Elements of crystallography

Prof. Antoine GUITTON

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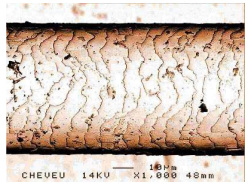
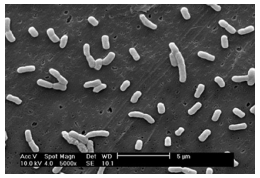
antoine.guitton@univ-Lorraine.fr

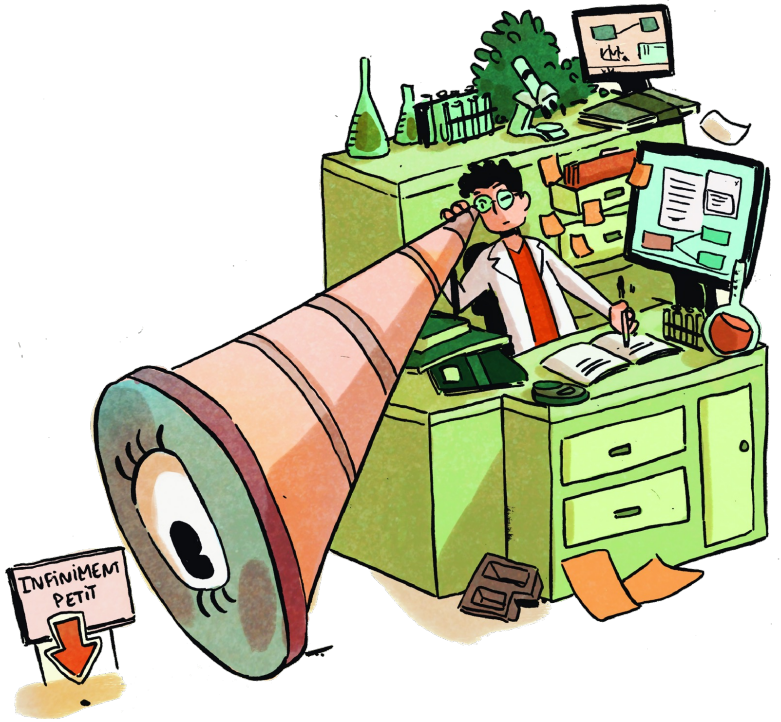
Some orders of magnitude

- **Micrometer (1 µm = 0.000001 m = 10^{-6} m)**





- Hair diameter = 50-100 µm
- Size of a bacteria = 0.1-10 µm



A. Guitton, Science en 4 Saisons – Hiver, *EDP Sciences (2023)*

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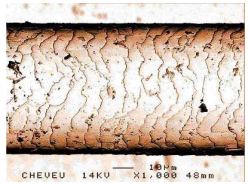

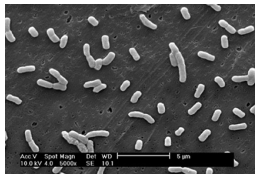

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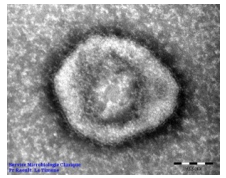

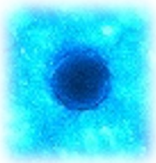

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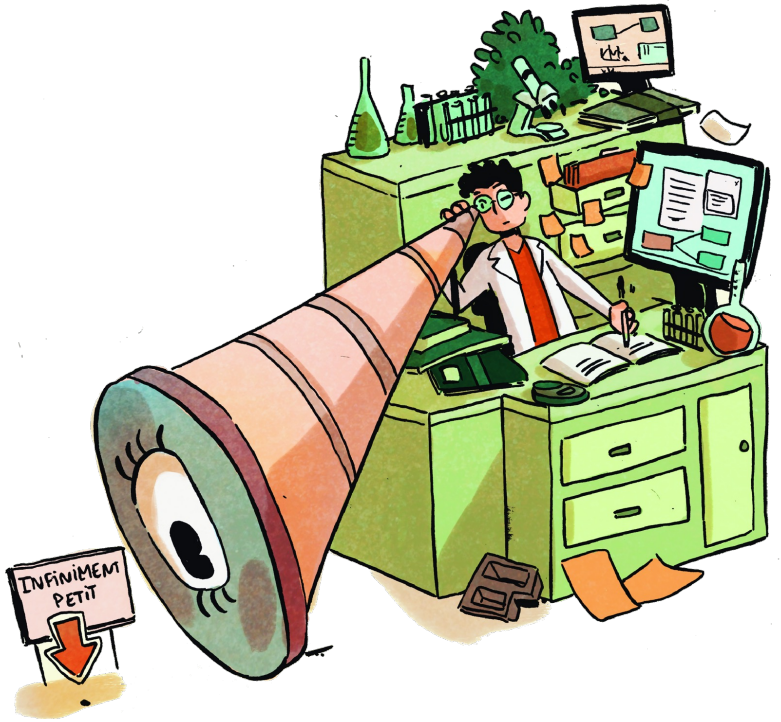

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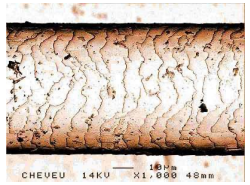

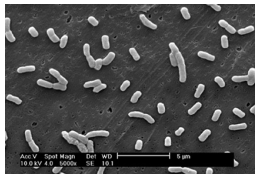

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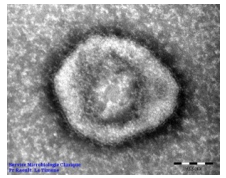

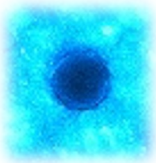

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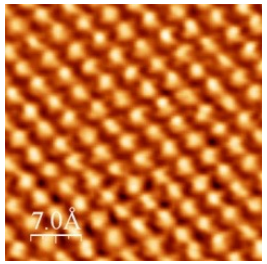

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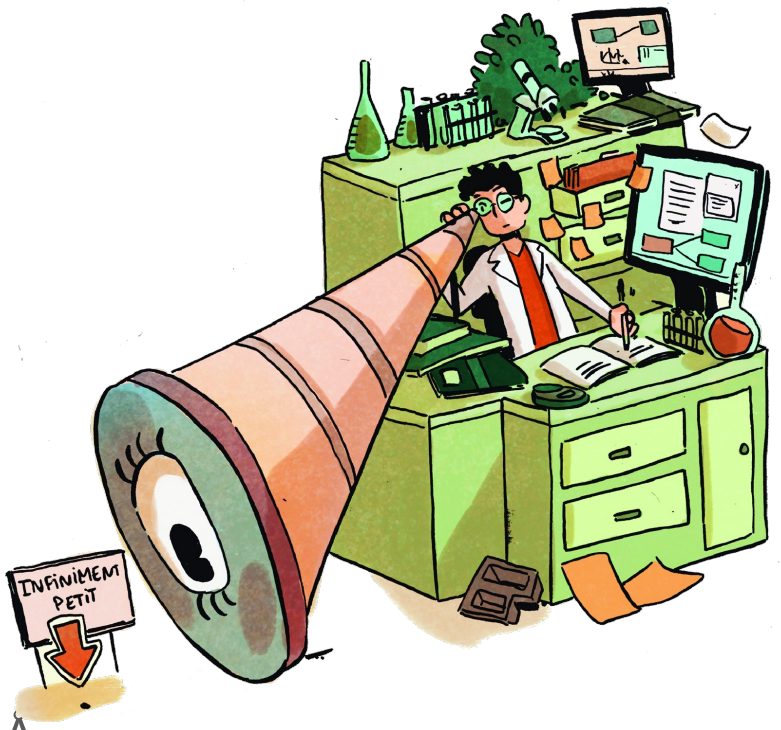

