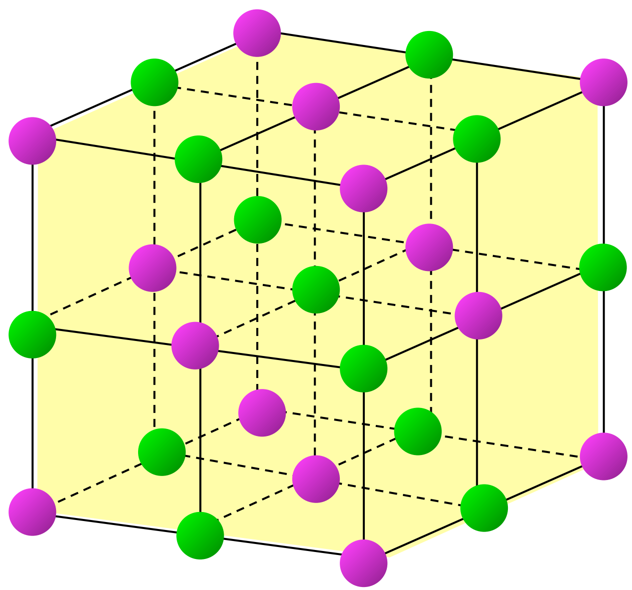
Basic crystallography



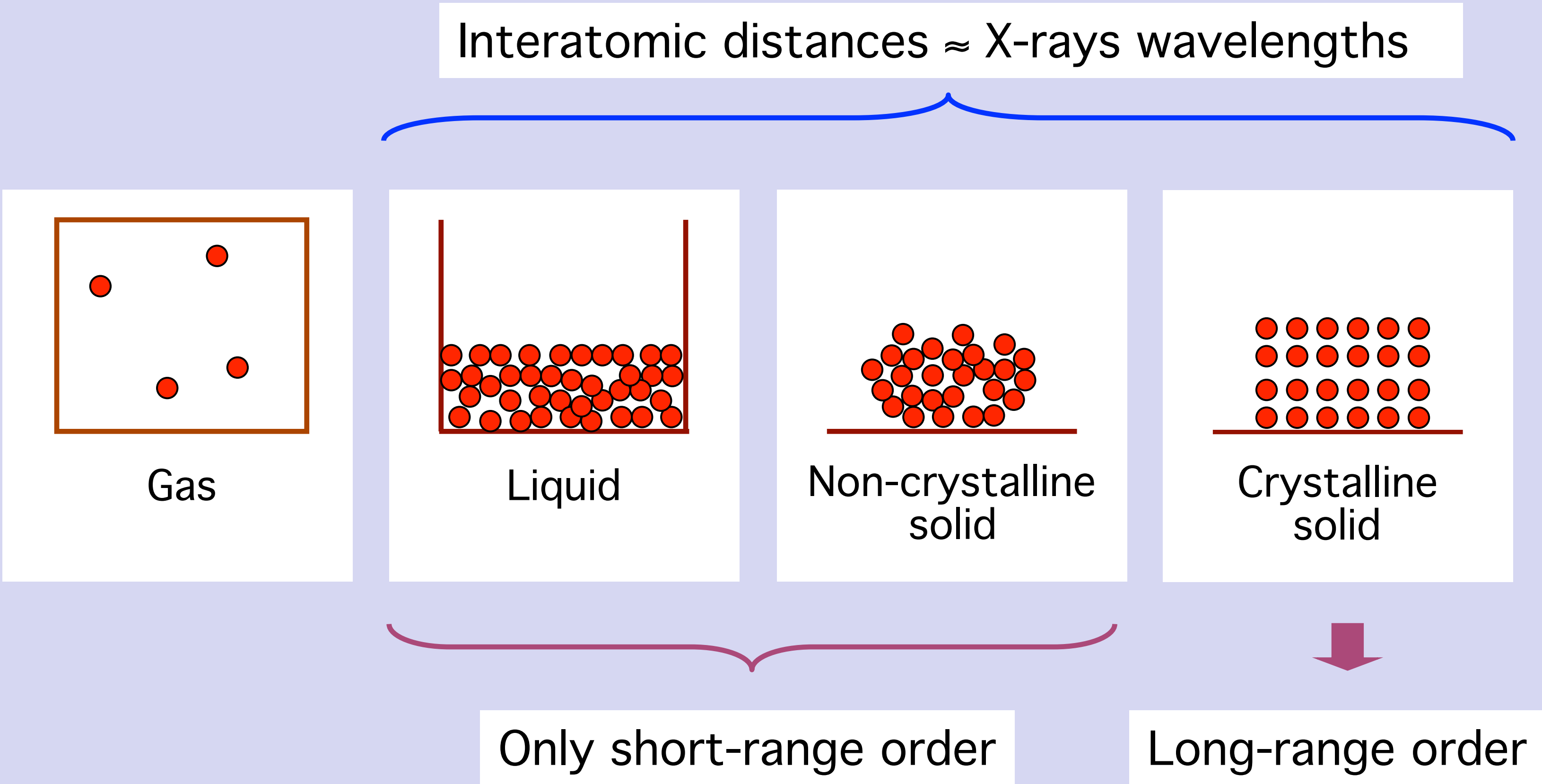
Paolo Fornasini
Department of Physics
University of Trento, Italy

Overview

- X-rays and materials structure
- Crystal lattices an cells
- Symmetry classifications
- Some relevant crystal structures
- Close packing

- X-rays and materials structure

Aggregates of atoms



Crystals

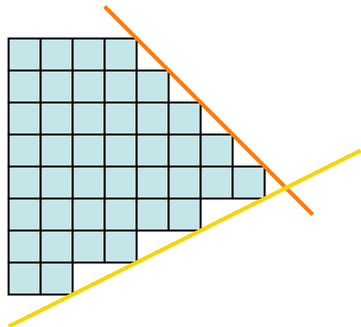
Paolo
Fornasini
Univ. Trento

Quartz crystal (SiO_2)

Macroscopic regularities
(e.g. constancy of angles)

→ Classification of crystals

→



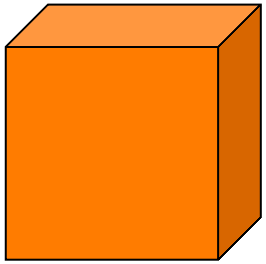
Regular packing
of microscopic structural units
R.J. Haüy (1743-1822)

Atoms and crystals

Paolo
Fornasini
Univ. Trento

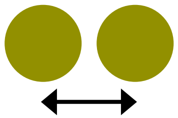
HYPOTHESIS: Structural units = atoms

Example: NaCl



Atomic masses: Na 38.12×10^{-24} g
Cl 58.85×10^{-24} g

Cubic structure
1 cm^3 m = 2.165 g
N = 44.6×10^{21} atoms

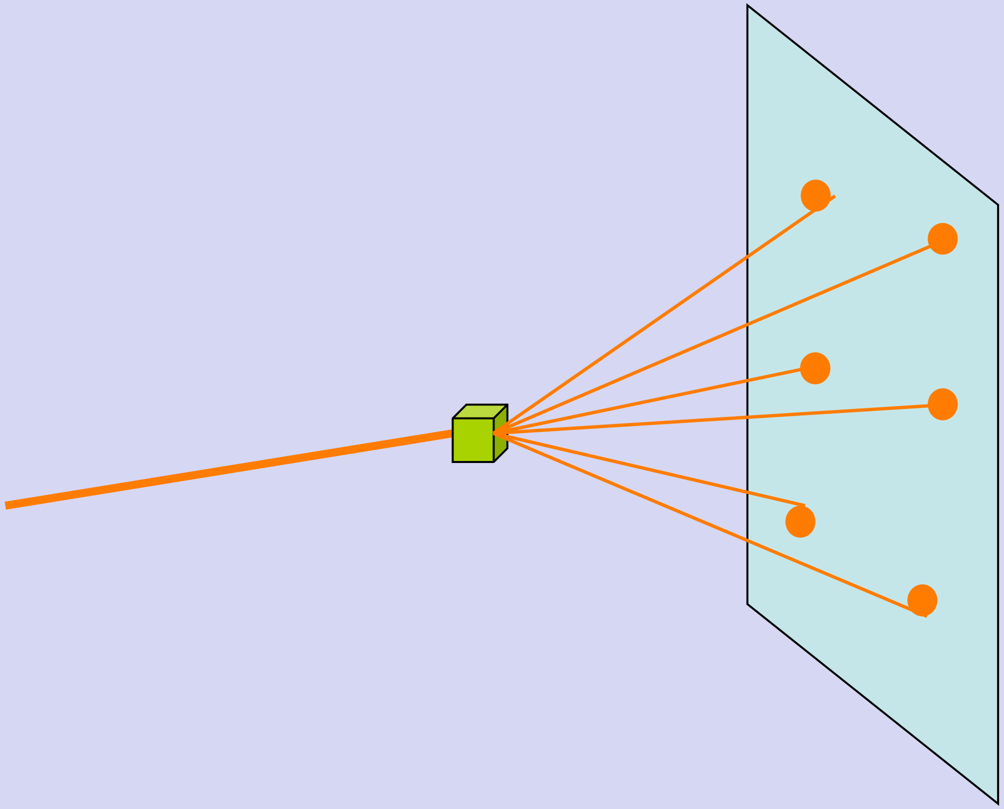


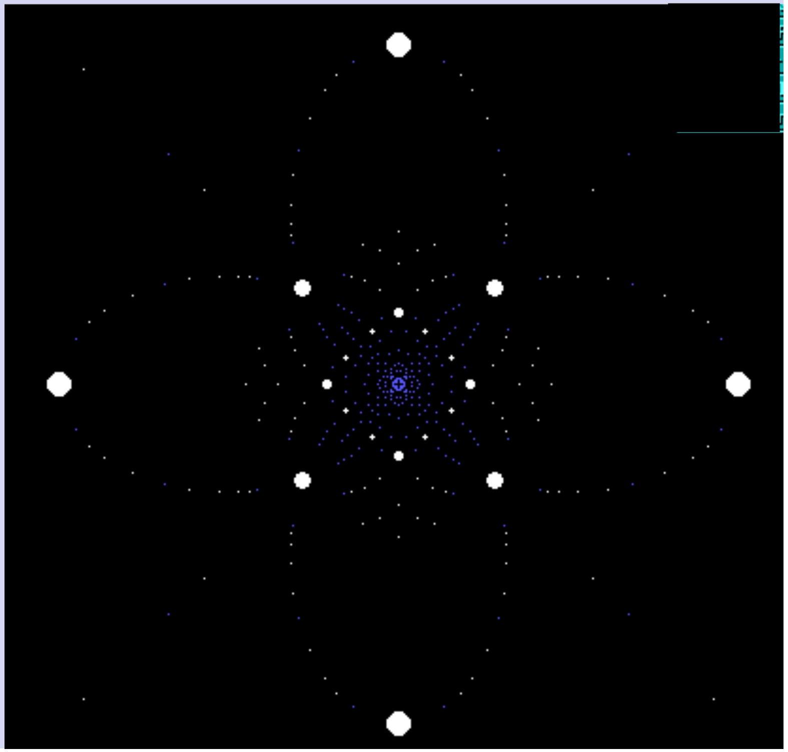
0.28 nm = 2.8 Å

CONCLUSION: Inter-atomic distances
Atomic dimensions
≈ X-ray wavelengths

X-ray diffraction from crystals

Paolo
Fornasini
Univ. Trento



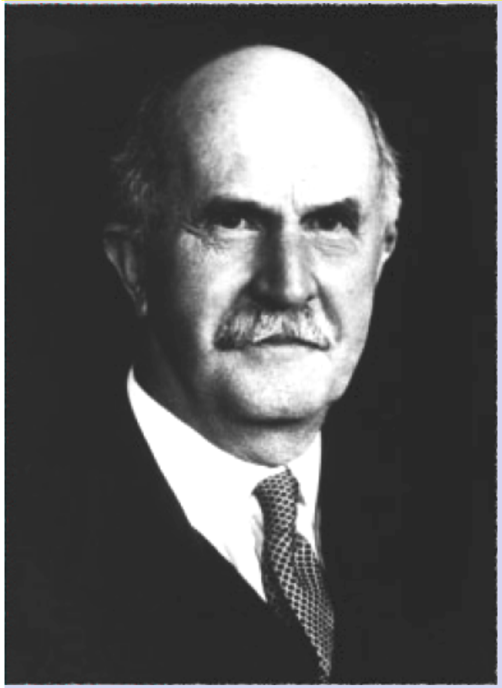


Munich, 1912:
- Max von Laue
- W. Friedrich & P.Knipping

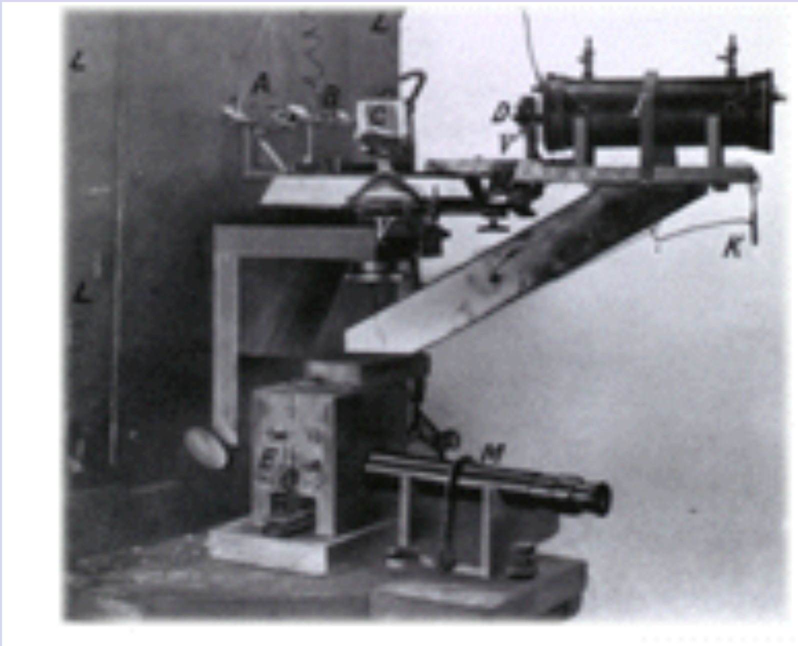
Crystallography

Paolo
Fornasini
Univ. Trento

Cambridge, 1912/13



William Henry Bragg
(1862-1942)



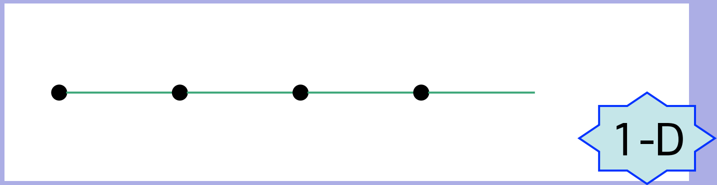
Bragg spectrometer

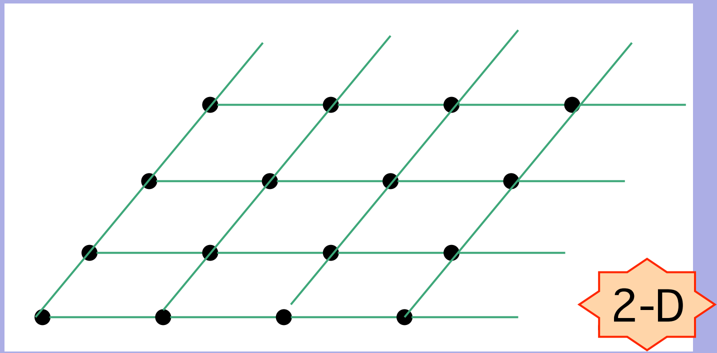
William Lawrence Bragg
(1890-1971)

