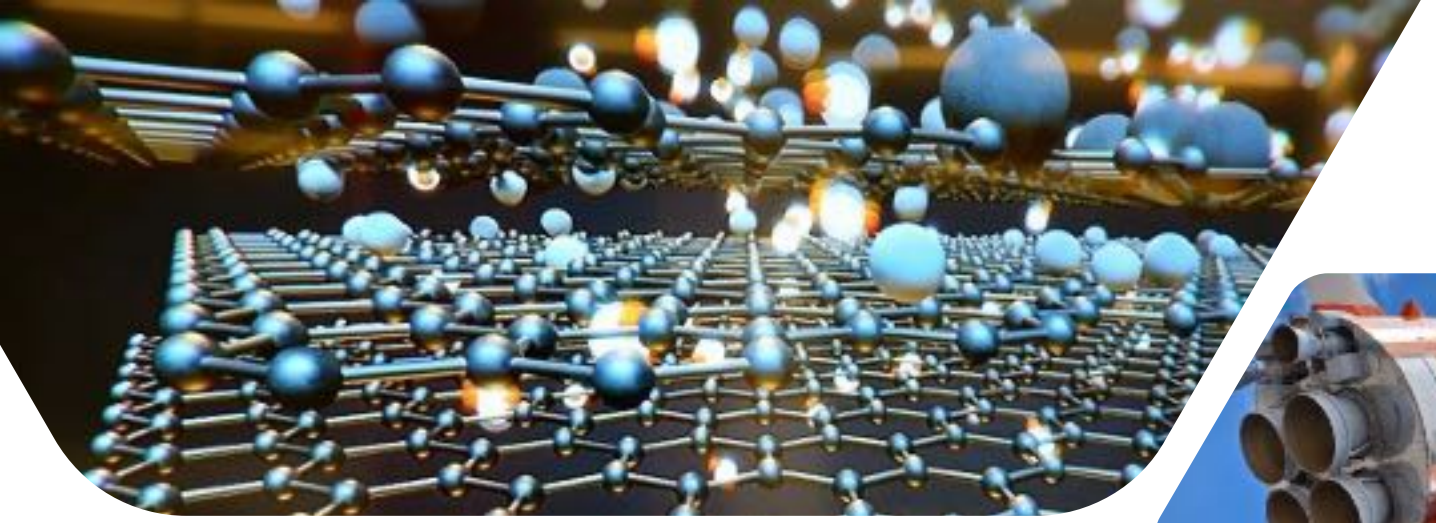
$$\frac{1}{d_{hkl}^2} = \left[\frac{h}{a}\begin{vmatrix} \frac{h}{a} & \cos\gamma & \cos\beta \\ \frac{k}{b} & 1 & \cos\alpha \\ \frac{l}{c} & \cos\alpha & 1 \end{vmatrix} + \frac{k}{b}\begin{vmatrix} 1 & \frac{h}{a} & \cos\alpha \\ \cos\gamma & \frac{k}{b} & \cos\alpha \\ \cos\beta & \frac{l}{c} & 1 \end{vmatrix} + \frac{l}{c}\begin{vmatrix} 1 & \cos\gamma & \frac{h}{a} \\ \cos\gamma & 1 & \frac{k}{b} \\ \cos\beta & \cos\alpha & \frac{l}{c} \end{vmatrix}\right] \cdot \begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}^{-1}$$

Trigonal (rhombohedral)

$$\frac{1}{d_{hkl}^2} = \left[(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + lh)(\cos^2\alpha - \cos\alpha)\right]\frac{1}{A^2(1 + 2\cos^3\alpha - 3\cos^2\alpha)}$$

Quiz

Peak No.	2θ	$sin^2\theta$	$\frac{sin^2\theta}{sin^2_{min}}$	$2 \times \frac{sin^2\theta}{sin^2_{min}}$	$3 \times \frac{sin^2\theta}{sin^2_{min}}$	$h^2 + k^2 + l^2$	hkl	a (Å)
1	38.43							
2	44.67							
3	65.02							
4	78.13							
5	82.33							
6	96.93							
7	111.83							
8	116.36							



END
Session 2

Professional Community & Collaborators

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Maykel Manawan

78.69 · Dr · Edit your information

Crystallography, X-ray/Neutron Diffraction

ICDD

Education Subcommittee

Introduction

Maykel Manawan currently works as a lecturer and researcher at Indonesia Defense University. An active member of the International Center for Diffraction Data, ICDD (Education sub-committee). Principal Investigator of the National Li-ion Battery Program (Battery Research Institute-Consortium). Member of Material Research Society Indonesia, MRS-INA. Member of Indonesian Magnetic Society. Member of Indonesia Neutron Scattering Society.

Skills and Expertise

Crystallography | Powder Diffraction | Neutron Diffraction | Protein X-ray Crystallography | Lithium Ion Batteries | Superconductivity and Superconduct... | Magnetic Materials and Magnetism | Density Functional Theory | Material Characterization | Ancient History

https://growkudos.com/projects/crystallography-and-diffraction

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TERIMA KASIH