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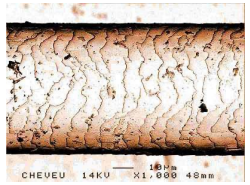

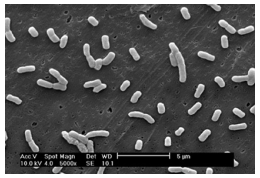

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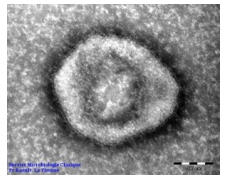

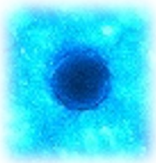

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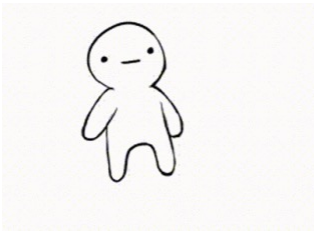

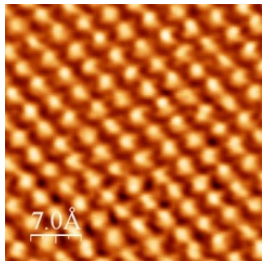

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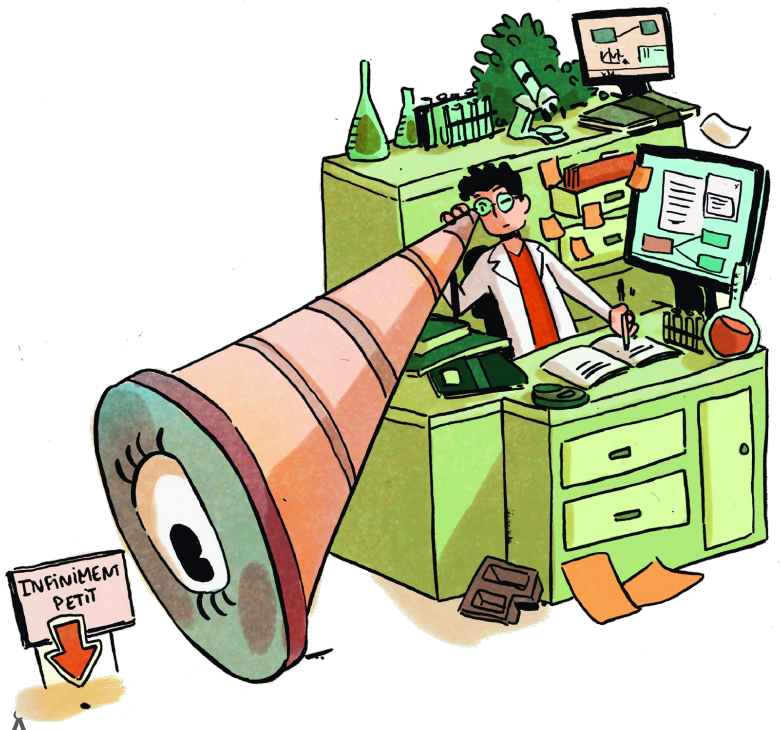

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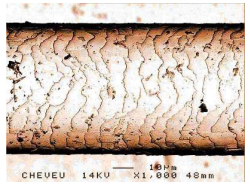

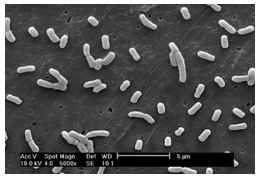

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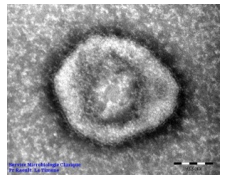

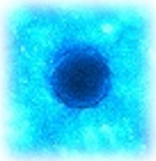

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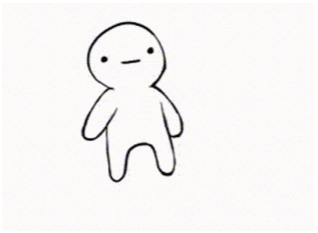

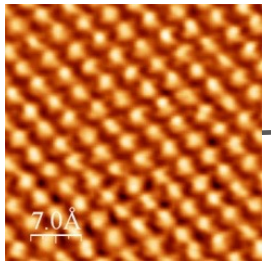

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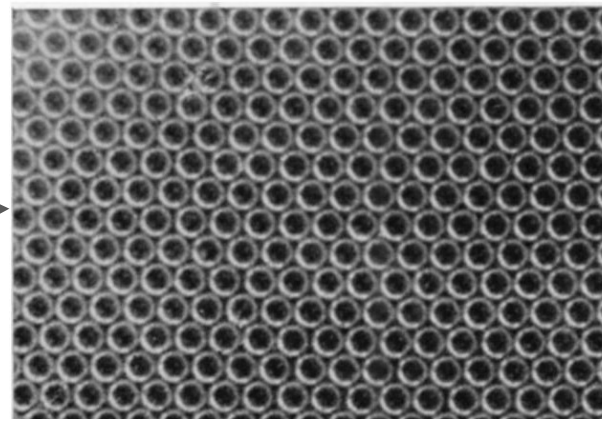
Stacking of spheres

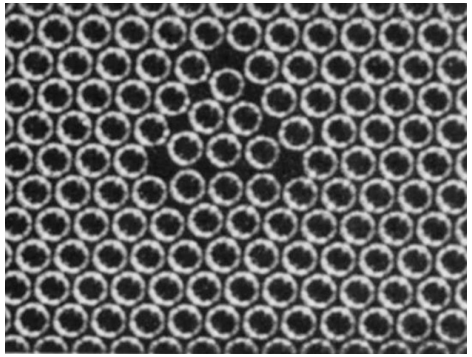
L. Bragg, J.F. Nye, *Proc. R. Soc. Lond.*, 1947