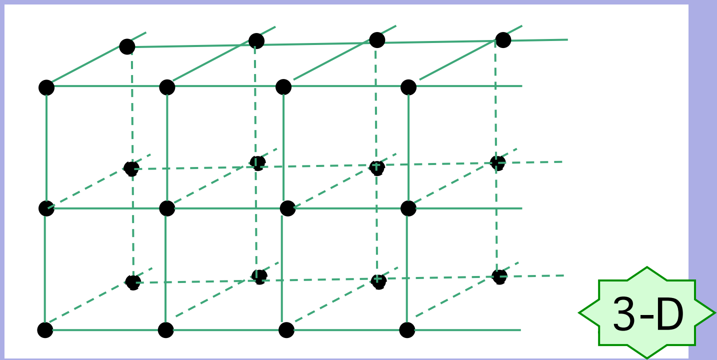
Crystal structure

Paolo
Fornasini
Univ. Trento

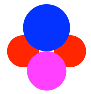
Bravais lattice + Basis



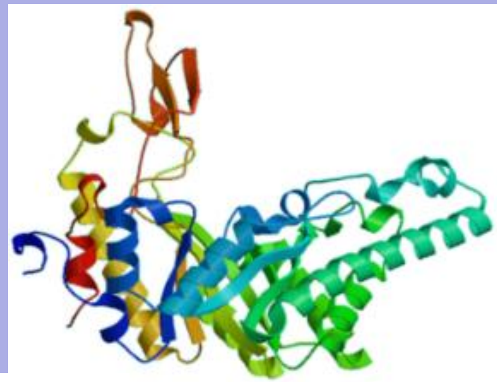




Atom



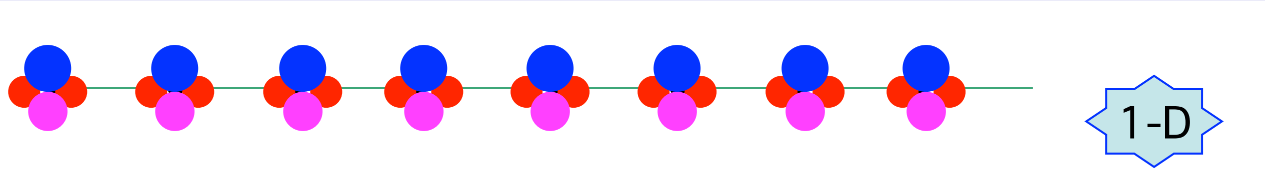
Molecule

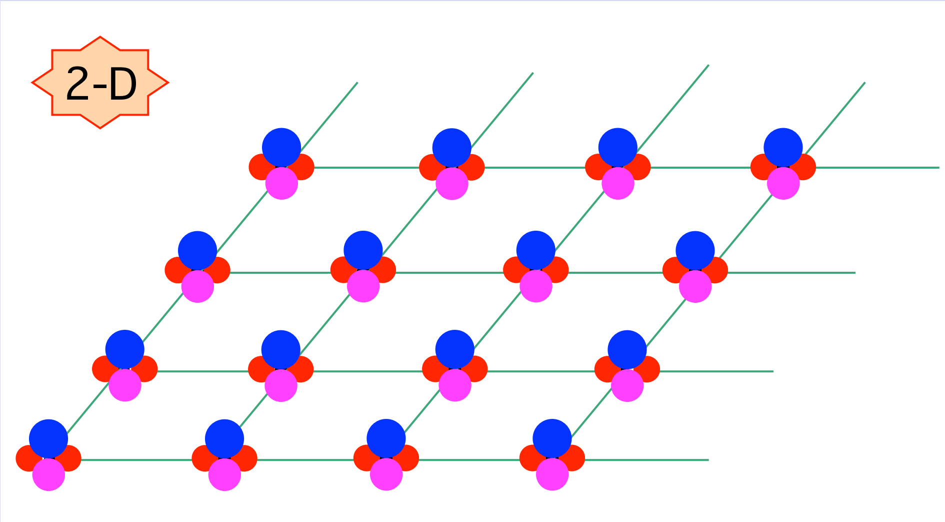


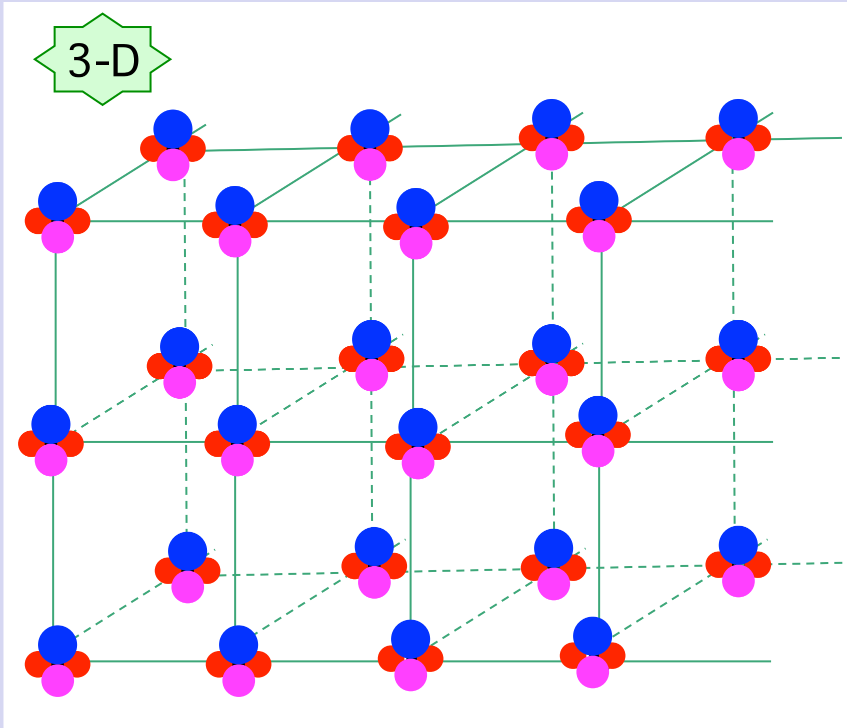
Protein

Bravais lattice + basis

Paolo
Fornasini
Univ. Trento



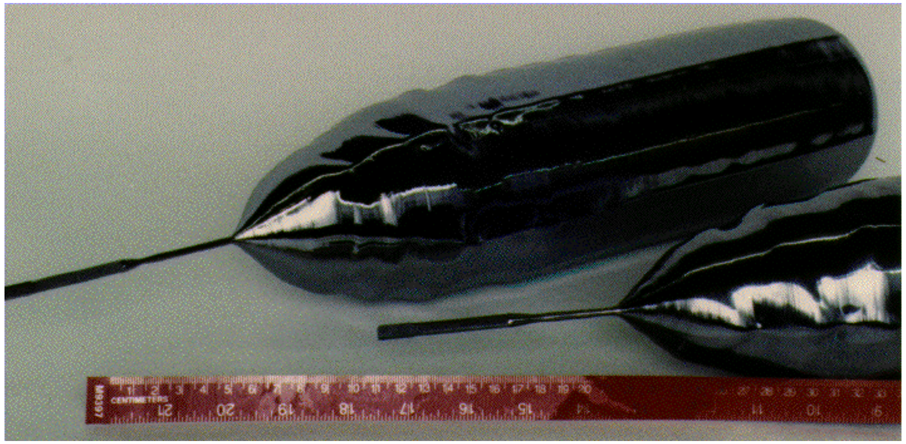


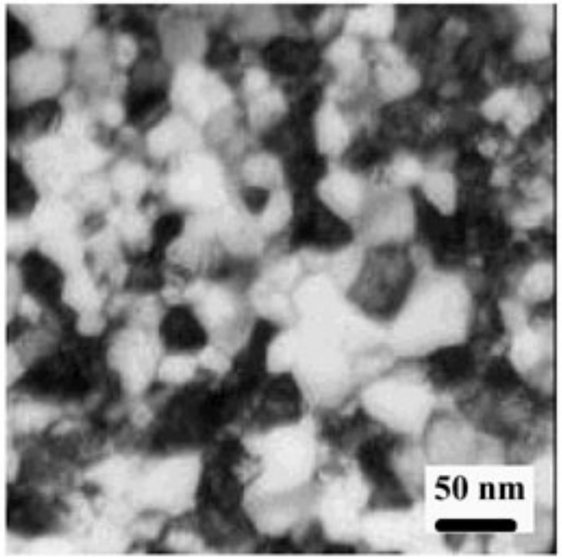


Macro and micro-crystals

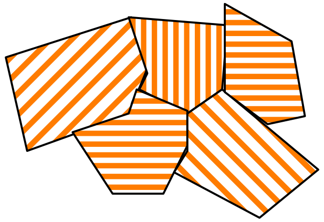
Paolo
Fornasini
Univ. Trento

Monocrystalline silicon, ∅ 13 cm





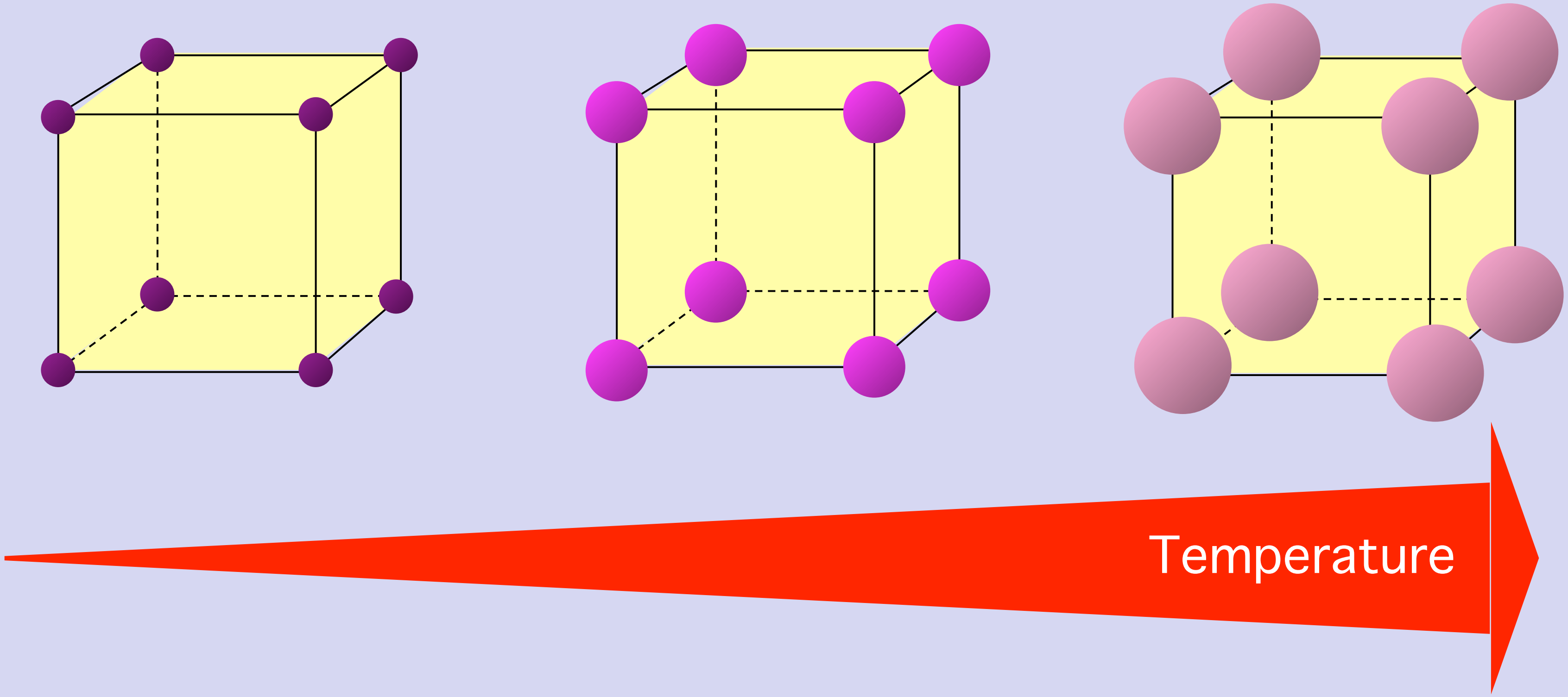
Cr, electron microscopy



Grain structure

Effects of temperature

Paolo
Fornasini
Univ. Trento



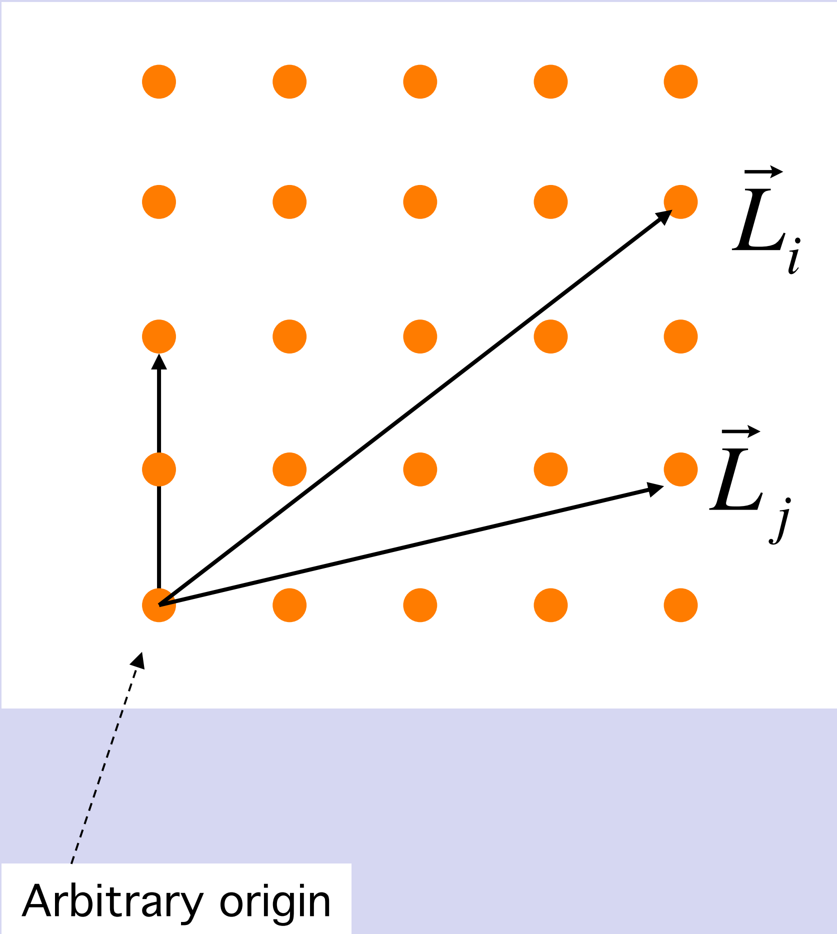
Thermal motion → Spread of atomic positions

Crystal lattices and cells

Lattice vectors (2D)

Paolo
Fornasini
Univ. Trento

2-D



Crystallographic basis (2D)

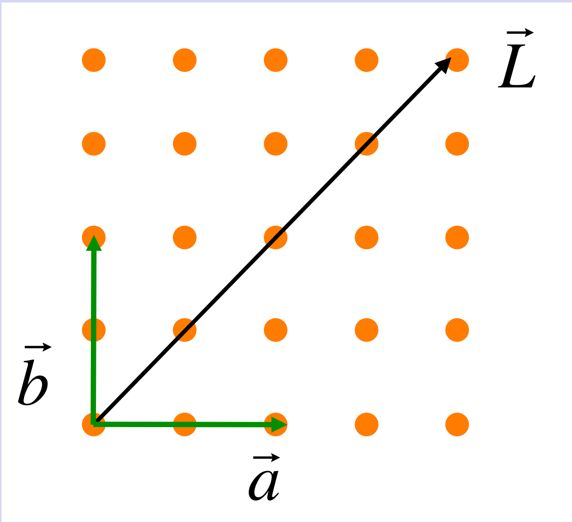
Paolo
Fornasini
Univ. Trento

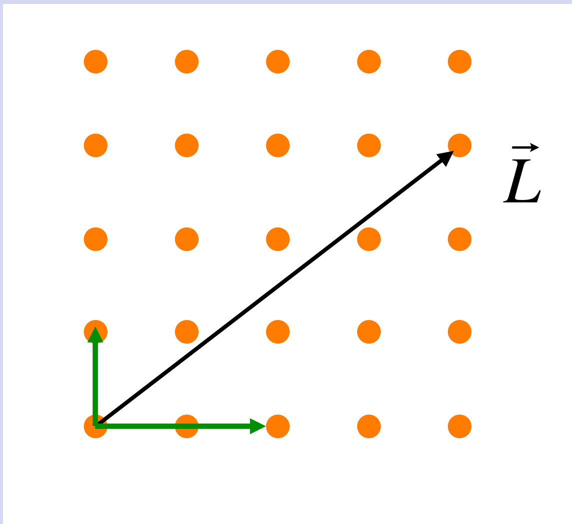
2-D

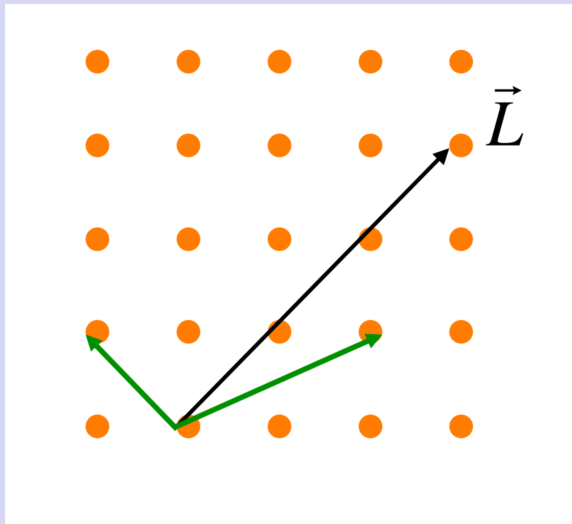
$$\vec{a},\vec{b} \Rightarrow n_1\vec{a} + n_2\vec{b} = \vec{L}$$

integer numbers

basis vectors







> conventional unit cells

Primitive basis (2D)