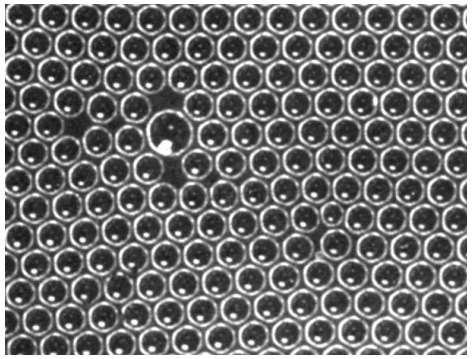
Defects in crystalline materials

0 dimension

Vacancy



Interstitial



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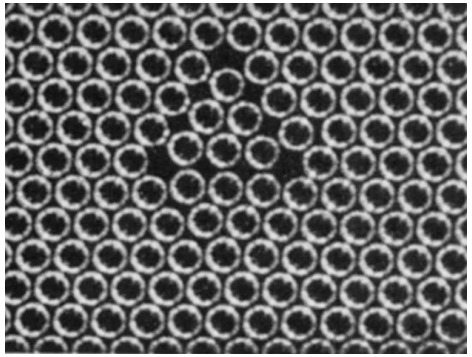

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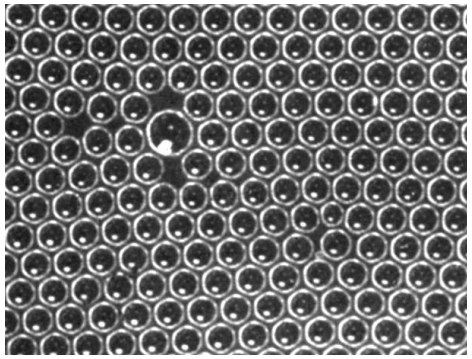
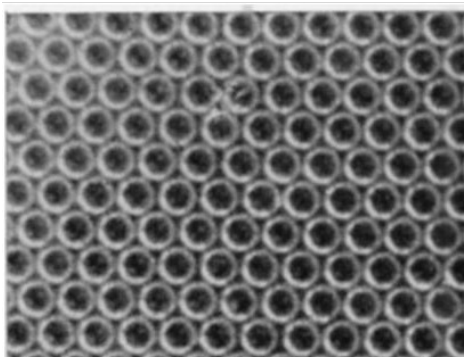


1 dimension

Dislocation



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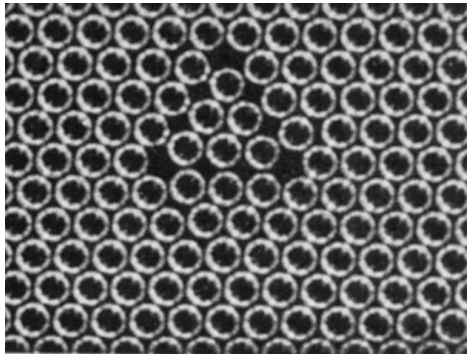

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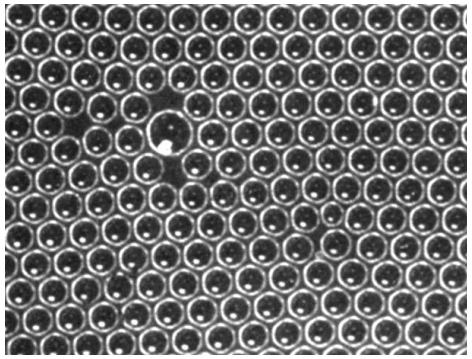

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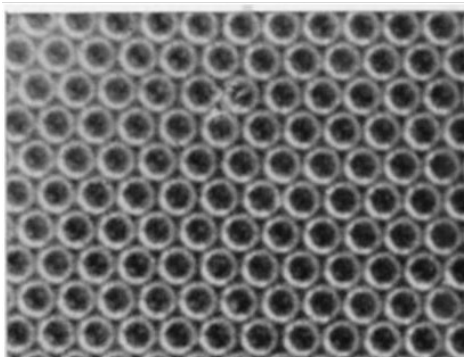
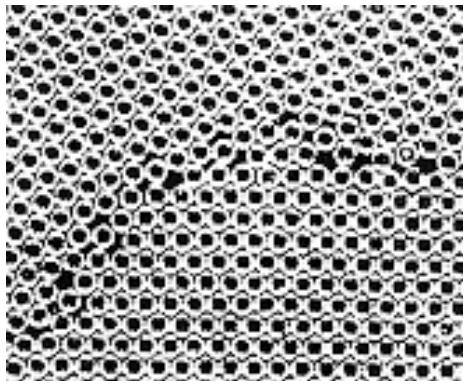


2 dimensions

Stacking fault

Grain boundaries



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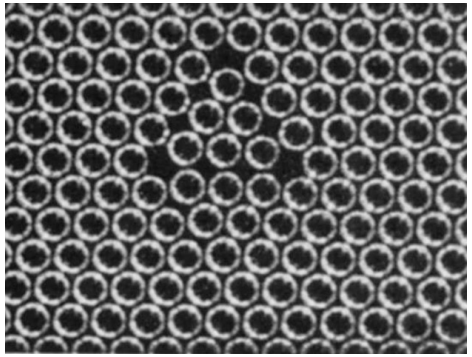

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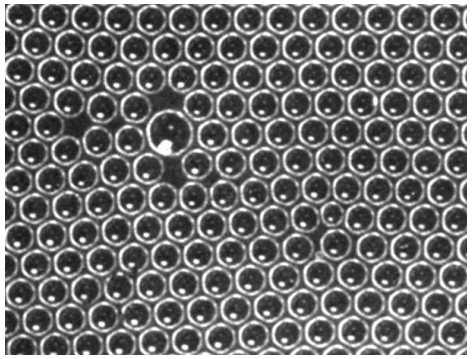

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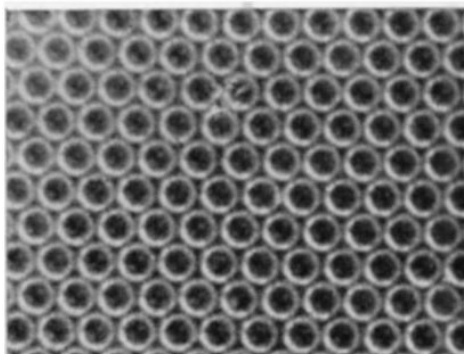

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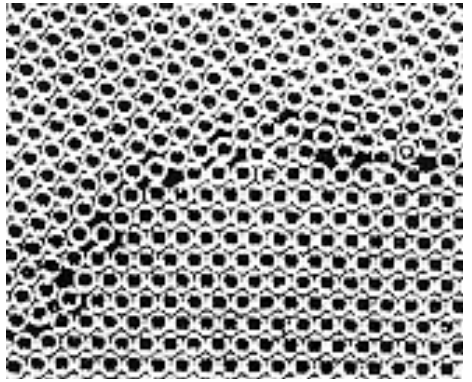

3 dimensions

Inclusions, precipitates…

"Crystals are like people; it is the defects in them which tend to make them interesting!"
(Colin J. Humphreys)

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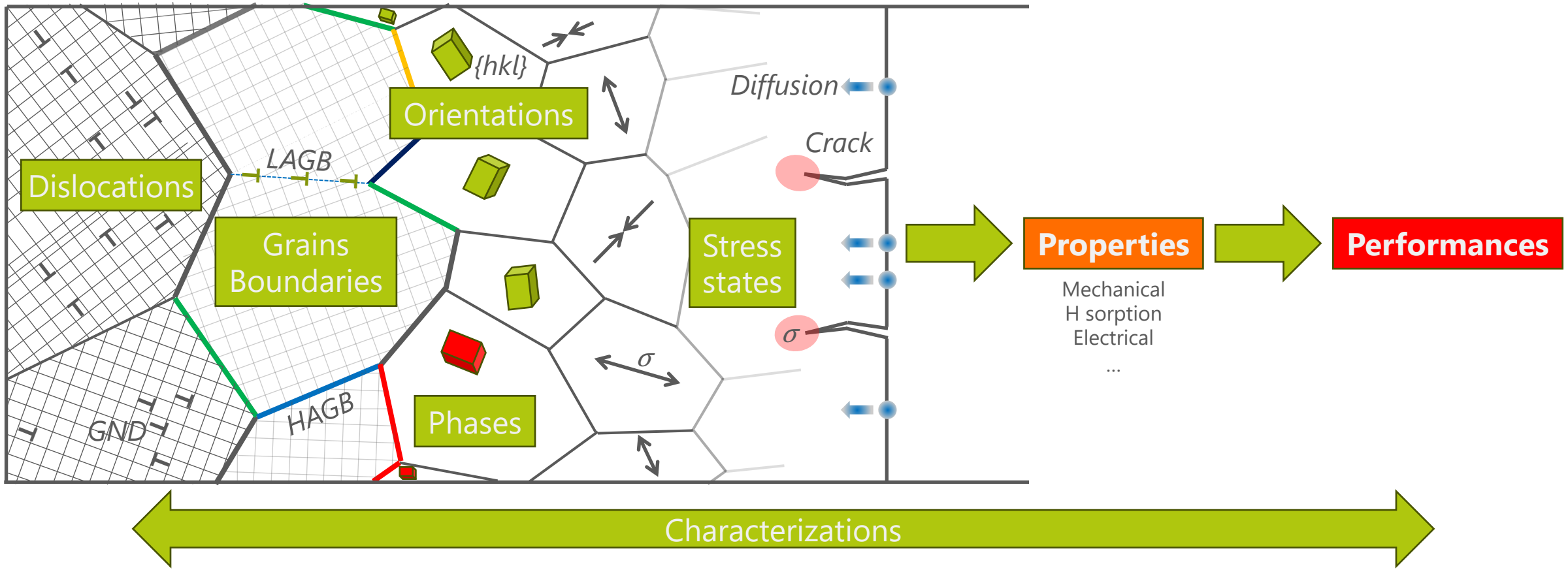
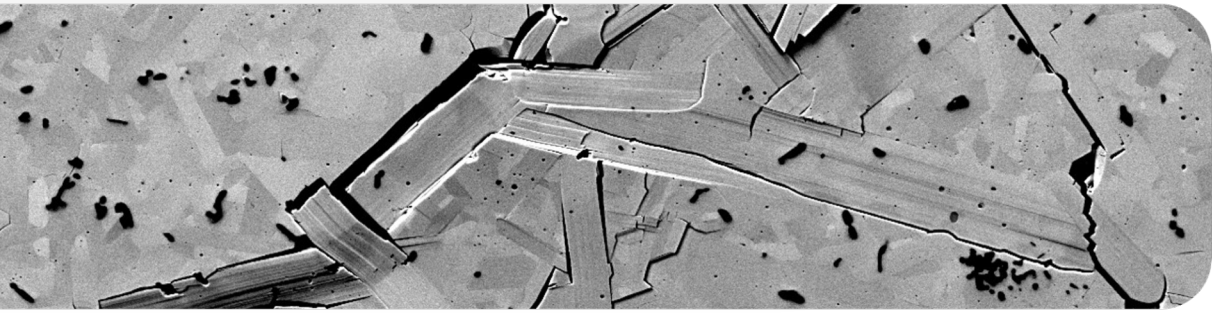
Micro-/nano-structures

Microstructure (~1 µm →1 mm) and nanostructure (~1 nm →100 nm) refer to the internal features of a material, at the micrometer and nanometer scales respectively, influencing its properties





Crystallographic structures without the “help” of mathematicians

Lattices and Bravais types

- **Lattice:**
  - A lattice is a set of points generated by translations of a basis:

    $$\mathcal{L} = \{\boldsymbol{\mathcal{R}} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2} + n_3\boldsymbol{a_3} \mid n_i \in \mathbb{Z}\}$$

  - Infinite, periodic, and translationally invariant.

A. Bravais, *J. École Polytech.* 19, 1–128 (1850)

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- **Unit cell:**
  - The fundamental repeating unit of a lattice, defined by vectors $\boldsymbol{a_1}$, $\boldsymbol{a_2}$ and $\boldsymbol{a_3} \Rightarrow \boldsymbol{\mathcal{C}} = (\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3})$.
  - Volume:
    $$V = \|\boldsymbol{a_1} \cdot (\boldsymbol{a_2} \times \boldsymbol{a_3})\|$$

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- **The centering types:**
  - It describes how many lattice points are placed within a unit cell:
    - Primitive (P): only at corners
    - Body-centered (I): one point at the center
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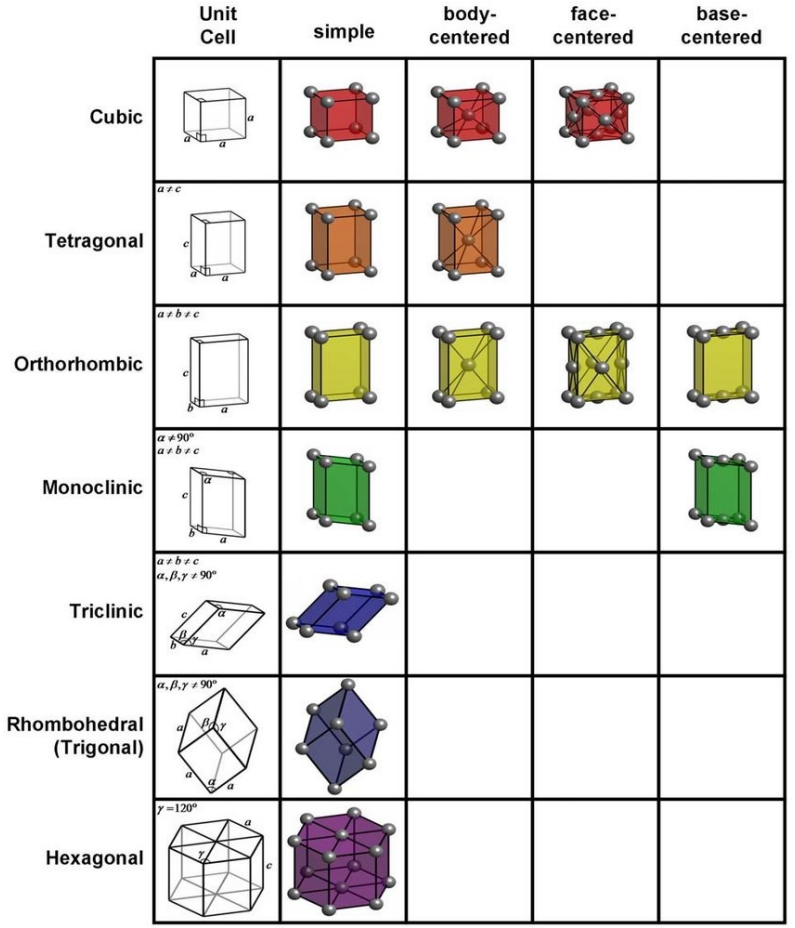
- **Bravais lattice:**
  - It is a distinct class of lattice that can fill all 3D space by translation alone, such that every lattice point is equivalent.
  - There are exactly 14 Bravais lattices in 3D. Any other lattice can be reduced to one of them by translation, rotation, or a change of unit cell.