Paolo
Fornasini
Univ. Trento

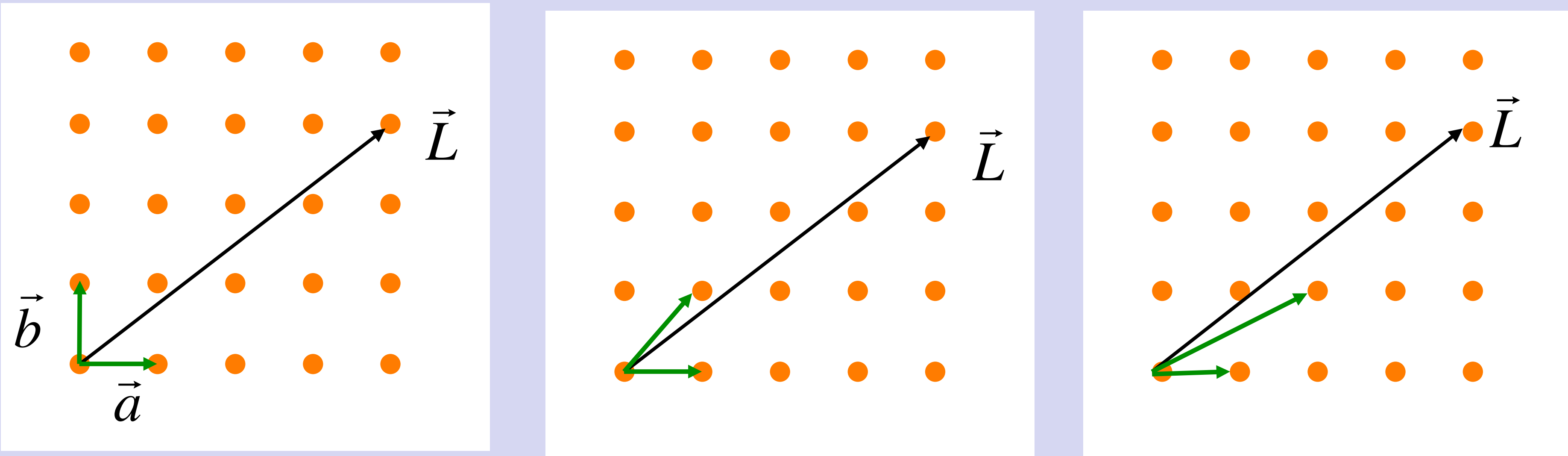
2-D

For every lattice vector

$$\vec{L} = n_1\vec{a} + n_2\vec{b}$$

integers

primitive vectors



Different choices of primitive vectors $\vec{a}, \vec{b}$

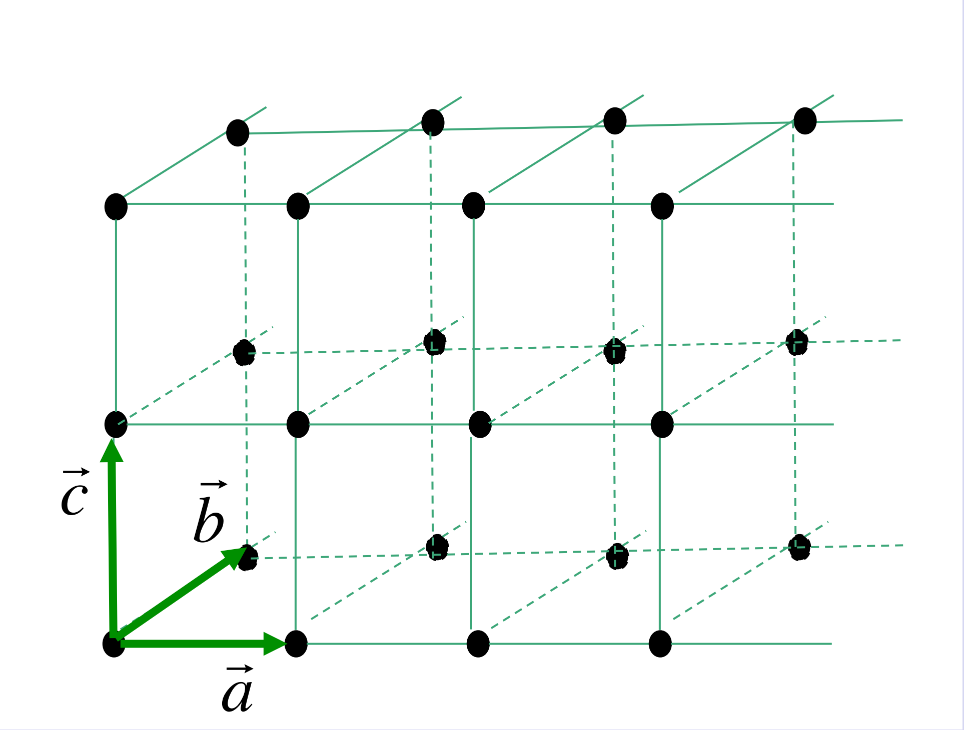
Primitive basis (3D)

Paolo
Fornasini
Univ. Trento

$$\vec{L} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

or

$$\vec{L} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

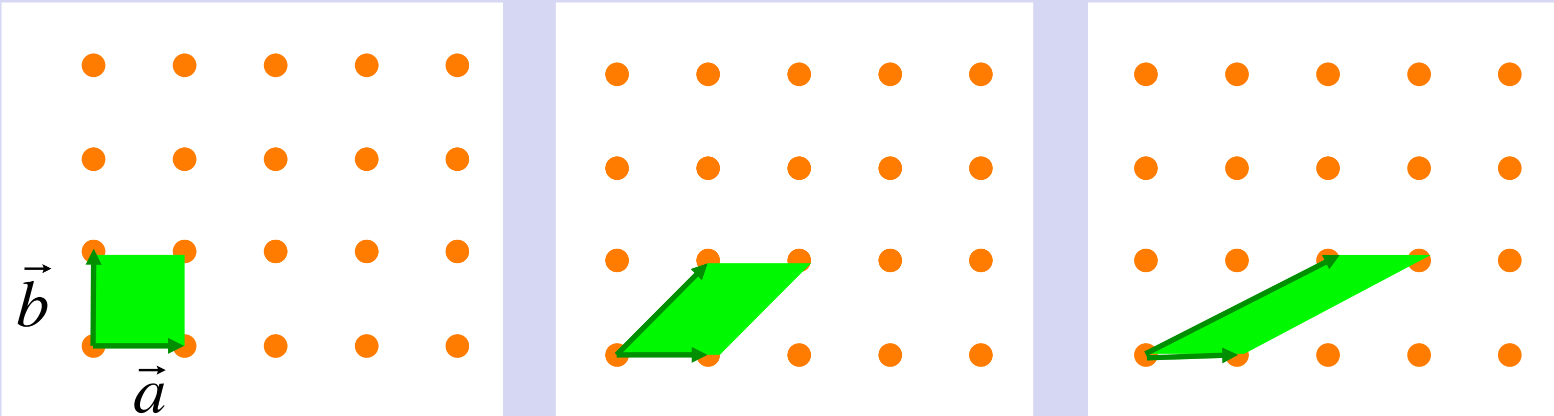


Different choices of primitive vectors $\vec{a},\vec{b},\vec{c}$

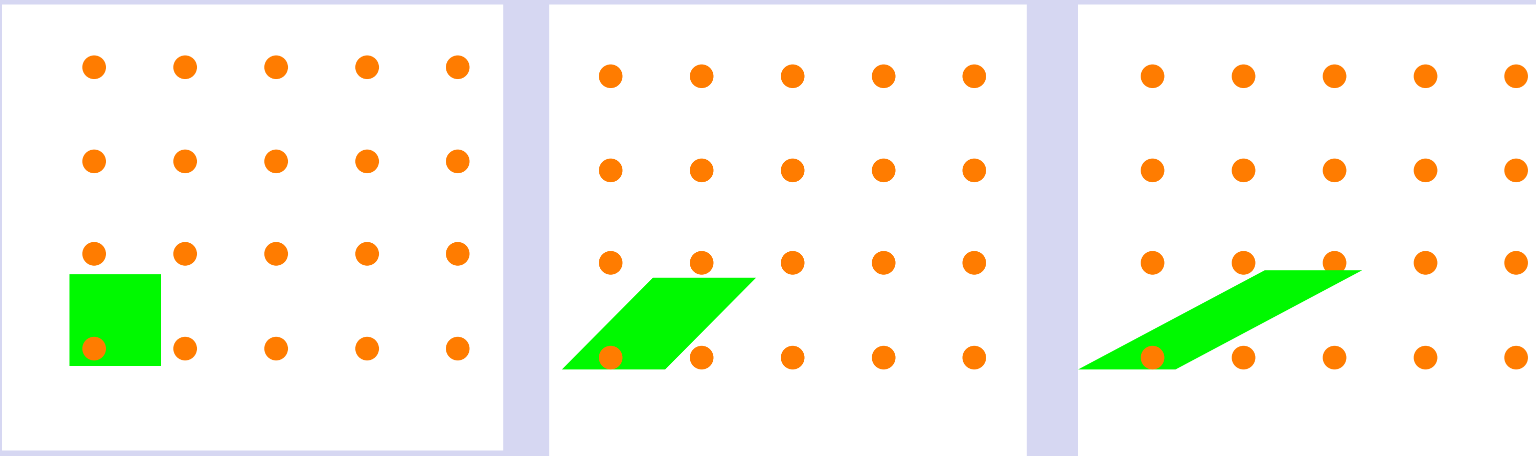
Primitive cells (2D)

2-D

Paolo
Fornasini
Univ. Trento



Different choices of primitive unit cells

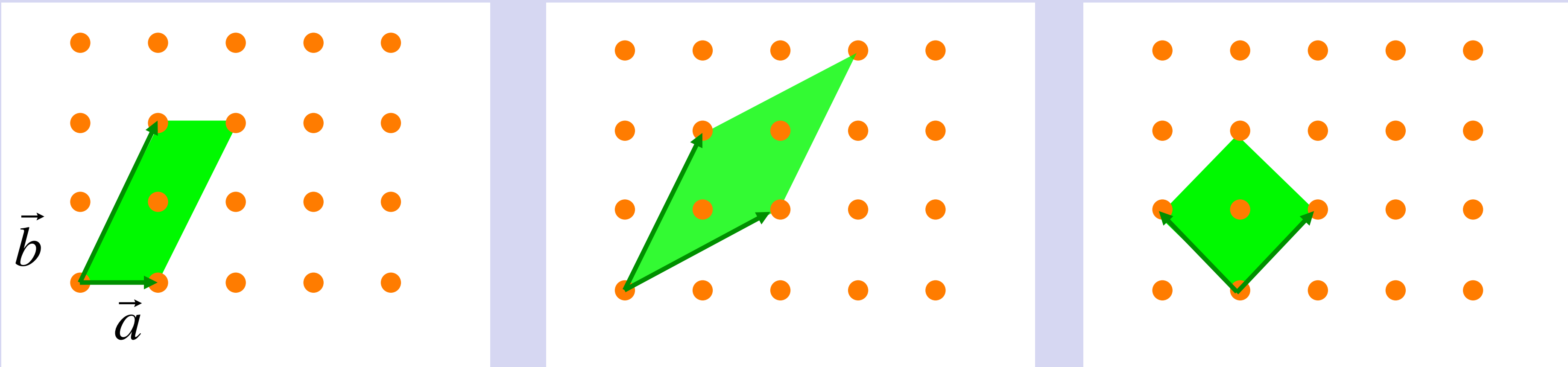


Primitive cell = 1 lattice point

Conventional unit cells (2D)

Paolo
Fornasini
Univ. Trento

2-D



Crystallographic non-primitive basis

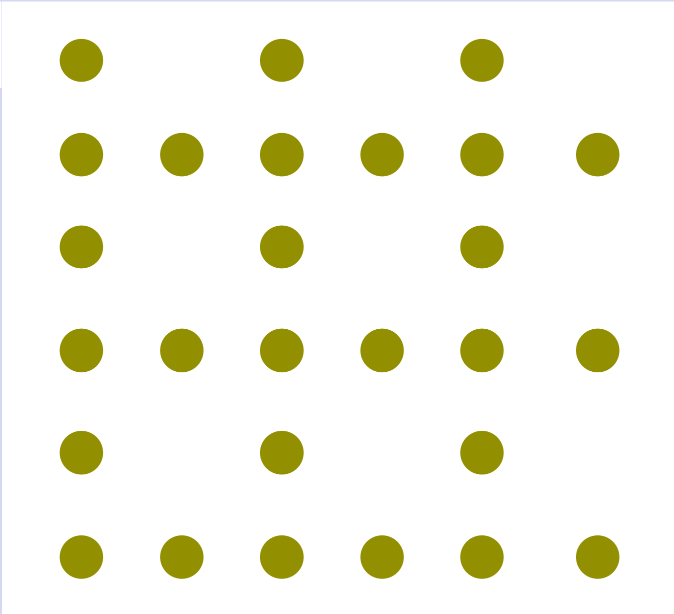
More than 1 lattice point per unit cell

Non-Bravais lattices

Paolo
Fornasini
Univ. Trento

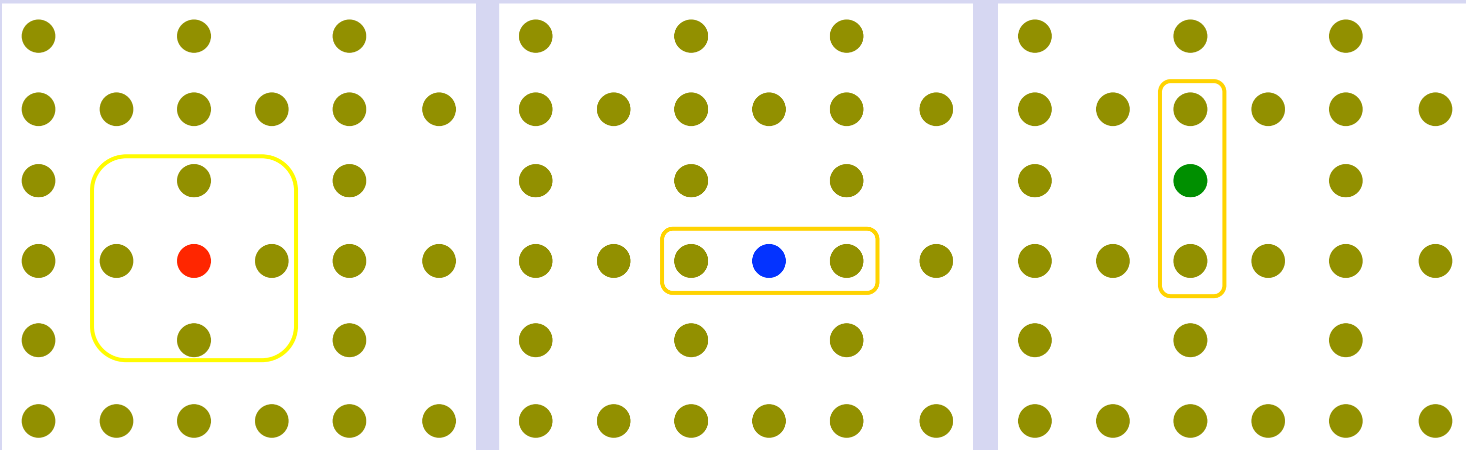
2-D

Atoms



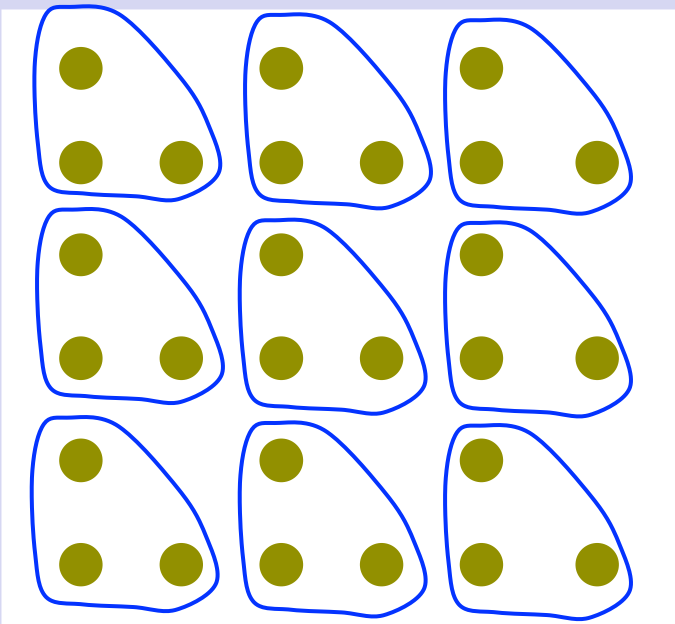
$$\vec{L} \neq n_1 \vec{a} + n_2 \vec{b}$$