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Distribution of crystalline materials by crystal system

System	Common Examples
Cubic	Fe, Al, NaCl
Hexagonal	Mg, Zn, Graphite
Tetragonal	Sn (β), TiO_2 (rutile)
Orthorhombic	Sulfur, $CaSO_4$
Monoclinic	$KAl(SO_4)_2 \cdot 12H_2O$, Glucose
Trigonal	Quartz α, Calcite, Bi
Triclinic	$CuSO_4 \cdot 5H_2O$, $K_2Cr_2O_7$

Distribution of crystalline materials by crystal system

System	Common Examples
Cubic	Fe, Al, NaCl
Hexagonal	Mg, Zn, Graphite
Tetragonal	Sn (β), TiO_2 (rutile)
Orthorhombic	Sulfur, $CaSO_4$
Monoclinic	$KAl(SO_4)_2 \cdot 12H_2O$, Glucose
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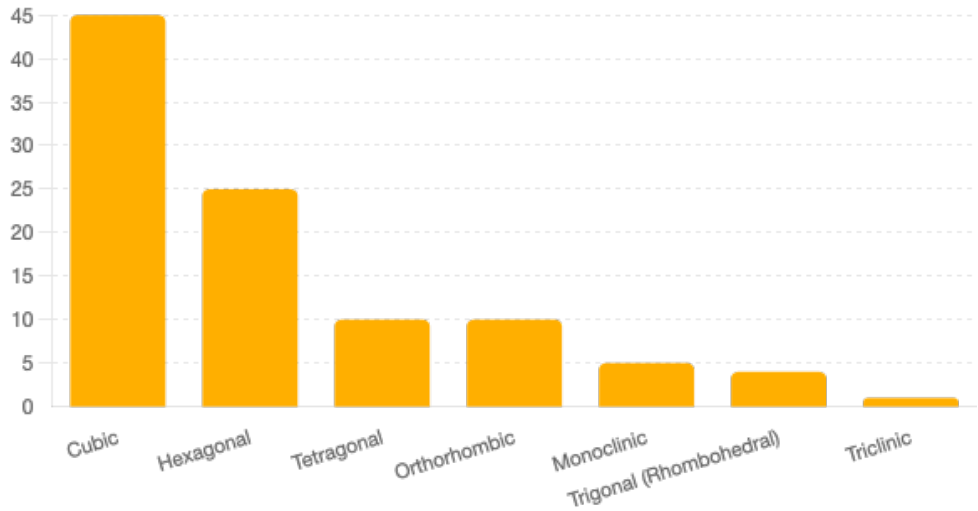

Approximate distribution based on inorganic crystal structures and common metallic and ceramic materials.
Organic compounds and minerals show different trends.

Metric tensor and lattice geometry

❖ What is the metric tensor $\mathcal{G}$?

- The metric tensor is a symmetric second-order tensor that encodes scalar products between the basis vectors $\boldsymbol{\mathcal{C}} = (\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3})$.
- It allows computation of distances, angles, and volumes even in non-orthonormal bases.

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- Volume of the unit cell

$$V = \sqrt{\det \boldsymbol{\mathcal{G}}}$$

Metric tensor and lattice geometry

❖ Metric tensor for cubic system:

- In cubic structure, $\boldsymbol{\mathcal{C}} = (\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3})$ in Cartesian coordinates $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ are:

$$\boldsymbol{a_1} = a\boldsymbol{x}\,;\boldsymbol{a_2} = a\boldsymbol{y}\,;\boldsymbol{a_3} = c\boldsymbol{z}$$

$$\boldsymbol{\mathcal{G}_{Cub}} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix} = a^2\boldsymbol{I_3}$$

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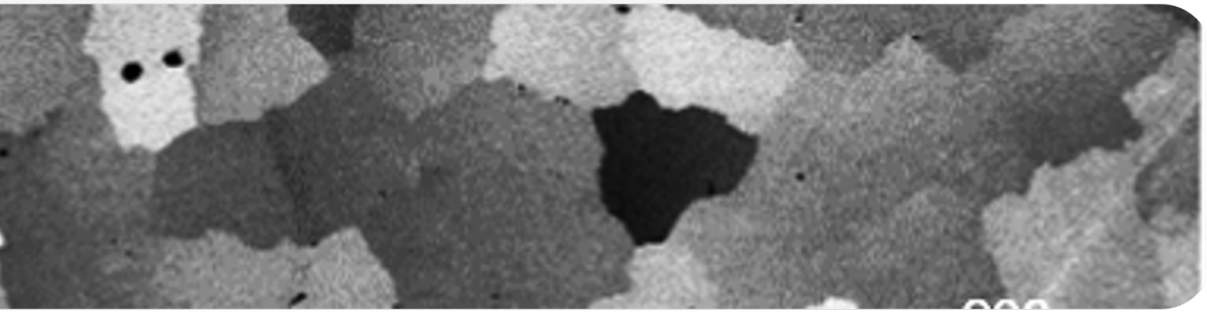
$$\boldsymbol{a_1} = a\boldsymbol{x}\,;\boldsymbol{a_2} = a\left(-\frac{1}{2}\boldsymbol{x} + \frac{\sqrt{3}}{2}\boldsymbol{y}\right);\boldsymbol{a_3} = c\boldsymbol{z}$$

$$\mathcal{G}_{Hex} = \begin{pmatrix} a^2 & -\frac{1}{2}a^2 & 0 \\ -\frac{1}{2}a^2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$$



Crystallographic structures with the “help” of mathematicians

Group theory and notation

What is a group?

- A group ($\mathfrak{G}$) is a mathematical structure consisting of a set of elements and an operation ($*$) satisfying:
  - Closure: If $a, b \in \mathfrak{G}$, then $a * b \in \mathfrak{G}$
  - Associativity: If $a, b, c \in \mathfrak{G}$, then $(a * b) * c = a * (b * c)$
  - Identity: There exists $e \in \mathfrak{G} \mid e * a = a * e = a$
  - Inverse: $\forall a \in \mathfrak{G}, \exists a^{-1} \in \mathfrak{G} \mid a * a^{-1} = e$
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Symmetry group of a crystal

- A symmetry group is the set of all symmetry operations that leave the crystal unchanged.
- These form a mathematical group under composition.
- Crystals are described by:
  - Point groups (symmetry of the shape)
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Hermann-Mauguin notation (International notation)

- A compact way to describe the symmetry elements of a crystal structure in 1D, 2D, or 3D space.

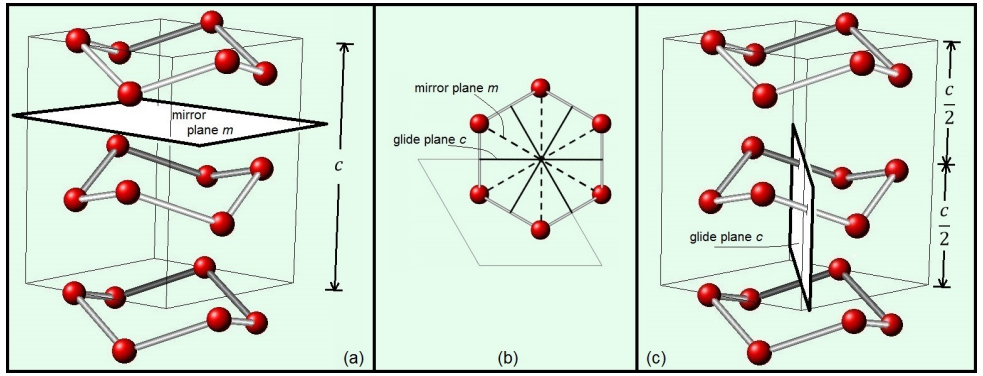
Structure of the notation

$$Ln_1n_2n_3$$

- L: lattice type
  - P = Primitive
  - I = Body-centered
  - F = Face-centered
  - A, B, C = Base-centered
  - R = Rhombohedral
- n_i: Symmetry elements along crystallographic axes
  - $1, 2, 3, 4, 6$: n-fold rotation ($\frac{360°}{n}$ rotation)
  - $\blacksquare_i$: the fractional translation along the rotation axis
  - $\bar{1}, \bar{3}, \bar{4}, \bar{6}$: rotoinversion (rotation + inversion)
  - m: mirror plane
  - n, a, b, c, d, e: glide planes

Group theory and notation

- Example: $P6_3/mmc$



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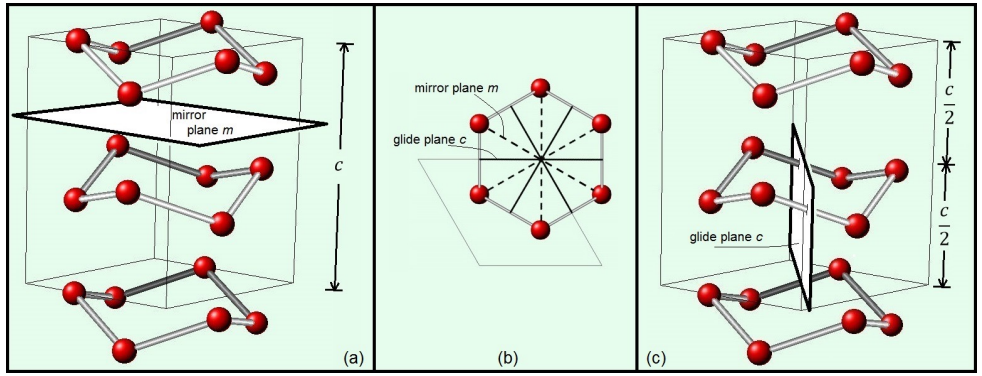

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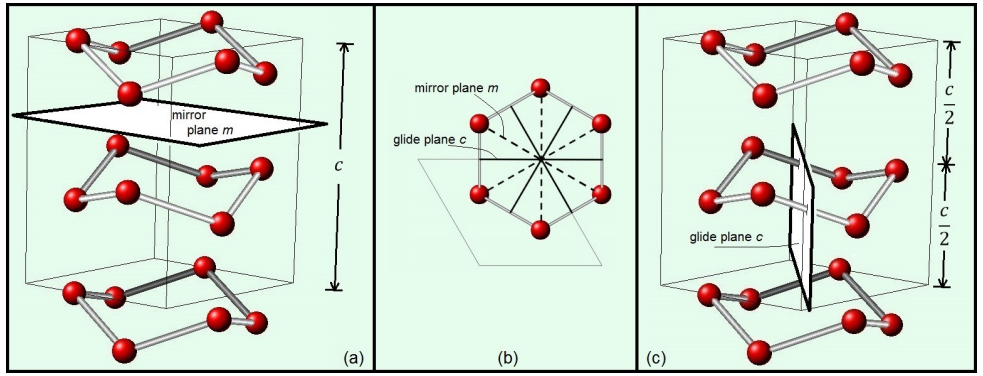
    - Followed by a translation of $\frac{3}{6} = \frac{1}{2}$ of the unit cell along the $\boldsymbol{a_3}$-axis



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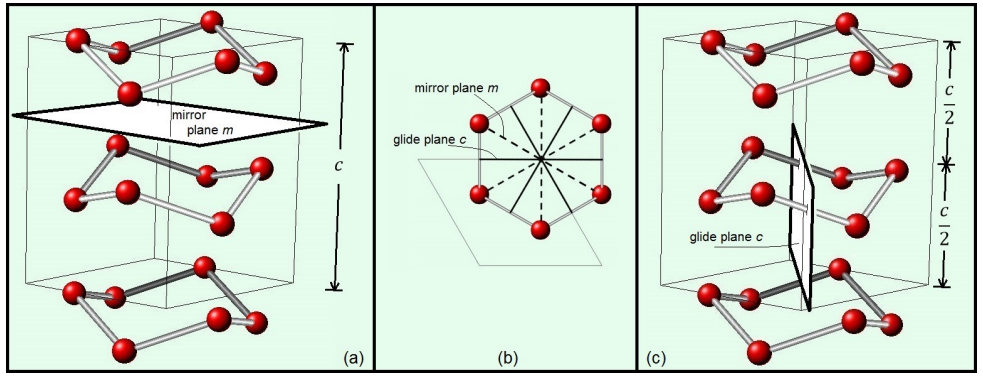
    - The slash (/) indicates this perpendicularity