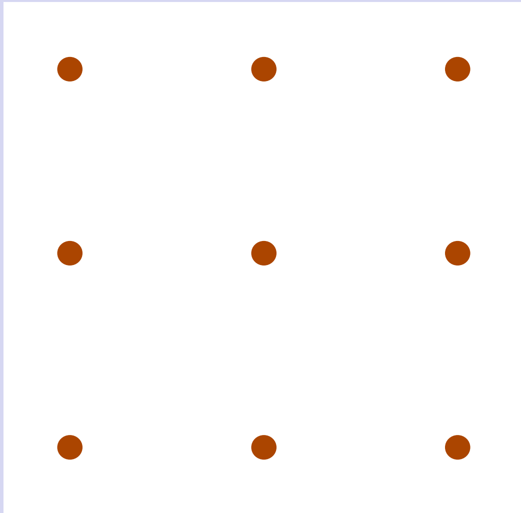
Un-equivalent sites



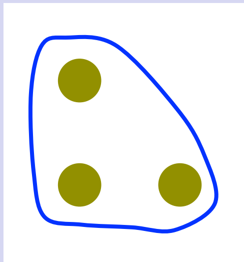
Bravais lattices

Paolo
Fornasini
Univ. Trento





Bravais lattice

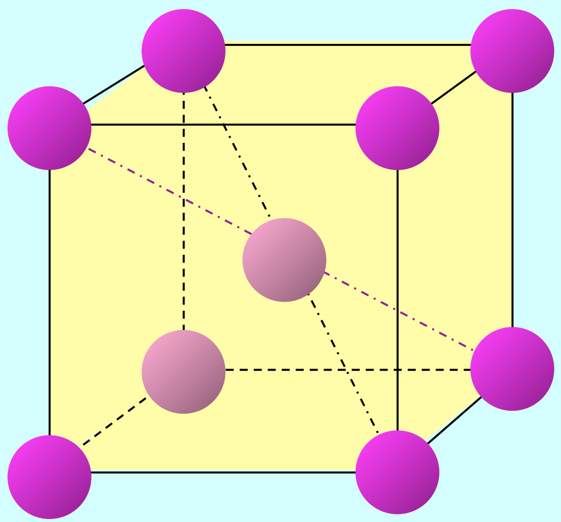


Basis

Conventional cells (3D)

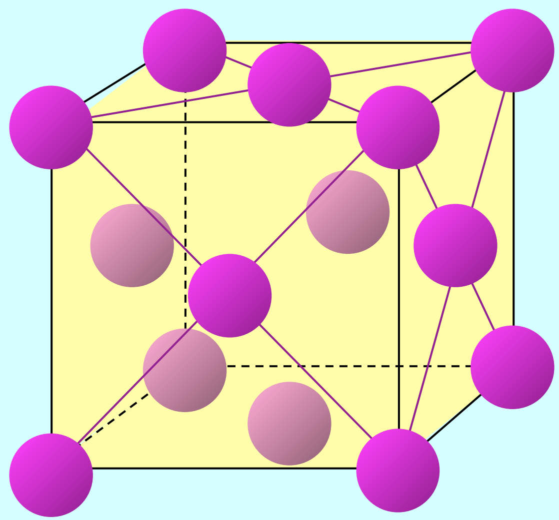
Paolo
Fornasini
Univ. Trento

3-D



Body centered cubic
BCC

2 Bravais lattice points per conventional cell



Face centered cubic
FCC

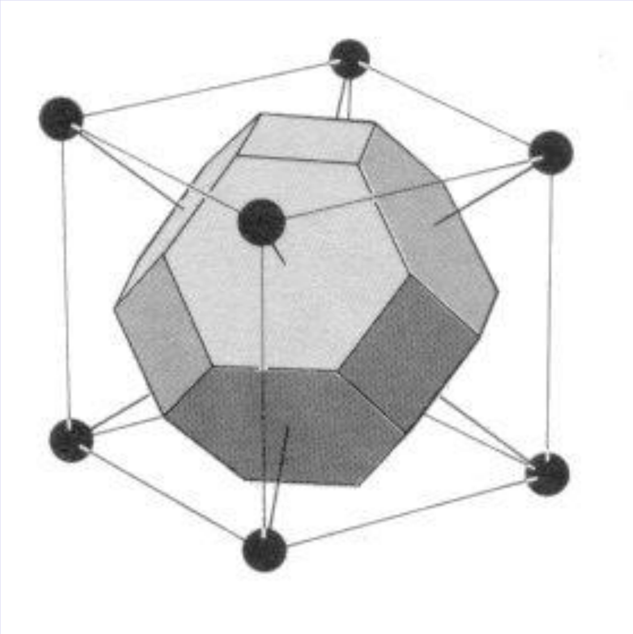
4 Bravais lattice points per conventional cell

3D Wigner-Seitz cells

Paolo
Fornasini
Univ. Trento

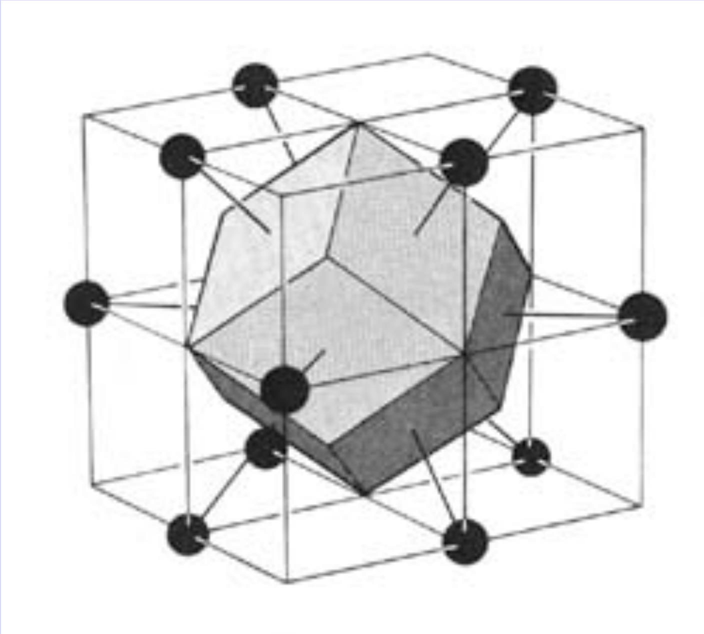
3-D

bcc Bravais lattice



Truncated octahedron:
8 hexagonal faces
6 square faces

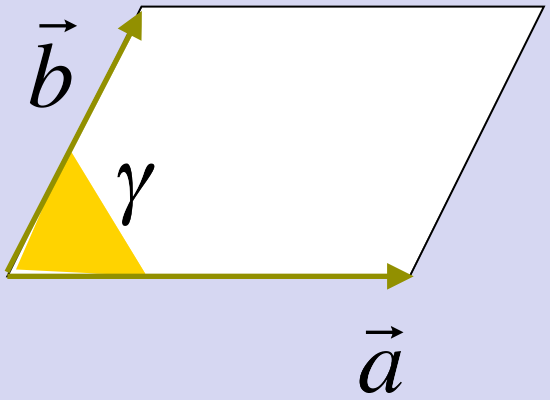
fcc Bravais lattice



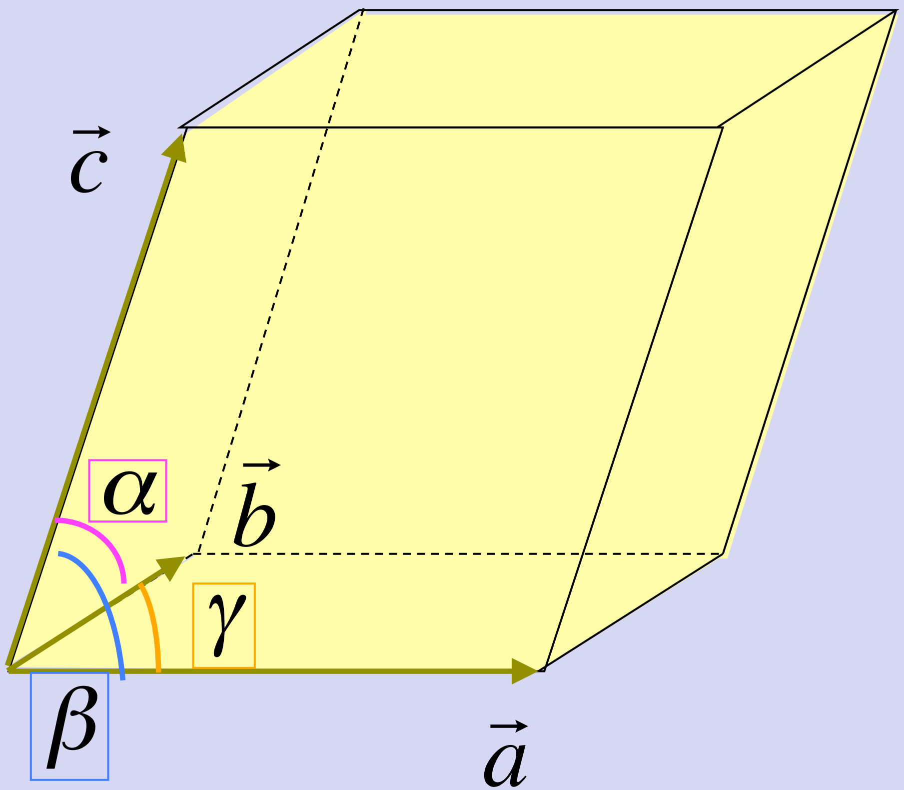
Rhombic dodecahedron:
12 faces

Characterization of unit cells

2-D



3-D

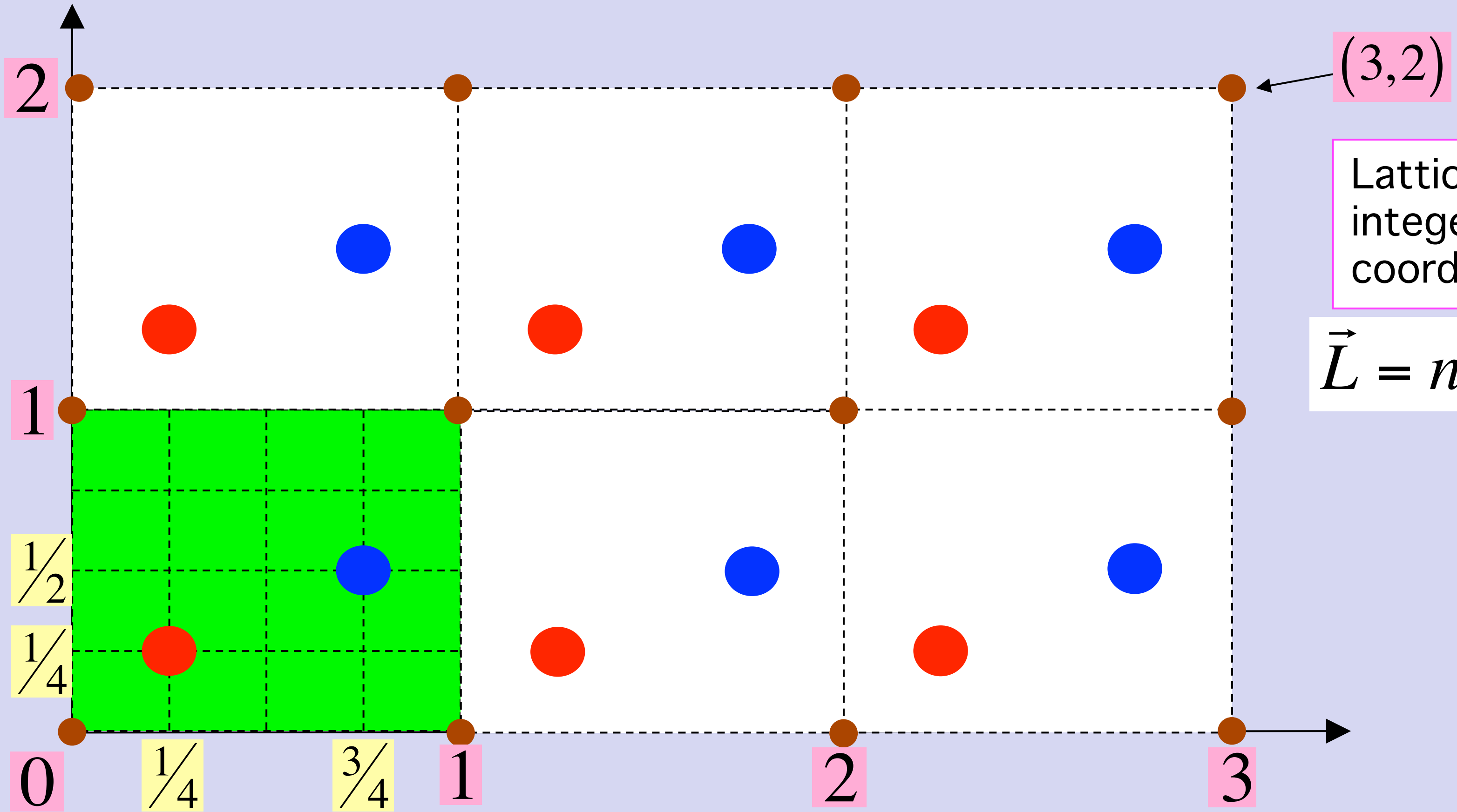


$a \quad b \quad c$ latin

$\alpha \quad \beta \quad \gamma$ greek

Internal coordinates (primitive cells)

Paolo
Fornasini
Univ. Trento



Lattice points: integer coordinates

$$\vec{L} = n_1\vec{a} + n_2\vec{b}$$

Inside cell: fractional coordinates

Red: $\left(\frac{1}{4},\frac{1}{4}\right)$ Blue: $\left(\frac{3}{4},\frac{1}{2}\right)$

Symmetry

Motions in n-dim. Euclidean spaces

Paolo
Fornasini
Univ. Trento

Rotation matrix

Translation vector

$$\begin{pmatrix} x'_1 \\ \vdots \\ x'_n \end{pmatrix} = \begin{pmatrix} R_{11} & \dots & R_{1n} \\ \vdots & & \vdots \\ R_{n1} & \dots & R_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} T_1 \\ \vdots \\ T_n \end{pmatrix}$$

$$\mathrm{x}' = \mathbf{R}\,\mathrm{x} + \mathrm{T} = \{\mathbf{R}|\mathrm{T}\}\,\mathrm{x}$$

Augmented matrix

$$\begin{pmatrix} x'_1 \\ \vdots \\ x'_n \\ \hline 1 \end{pmatrix} = \left(\begin{array}{ccc|c} R_{11} & \dots & R_{1n} & T_1 \\ \vdots & & \vdots & \vdots \\ R_{1n} & \dots & R_{nn} & T_n \\ \hline 0 & \dots & 0 & 1 \end{array}\right) \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{pmatrix}$$

$$\tilde{x}' = \tilde{\boldsymbol{R}}\tilde{\boldsymbol{x}}$$

$$\{\mathbf{R}|\mathrm{T}\}^{-1} = \{\mathbf{R}^{-1}|-\mathbf{R}^{-1}\,\mathrm{T}\}$$

Inversion

$$\tilde{\boldsymbol{R}}^{-1}$$

$$\mathrm{x}'' = \{\mathbf{R}'|\mathrm{T}'\}\{\mathbf{R}|\mathrm{T}\}\,\mathrm{x} = \{\mathbf{R}'\mathbf{R}\,|\mathbf{R}\,\mathrm{T} + \mathrm{T}'\}\,\mathrm{x}$$

Composition

$$\tilde{\boldsymbol{R}}'' = \tilde{\boldsymbol{R}}'\tilde{\boldsymbol{R}}$$

Types of motion (n=3)

Paolo
Fornasini
Univ. Trento

Rotation — Translation

$$\begin{pmatrix} x'_1 \\ \vdots \\ x'_n \end{pmatrix} = \begin{pmatrix} R_{11} & \dots & R_{1n} \\ \vdots & & \vdots \\ R_{n1} & \dots & R_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} T_1 \\ \vdots \\ T_n \end{pmatrix}$$

- $\mathbf{R} = \mathbf{I}$ — Pure translations
- At least 1 fixed point
  - $\det(\mathbf{R}) = +1$ — Rotations
  - $\det(\mathbf{R}) = -1$
    - Inversion — $\mathbf{R} = -\mathbf{I}$
    - Reflections — $\mathbf{R} \neq -\mathbf{I}, \quad \mathbf{R}^2 = \mathbf{I}$
    - Roto-iniversions
- Other (no fixed points)
  - $\det(\mathbf{R}) = +1$ — Screw rotations
  - $\det(\mathbf{R}) = -1$ — Glide reflections

Symmetry operations

Paolo
Fornasini
Univ. Trento

Symmetry operation of a given object = Motion which maps the object onto itself

Group properties
- Closure
- Inverse transformation
- Identity operation
- Associative law

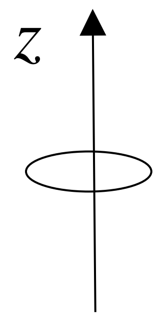
Crystallographic symmetry operations

A motion is a crystallographic symmetry operation
if a crystal structure exists
for which it is a symmetry operation.

Lattice rotations

3-D

Paolo
Fornasini
Univ. Trento



Proper rotation

$$\mathbf{R}(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Improper rotation

$$\mathbf{R}(\phi) = \begin{pmatrix} -\cos\phi & \sin\phi & 0 \\ -\sin\phi & -\cos\phi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\mathrm{tr}(\mathbf{R}) = \pm(1 + 2\cos\phi)$$

Lattice, primitive basis

$$\vec{L} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Rotation

$$\begin{pmatrix} n'_1 \\ n'_2 \\ n'_3 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

n_i, n'_i integers ⇒ R_{ij} integers ⇒ $\mathrm{tr}(\mathbf{R}) = \pm(1 + 2\cos\phi) = \text{integer}$

⇒ $\phi = 0, 60, 90, 120, 180 \ldots \text{degrees}$

restrictions on crystal rotations

Types of crystal symmetries

3-D

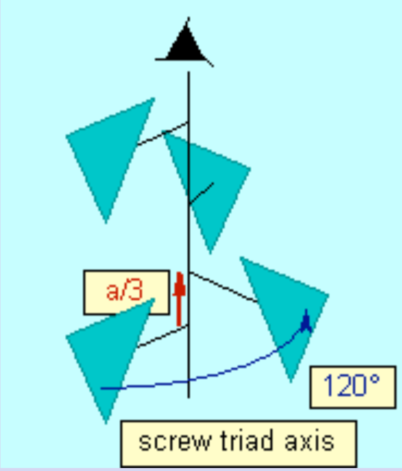
Paolo
Fornasini
Univ. Trento

Possible rotation axes: $C_n = C_1, C_2, C_3, C_4, C_6$ $n = 1, 2, 3, 4, 6$

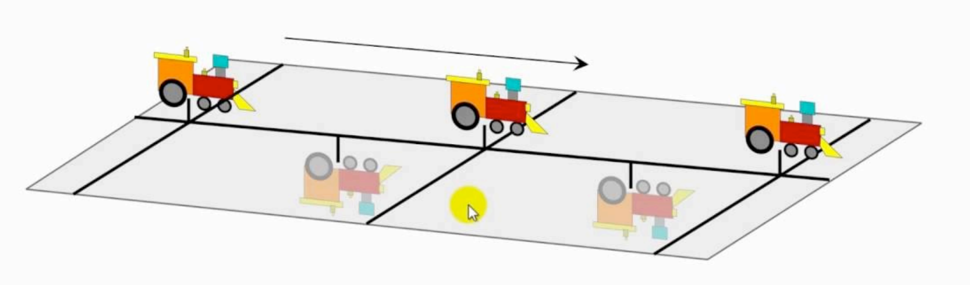
Schoenflies International

Pure translations: $\vec{T} = \vec{L}$ Motion = lattice vector

Screw rotations: Rotation + fractional translation



Glide reflections: Reflection + fractional translation



Structure of space groups

3-D

Paolo
Fornasini
Univ. Trento

Pure translations

Proper & improper rotations
Screw rotations
Glide reflections

Augmented matrices

I	$\tilde{\boldsymbol{R}}_1$	$\tilde{\boldsymbol{R}}_2$	$\tilde{\boldsymbol{R}}_3$	$\cdots$	$\tilde{\boldsymbol{R}}_N$
T_{L_1}	$T_{L_1}\tilde{\boldsymbol{R}}_1$	$T_{L_1}\tilde{\boldsymbol{R}}_2$	$T_{L_1}\tilde{\boldsymbol{R}}_3$	$\cdots$	$T_{L_1}\tilde{\boldsymbol{R}}_N$
T_{L_2}	$T_{L_2}\tilde{\boldsymbol{R}}_1$	$T_{L_2}\tilde{\boldsymbol{R}}_2$	$T_{L_2}\tilde{\boldsymbol{R}}_3$	$\cdots$	$T_{L_2}\tilde{\boldsymbol{R}}_N$
T_{L_3}	$T_{L_3}\tilde{\boldsymbol{R}}_1$	$T_{L_3}\tilde{\boldsymbol{R}}_2$	$T_{L_3}\tilde{\boldsymbol{R}}_3$	$\cdots$	$T_{L_3}\tilde{\boldsymbol{R}}_N$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$

Infinite subgroup (commutative invariant)

Finite number of infinite cosets

Symmorphic groups

3-D

Paolo
Fornasini
Univ. Trento

Only Proper & improper rotations → Symmorphic space groups

Proper & improper rotations
+ Screw rotations + Glide reflections → Non-Symmorphic space groups

Pure translations

I	$\tilde{R}_1$	$\tilde{R}_2$	$\tilde{R}_3$	$\cdots$	$\tilde{R}_N$
T_{L_1}	$T_{L_1}\tilde{R}_1$	$T_{L_1}\tilde{R}_2$	$T_{L_1}\tilde{R}_3$	$\cdots$	$T_{L_1}\tilde{R}_N$
T_{L_2}	$T_{L_2}\tilde{R}_1$	$T_{L_2}\tilde{R}_2$	$T_{L_2}\tilde{R}_3$	$\cdots$	$T_{L_2}\tilde{R}_N$
T_{L_3}	$T_{L_3}\tilde{R}_1$	$T_{L_3}\tilde{R}_2$	$T_{L_3}\tilde{R}_3$	$\cdots$	$T_{L_3}\tilde{R}_N$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$

- Classifications of crystals

Symmetry classifications

2-D

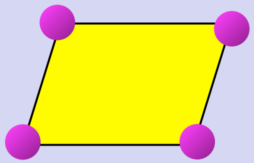
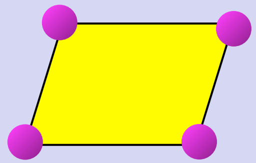
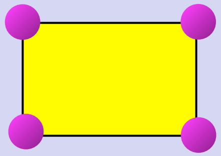
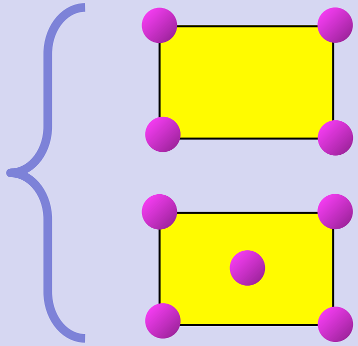
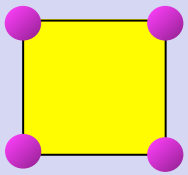
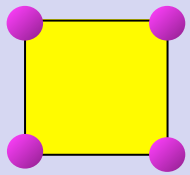
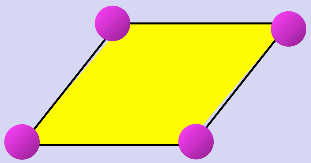
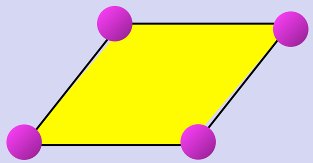
Paolo
Fornasini
Univ. Trento

	Point symmetry	Point + translational symmetry
Bravais lattices	4 families (4 systems)	5 Bravais lattices
Crystal structures	10 crystal classes	17 plane group types Wallpaper groups

2-D lattices

2-D

Paolo
Fornasini
Univ. Trento

4 families = 4 crystal systems			5 Bravais lattices	
m – Oblique (monoclinic)		$a \neq b, \gamma \neq 90^\circ$		mp
o – Rectangular (orthorhombic)		$a \neq b, \gamma = 90^\circ$		op oc
t – Square (tetragonal)		$a = b, \gamma = 90^\circ$		tp
h – Hexagonal		$a = b, \gamma = 120^\circ$		hp

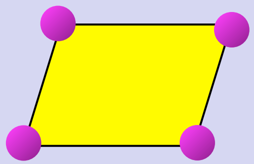
2-D example: oblique family

2-D

Paolo
Fornasini
Univ. Trento

LATTICE

Oblique family
2-fold rotation axis



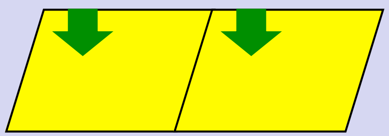
1 Bravais lattice

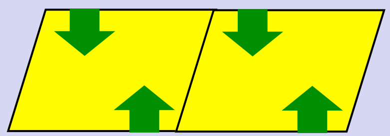
STRUCTURE

2 crystal classes = 2 plane group types

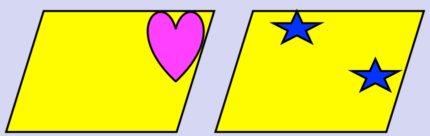
A - Only identity

B – 2-fold rotation axis

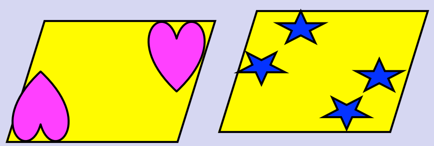




Infinite possible bases



....



....

2-D example: rectangular family

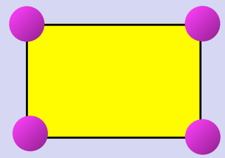
2-D

Paolo
Fornasini
Univ. Trento

LATTICE

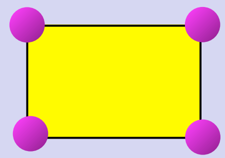
Point symmetry

Rectangular family
> 2-fold rotation axis
> mirror planes

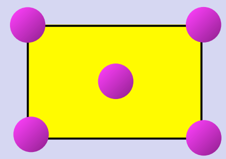


+ transl. symmetry

2 Bravais lattices



P
primitive



C
centred

STRUCTURE

Point symmetry

2 plane crystal classes

+ transl. symmetry

7 plane group types

Symmetry classifications

3-D

Paolo
Fornasini
Univ. Trento

	Point symmetry		Point + translational symmetry
Bravais lattices	6 crystal families	7 crystal systems	14 Bravais lattices
Crystal structures	32 crystal classes		230 space group types 73 symmorphic 157 non-symmorphic

Crystal families

3-D

Paolo
Fornasini
Univ. Trento

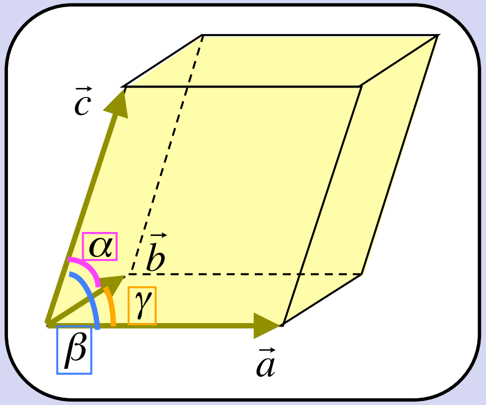
	Crystal family	Crystal system	Required symmetries of point group
a	Triclinic (anorthic)		None
m	Monoclinic		1 twofold axis of rotation or 1 mirror plane
o	Orthorhombic		3 twofold axes of rotation or 1 twofold axis of rotation and two mirror planes.
t	Tetragonal		1 fourfold axis of rotation
h	Hexagonal	Trigonal	1 threefold axis of rotation
		Hexagonal	1 sixfold axis of rotation
c	Cubic		4 threefold axes of rotation
	Total: 6	7	

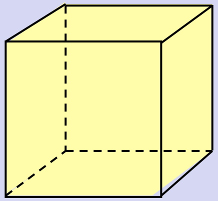
7 crystal systems (6 families)

3-D

Paolo
Fornasini
Univ. Trento

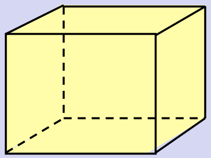
7 different cells that can fill 3-d space





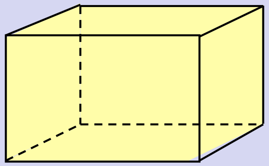
$a = b = c$
$\alpha = \beta = \gamma$

Cubic



$a = b \neq c$
$\alpha = \beta = \gamma$

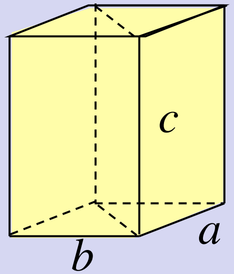
Tetragonal



$a \neq b \neq c$
$\alpha = \beta = \gamma$

Orthorombic

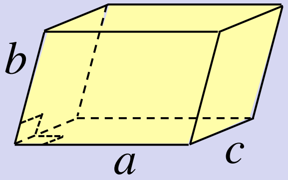
Hexagonal family



$a = b \neq c$
$\alpha = \beta = 90^\circ$
$\gamma = 120^\circ$

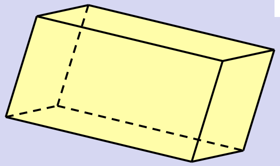
Hexagonal crystal ystem

Trigonal crystal system



$a \neq b \neq c$
$\alpha = \beta = 90^\circ$
$\gamma \neq 120^\circ$

Monoclinic



$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90^\circ$

Triclinic

14 Bravais lattices (A)

3-D

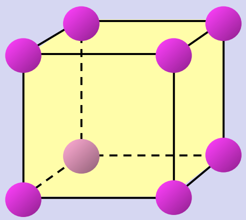
Paolo
Fornasini
Univ. Trento

6 crystal families

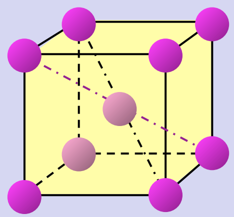
14 Bravais lattices

P = primitive
I = body centered
F = face centered
S = side centered (A,B,C)
R = rhombohedral

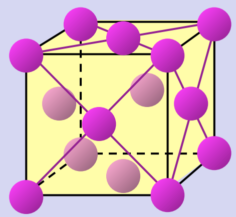
c - Cubic



cP

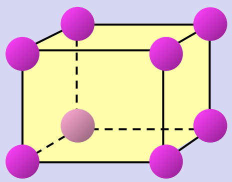


cI

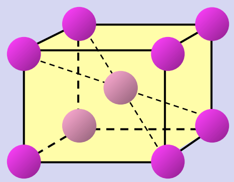


cF

t - Tetragonal



tP



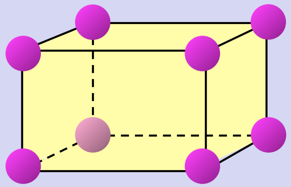
tI

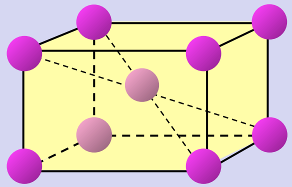
14 Bravais lattices (B)

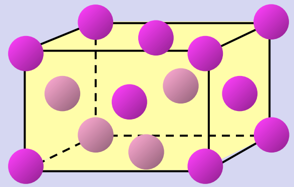
3-D

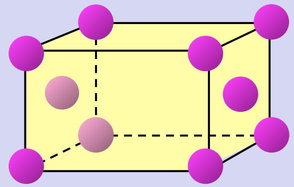
Paolo
Fornasini
Univ. Trento

o - Orthorombic

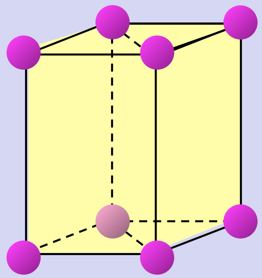

oP


oI

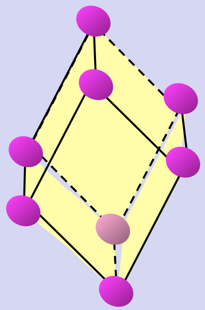

oF


oS

h - Hexagonal

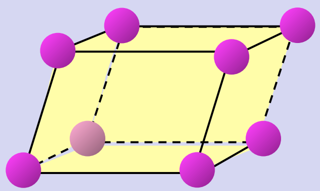

hexagonal

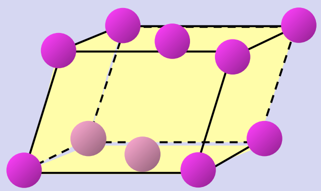
hP


rhomboedral

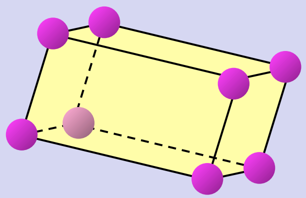
hR

m - Monoclinic


mP


mS

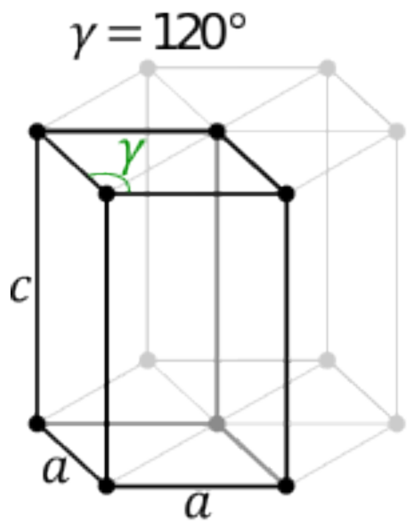
a - Triclinic


aP

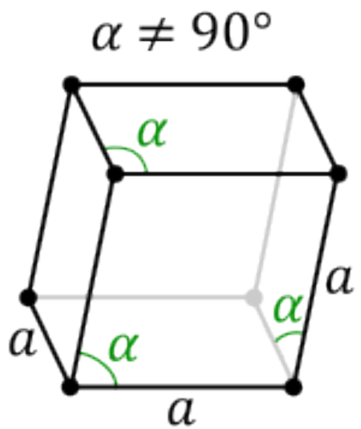
Hexagonal and Rhombohedral lattices

3-D

Paolo
Fornasini
Univ. Trento

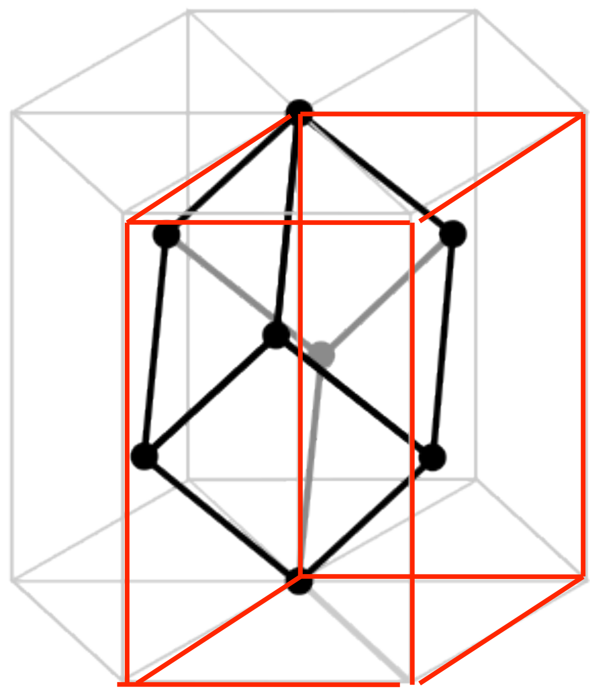


Hexagonal
cell



Rhombohedral
cell

Conventional hexagonal cell
for the rhombohedral lattice
(3 lattice point per cell)