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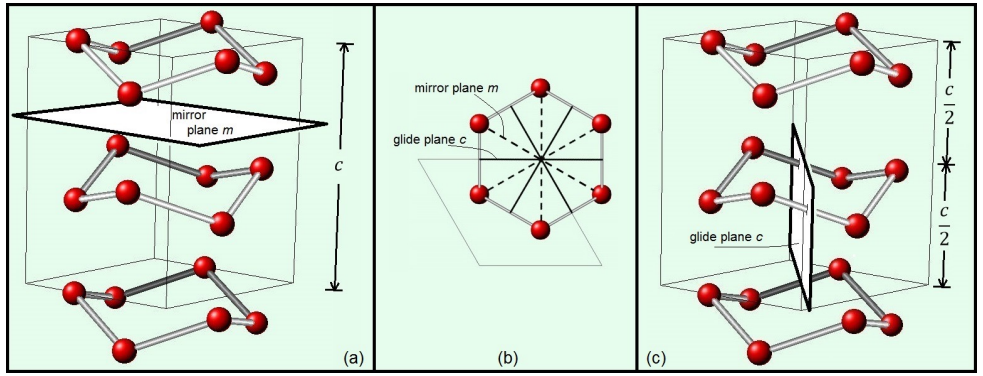
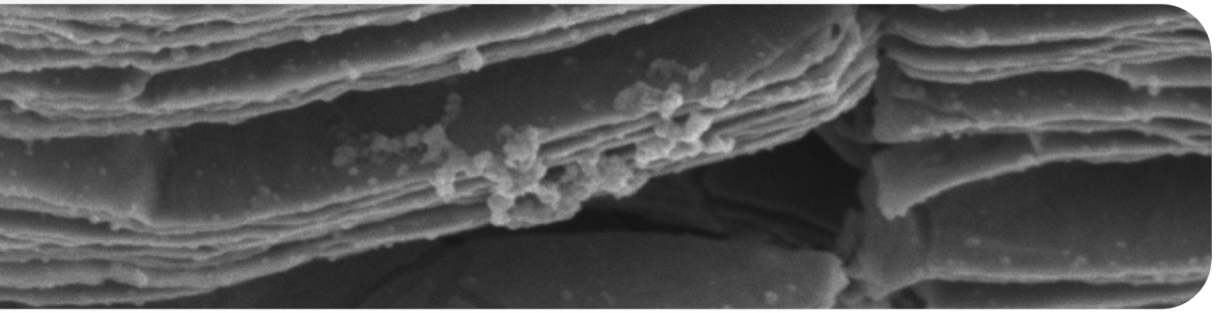
  - mc: Vertical mirror and glide planes
    - The first m indicates a vertical mirror plane, parallel to $\boldsymbol{a_3}$
    - The c denotes a glide plane:

    ⇒ A mirror operation combined with a translation of $\frac{1}{2}$ along the $\boldsymbol{a_3}$-axis

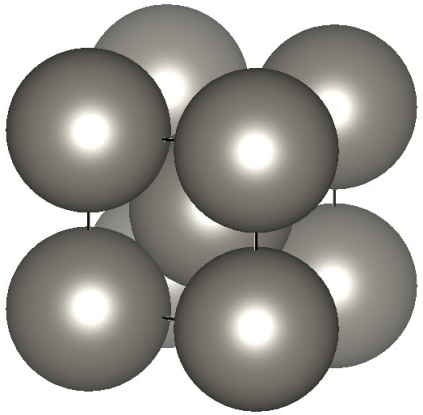


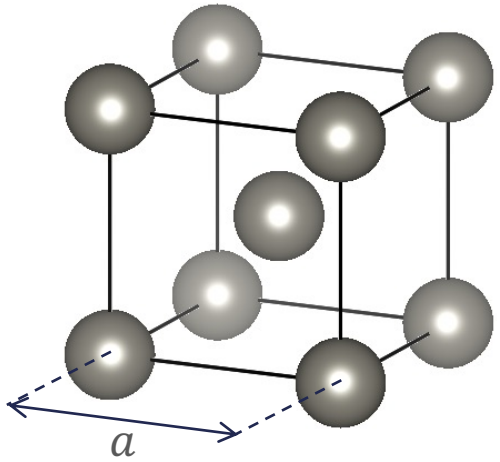


Some crystallographic structures

Body-Centered Cubic (BCC) – $Im\bar{3}m$

❖ **Geometrical description**





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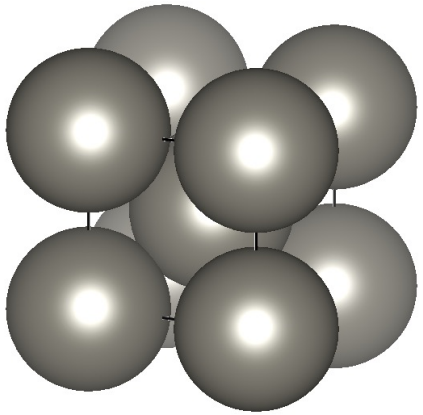

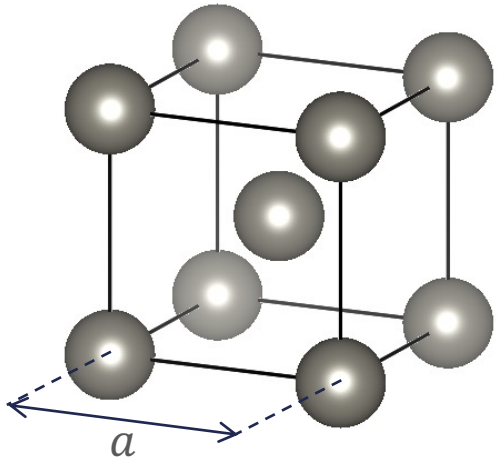

- **Geometrical description**
  - Atoms located at the 8 corners of the cube, plus 1 atom at the center of the cube.
  - The central atom is not shared with any other cell.
- **Number of atoms per unit cell**

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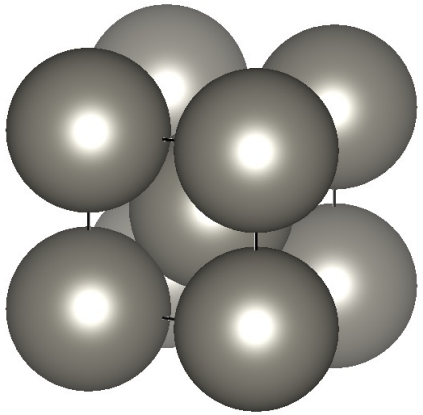

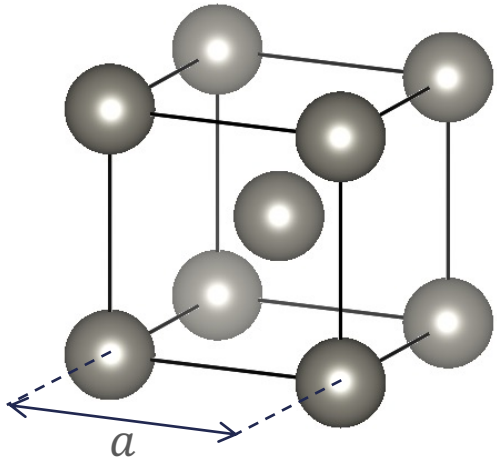

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- **Relationship between lattice parameter and atomic radius**