Comparison of classifications

3-D

Paolo
Fornasini
Univ. Trento

Difference between: Hexagonal – trigonal - rhombohedral

Point symmetry

Point + translational symmetry

Crystal family	Crystal system	Required symmetries of point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic		None	2	2	1	Triclinic
Monoclinic		1 twofold axis of rotation or 1 mirror plane	3	13	2	Monoclinic
Orthorhombic		3 twofold axes of rotation or 1 twofold axis of rotation and two mirror planes.	3	59	4	Orthorhombic
Tetragonal		1 fourfold axis of rotation	7	68	2	Tetragonal
Hexagonal	Trigonal	1 threefold axis of rotation	5	7	1	Rhombohedral
				18	1	Hexagonal
	Hexagonal	1 sixfold axis of rotation	7	27		
Cubic		4 threefold axes of rotation	5	36	3	Cubic
Total: 6	7		32	230	14	7

International symbols, point groups

3-D

Paolo
Fornasini
Univ. Trento

At most 3 symmetry elements. Order is relevant

Examples:

2

$2\ 3$

$m\ \overline{3}\ m$

- tertiary
- secondary
- primary

} symmetry element

a) n is an n-fold rotation axis, $n = 1, 2, 3, 4, 6$

b) $\overline{n}$ is an n-fold roto-inversion axis, say the combination of a rotation with an inversion, $\overline{n} = \overline{1}, \overline{3}, \overline{4}, \overline{6}$

$\overline{1}$ is the inversion point; the symbol $\overline{2}$ corresponds to m and is not used

c) m is a mirror plane

d) nm is an n-fold axis with n symmetry planes passing through it, e.g. $3m, 4m$

e) n/m is an n-fold axis with a symmetry plane perpendicular to it, e.g. $3/m$
if n is even, there is also a centre of symmetry

f) $n2$ is an n-fold axis with n two-fold axes perpendicular to it, e.g. $32, 42$

g) $\frac{n}{m}m$ or n/mmm is an n-fold axis with planes parallel and perpendicular to it

32 crystal classes

3-D

Paolo
Fornasini
Univ. Trento

Point-symmetry of crystal structures

System	Schoenflies	International	
Triclinic	C_1, C_i	$1, \bar{1}$	
Monoclinic	C_2, C_{1h}, C_{2h}	$2, m, 2/m$	
Orthorhombic	D_2, C_{2v}, D_{2h}	$222, mm2, mmm$	
Tetragonal	C_4, S_4, C_{4h}	$4, \bar{4}, 4/m$	
	$D_4, D_{2d}, C_{4v}, D_{4h}$	$422, \bar{4}2m, 4mm, 4/mmm$	
Trigonal	$C_3, C_{3i}, D_3, C_{3v}, D_{3d}$	$3, \bar{3}, 32, 3m, \bar{3}$	
Hexagonal	C_6, C_{3h}, C_{6h}	$6, \bar{6}, 6/m$	
	$D_6, D_{3h}, C_{6v}, D_{6h}$	$622, \bar{6}2m, 6mm, 6/m, mm$	
Cubic	T	23	Tetrahedron proper rot.
	T_d	$\bar{4}3m$	Tetrahedron symmetry
	$T_h = T \otimes C_i$	$m\bar{3}$	Full tetrahedral symmetry
	O	43	Octahedron proper rot.
	$O_h = O \otimes C_i$	$m\bar{3}m$	Full octahedral symmetry

Infinite possible bases for each class

International symbols, space groups

3-D

Paolo
Fornasini
Univ. Trento

Additional elements with respect to point groups

Examples: $F\,m\,\bar{3}\,m$

$F\,d\,\bar{3}\,m$ → Glide plane

a,b,c = axial
e = double
n = diagonal
d = "diamond"

$P\,3_1\,2\,1$ → Screw axis

n_p Righ-hand screw rotation 360/n deg.
+ translation (p/n) **t**
(**t** = shortest lattice translation parallel to the axis)

P primitive
F all-face-centred
I body-centred
S base-centred (S=A,B,C)
R rhombohedral

International Tables

Paolo
Fornasini
Univ. Trento

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

Volume A
SPACE-GROUP SYMMETRY

Edited by
THEO HAHN

Fifth edition

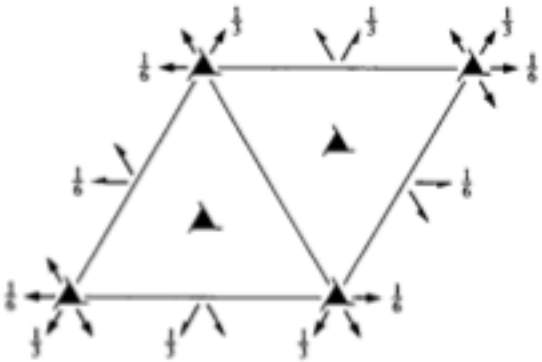
Published for
THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY
by
SPRINGER
2005

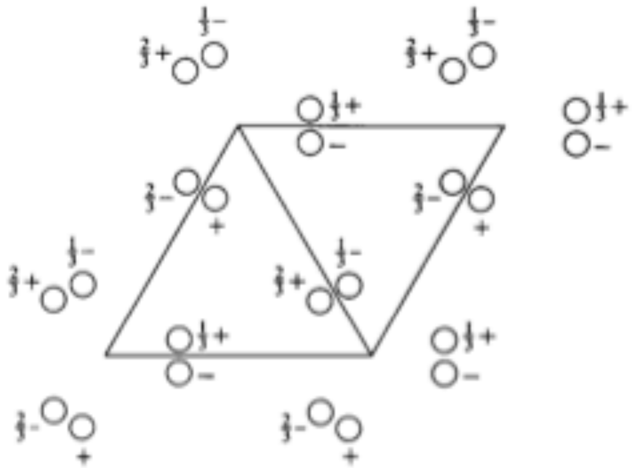
International Tables – example (pag.1)

Paolo
Fornasini
Univ. Trento

International Tables for Crystallography (2006). Vol. A, Space group 152, pp. 510–511.

$P3_121$	D_3^4	321	Trigonal
No. 152	$P3_121$		Patterson symmetry $P\bar{3}m1$





Origin on $2[1\,1\,0]$ at $3_1(1,1,2)1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})\quad 0,0,z$ (3) $3^-(0,0,\frac{2}{3})\quad 0,0,z$
(4) $2\quad x,x,0$ (5) $2\quad x,0,\frac{1}{3}$ (6) $2\quad 0,y,\frac{1}{6}$

International Tables – example (pag. 2)

Paolo
Fornasini
Univ. Trento

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=3n$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{2}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	
						Special: no extra conditions
3	b	. 2 .	$x,0,\frac{5}{6}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a	. 2 .	$x,0,\frac{1}{3}$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p\,3\,1\,m$	Along [100] $p\,2$	Along [210] $p\,1\,1\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$	$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{1}{3}$	Origin at $x,\frac{1}{2}x,\frac{1}{6}$

Maximal non-isomorphic subgroups

I [2] $P3_1 1 1$ ($P3_1$, 144) 1; 2; 3

{ [3] $P121$ ($C2$, 5) 1; 4
{ [3] $P121$ ($C2$, 5) 1; 5
{ [3] $P121$ ($C2$, 5) 1; 6

IIa none

IIb [3] $H3_1 21$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_1 12$, 151)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_2 21$ ($\mathbf{c}'=2\mathbf{c}$) (154); [4] $P3_1 21$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (152); [7] $P3_1 21$ ($\mathbf{c}'=7\mathbf{c}$) (152)

Minimal non-isomorphic supergroups

I [2] $P6_1 22$ (178); [2] $P6_4 22$ (181)

II [3] $H3_1 21$ ($P3_1 12$, 151); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (150)

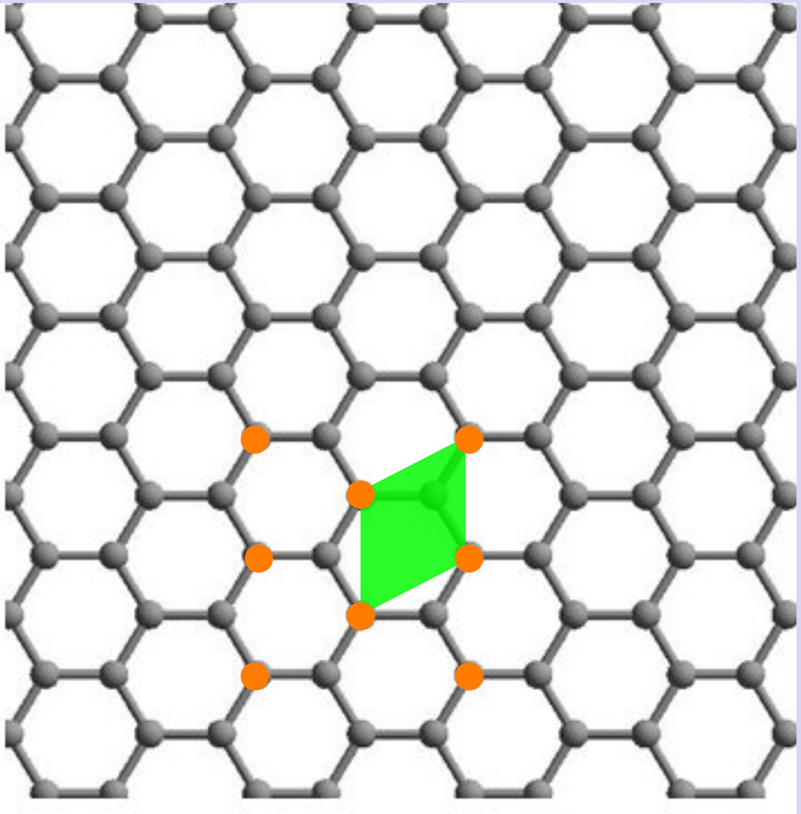
Some relevant crystal structures

Planar Graphene structure

Paolo
Fornasini
Univ. Trento

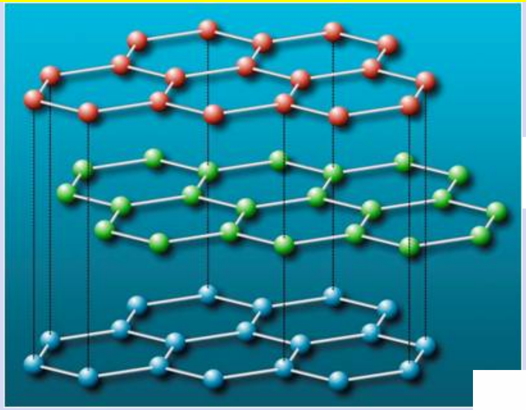
2-D

Honeycomb of C atoms, d=1.42 Å

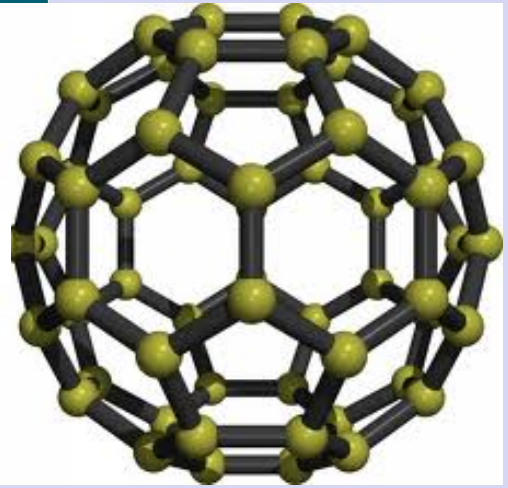


C atoms don't form a Bravais lattice

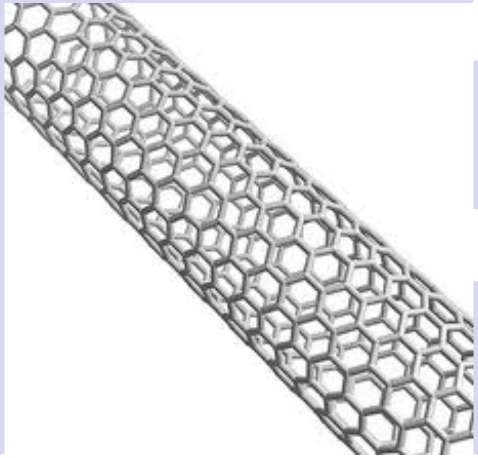
2 atoms per primitive cell



Graphite



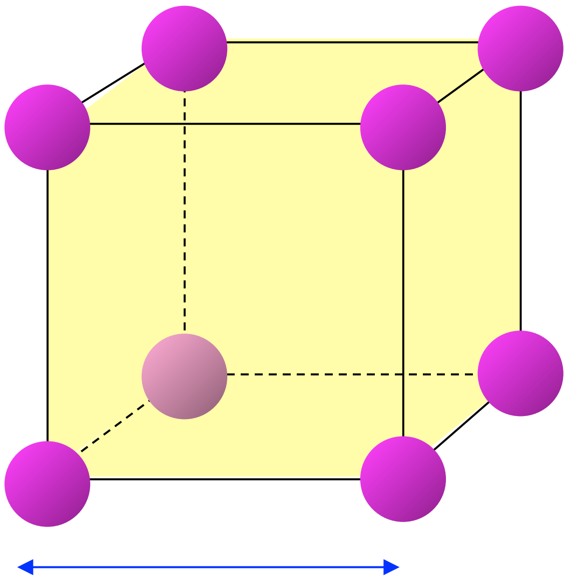
Fullerene



Nanotubes

Simple cubic lattice

Paolo
Fornasini
Univ. Trento

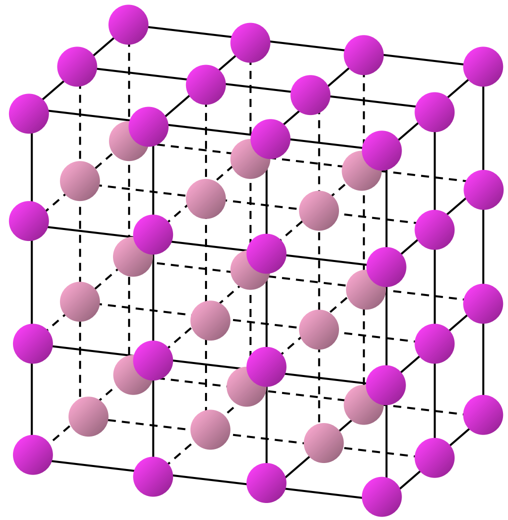


a
lattice parameter

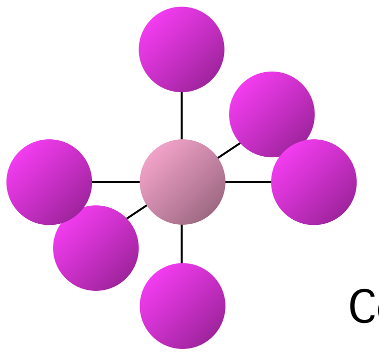
Primitive unit cell
(1 lattice point per cell)

84-Po   a=3.35 Å

Bravais crystal



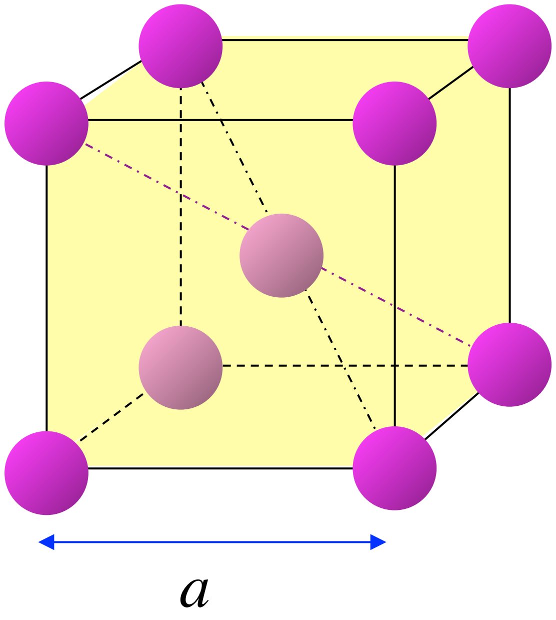
Space group: $P\,3\bar{3}m$



Coordination number = 6

Body centered cubic lattice (bcc)

Paolo
Fornasini
Univ. Trento

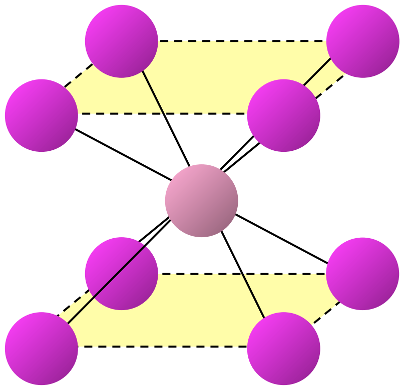


conventional unit cell
(2 lattice points per cell)

24-Cr	a=2.88 Å
26-Fe	a=2.87 Å
42-Mo	a=3.15 Å

Bravais crystal

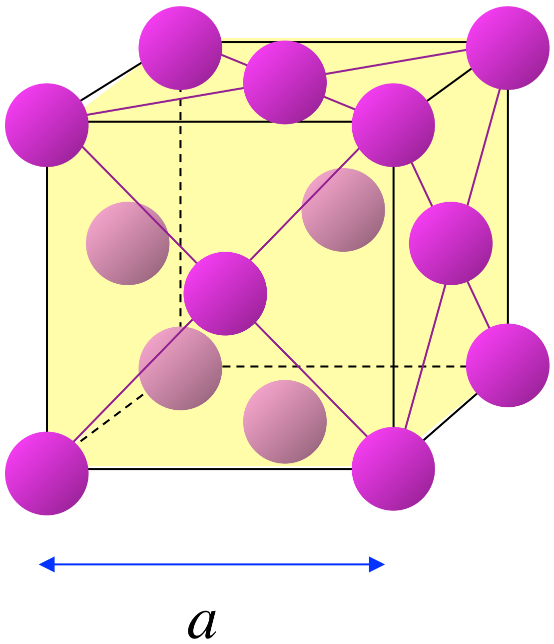
Space group: $I\,m\bar{3}m$



Coordination number = 8

Face centered cubic lattice (fcc)

Paolo
Fornasini
Univ. Trento

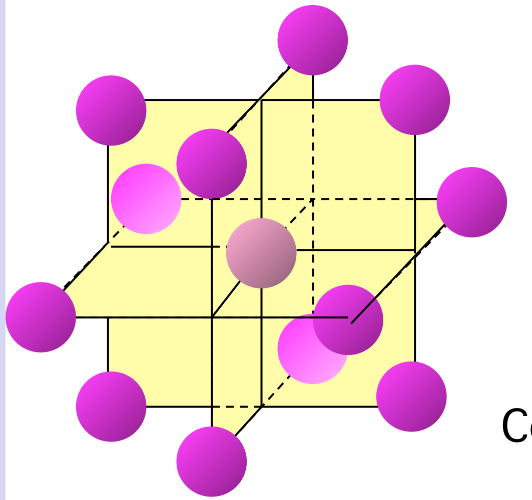


conventional unit cell
(4 lattice points per cell)

29-Cu	a=3.61 Å
47-Ag	a=4.09 Å
79-Au	a=4.08 Å

Bravais crystal

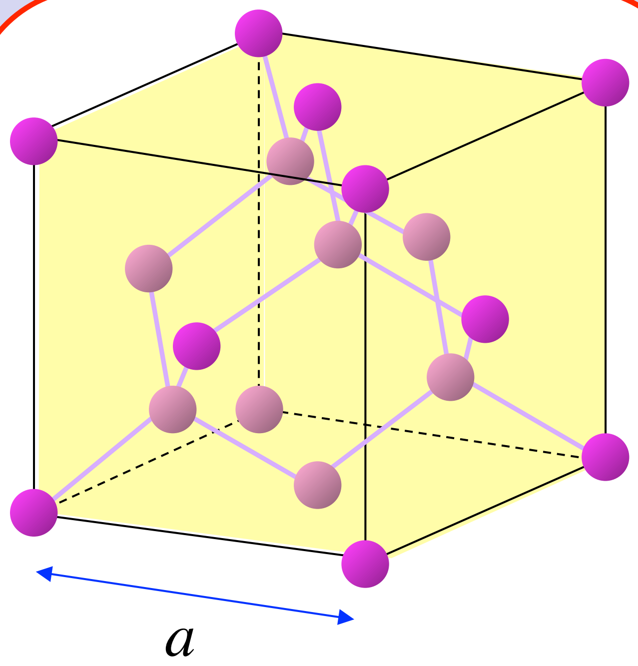
Space group: $F\, m\bar{3}m$



Coordination number = 12

Diamond structure

Paolo
Fornasini
Univ. Trento

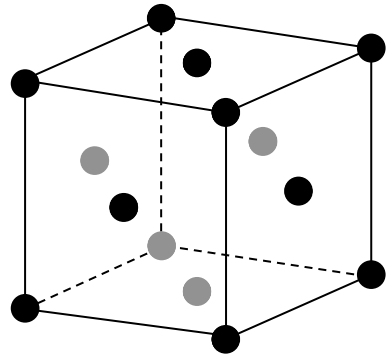


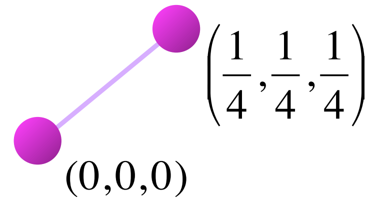
conventional unit cell
(8 atoms per cell)

6-C	a=3.57 Å
14-Si	a=5.43 Å
32-Ge	a=5.66 Å

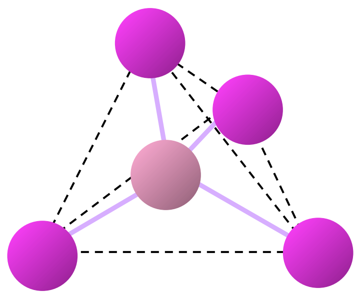
Non-Bravais crystal

fcc Bravais lattice + 2-atom basis





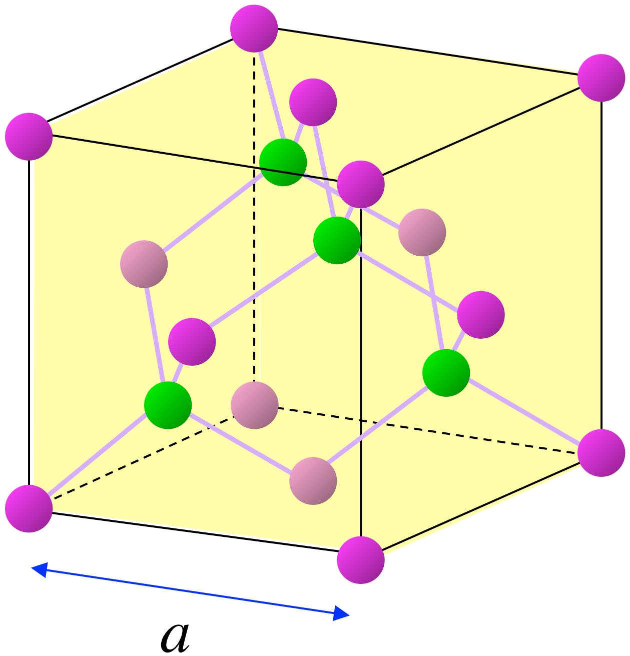
Space group: $F\,d\bar{3}m$



Coordination number = 4

Zincblende (sphalerite) structure

Paolo
Fornasini
Univ. Trento

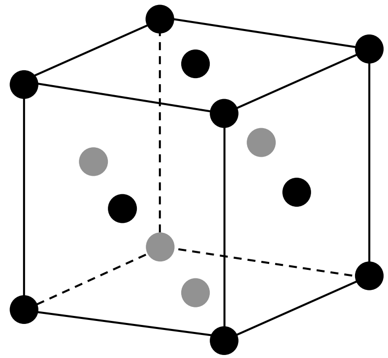


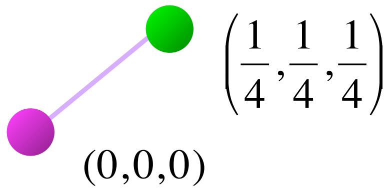
conventional unit cell
(8 atoms per cell)

ZnS	a=5.41 Å
GaAs	a=5.65 Å
SiC	a=4.35 Å

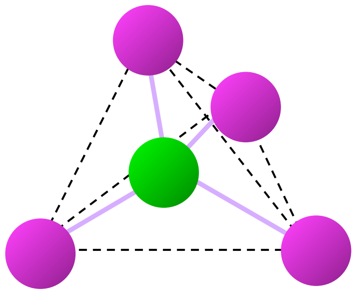
Non-Bravais crystal

fcc Bravais lattice + 2-atom basis





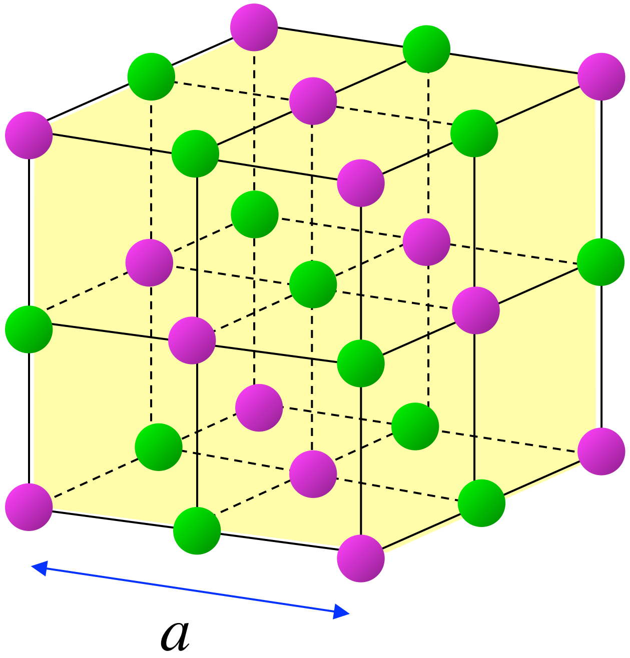
Space group: $F\bar{4}3m$ (different from diamond)



Cordination number = 4

Rock-salt (NaCl) structure

Paolo
Fornasini
Univ. Trento

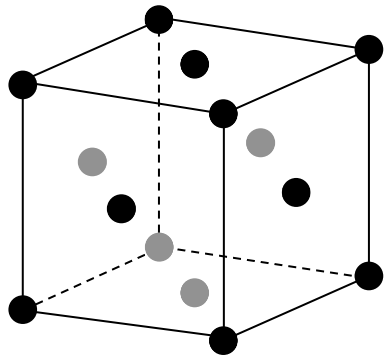


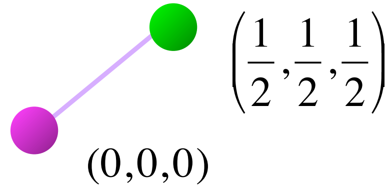
conventional unit cell
(8 atoms per cell)

NaCl	a=5.64 Å
KBr	a=6.60 Å
CaO	a=4.81 Å

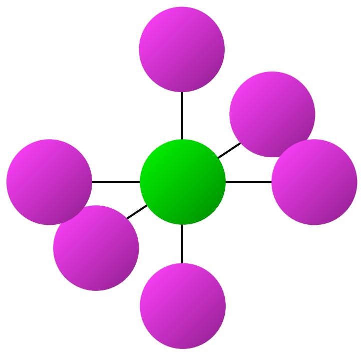
Non-Bravais crystal

fcc Bravais lattice + 2-atom basis





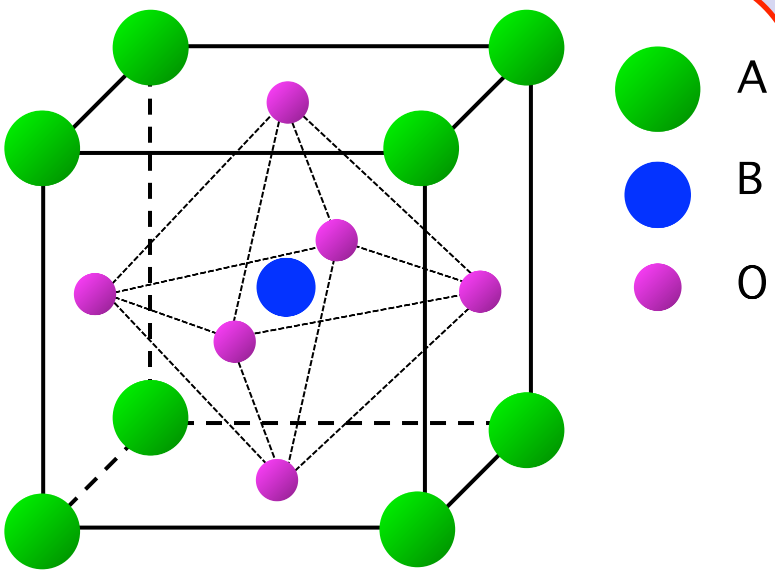
Space group: $F\,m\bar{3}m$ (same as for fcc)



Cordination number = 6

Perovskite (ideal) structure

Paolo
Fornasini
Univ. Trento



sc Bravais lattice

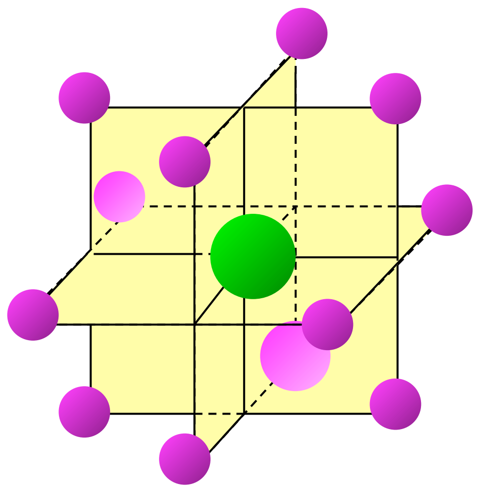
Space group: $P\,m\bar{3}m$

(high-T undistorted structure)

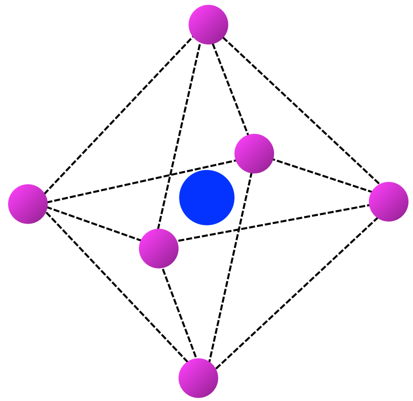
ABO_3

$CaTiO_3$ (perovskite)

$BaTiO_3$



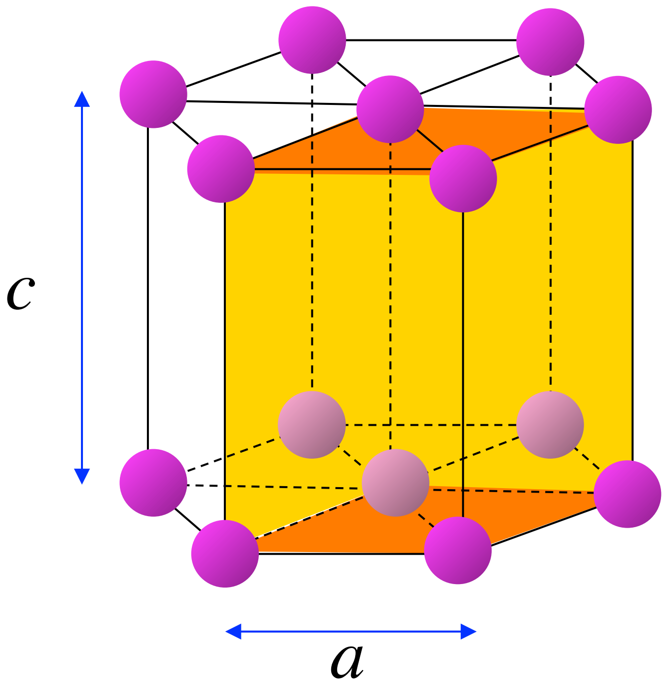
C.N. = 12



C.N. = 6
[octahedral]

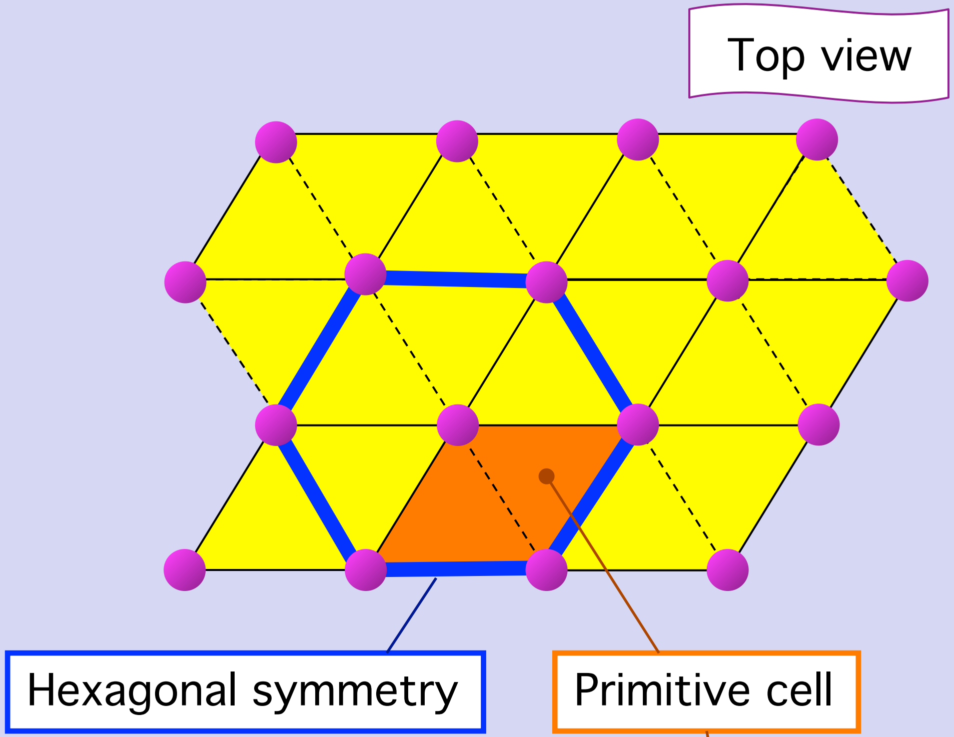
Simple hexagonal structure

Paolo
Fornasini
Univ. Trento

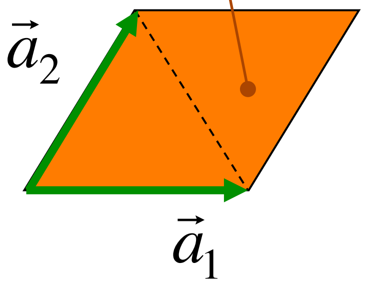


2 lattice parameters

Primitive unit cell
(1 lattice point per cell)

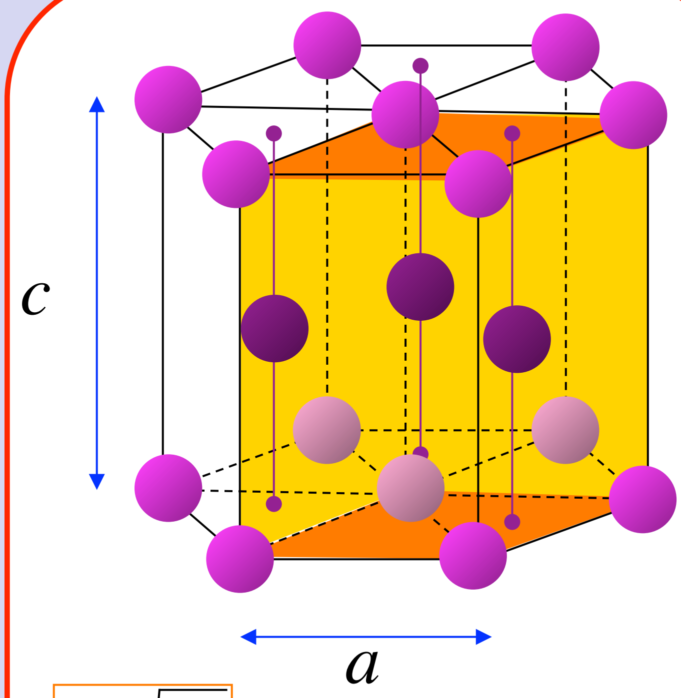


$$a_1 = a_2$$



Hexagonal close packed structure

Paolo
Fornasini
Univ. Trento



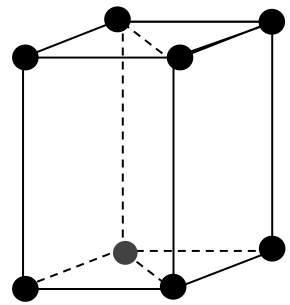
$$c = \sqrt{\frac{8}{3}}\,a$$

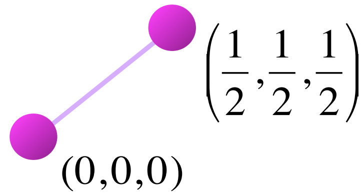
Conventional unit cell
(2 atoms per cell)

4-Be	a=2.29 Å
12-Mg	a=3.21 Å
48-Cd	a=2.98 Å

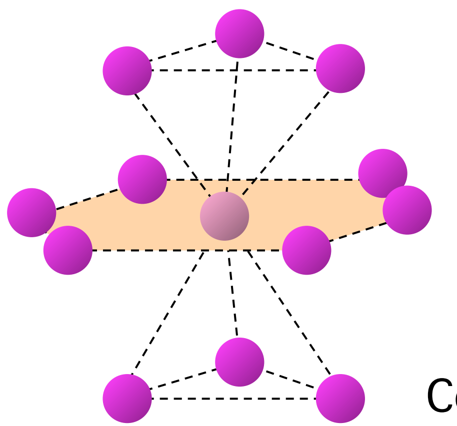
Non-Bravais lattice

primitive cell + 2-atom basis





Space group: $P\,6_3\,/\,mmc$

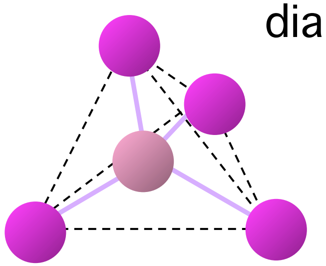


Cordination number = 12

Coordination number

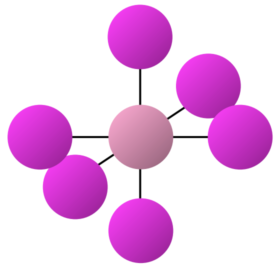
Paolo
Fornasini
Univ. Trento

diamond



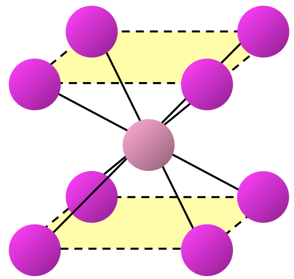
N=4

cubic



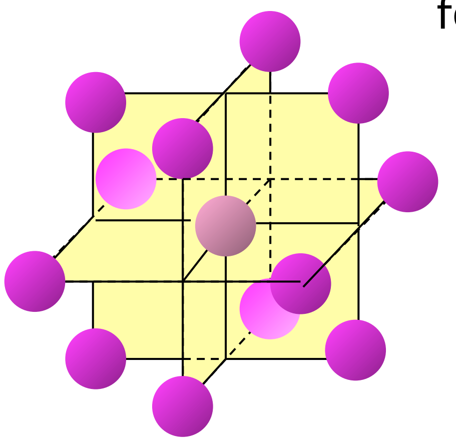
N=6

bcc

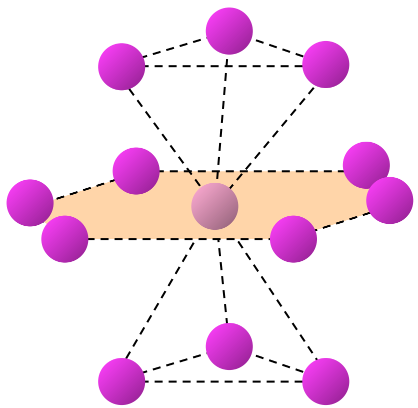


N=8

fcc



hcp



N=12

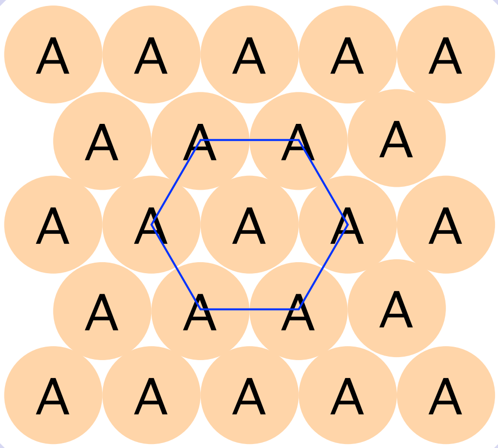
Close packing

Close-packing

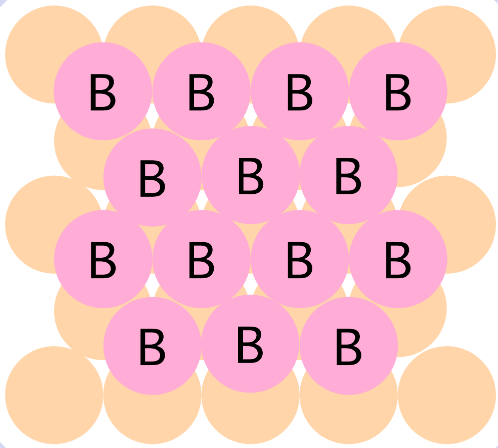
Close-packing of spheres in crystals

Paolo
Fornasini
Univ. Trento

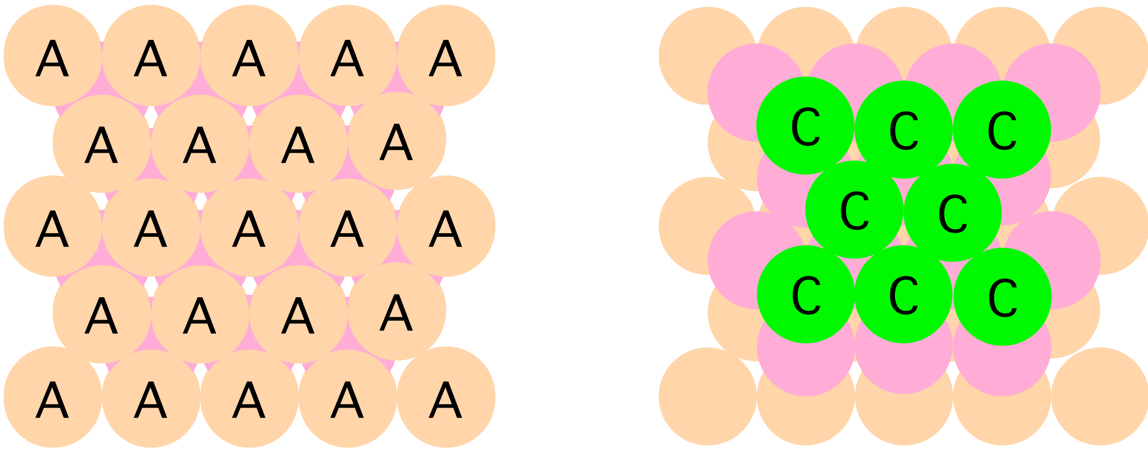
1st layer



2nd layer



3rd layer

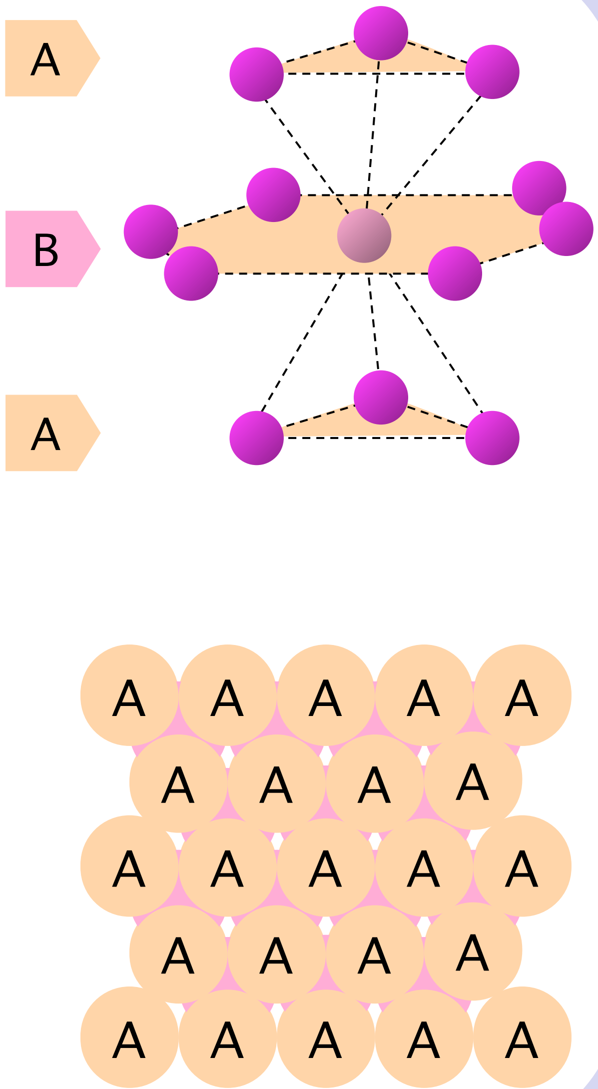


A B A

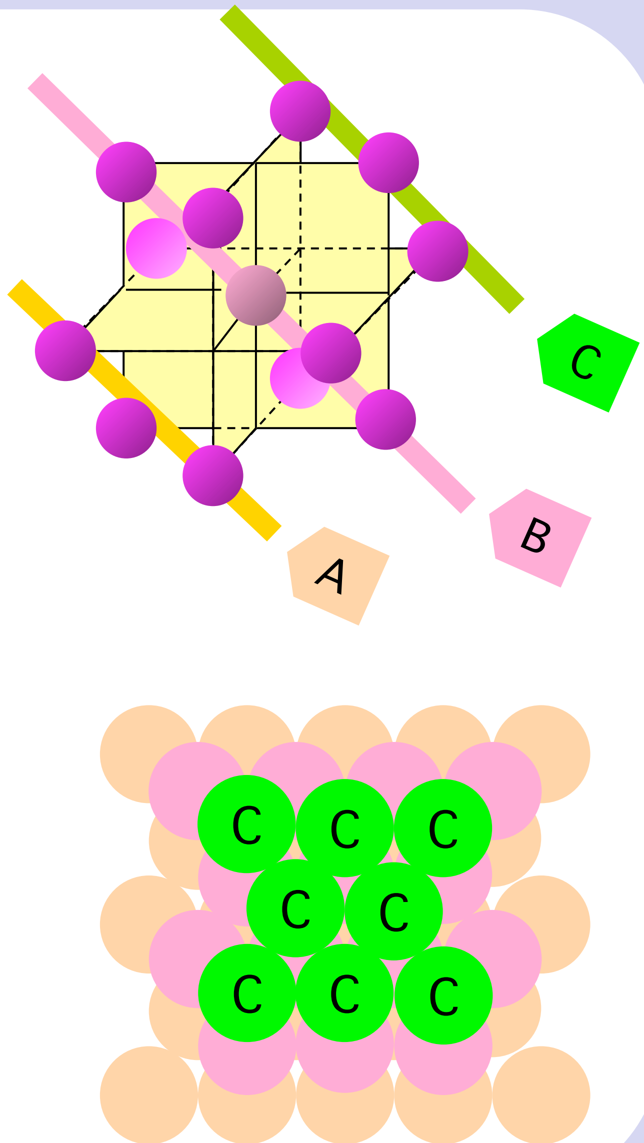
A B C

hcp versus fcc

Paolo
Fornasini
Univ. Trento



hcp

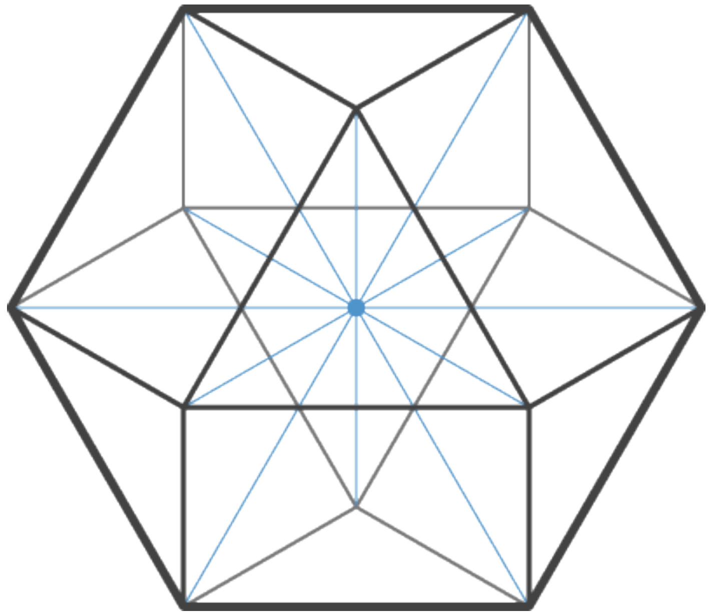


fcc

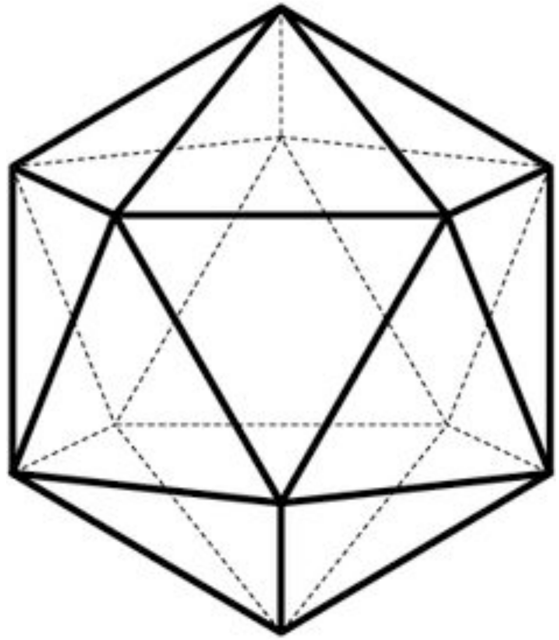
Close-packing - general

Paolo
Fornasini
Univ. Trento

Central atom surrounded by 12 nearest-neighbours



Cuboctahedron



Icosahedron

fcc and hcp

Lower surface energy – but:
incompatible with translational symmetryd