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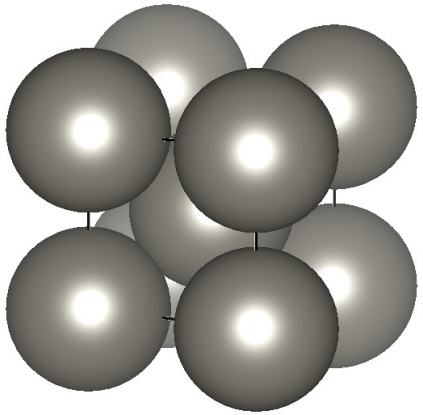

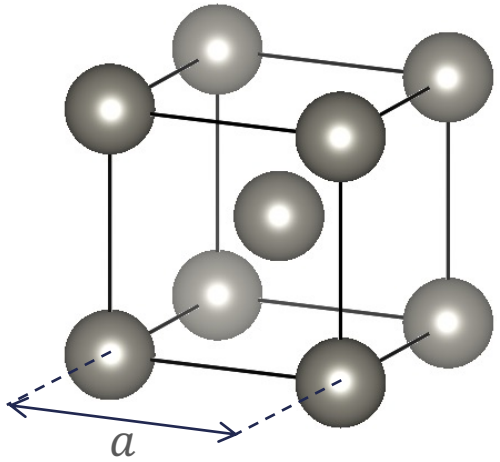

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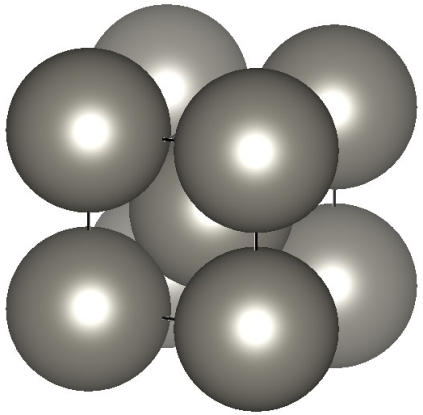

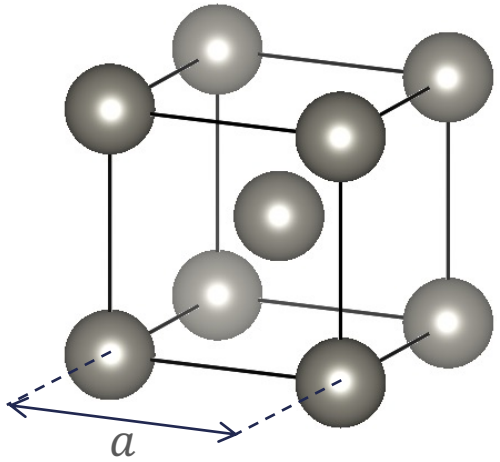

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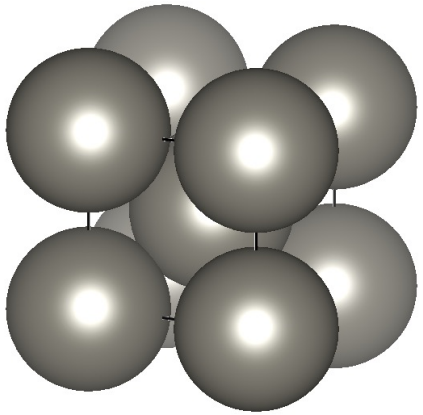

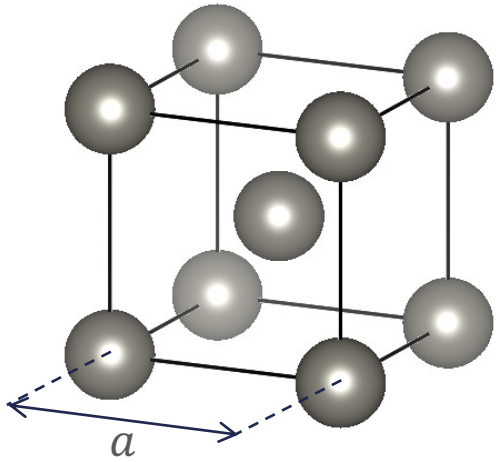

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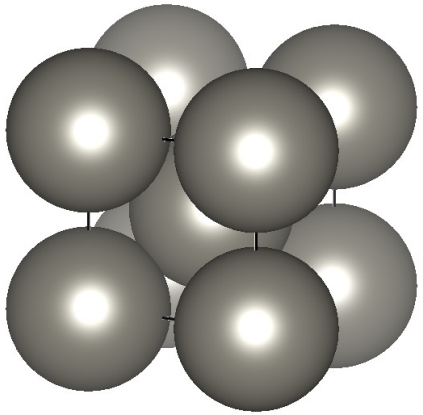
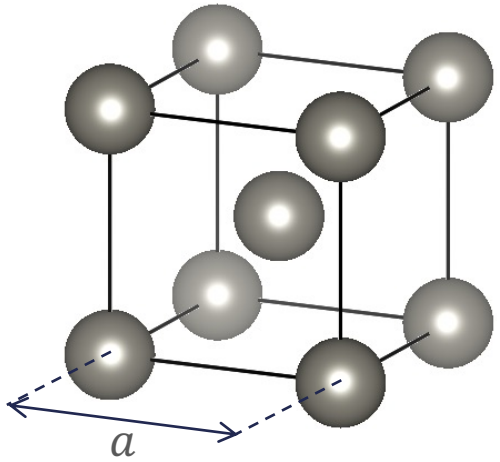
$$\eta = \frac{NV_{atom}}{V_{cell}} = \frac{\pi\sqrt{3}}{8} = 68\%$$

- **Coordination number**

Body-Centered Cubic (BCC) – $Im\bar{3}m$





- **Geometrical description**
  - Atoms located at the 8 corners of the cube, plus 1 atom at the center of the cube.
  - The central atom is not shared with any other cell.
- **Number of atoms per unit cell**

$$N = 8\times\frac{1}{8} + 1 = 2$$

- **Relationship between lattice parameter and atomic radius**
  - Atoms touch along the body diagonal:

$$4R = a\sqrt{3}$$

- **Volume of one unit cell**

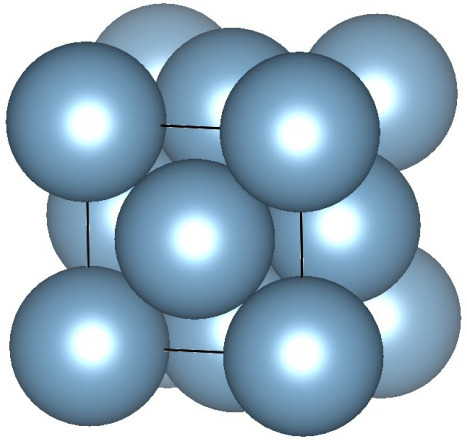
$$V_{cell} = a^3$$

- **Packing efficiency**

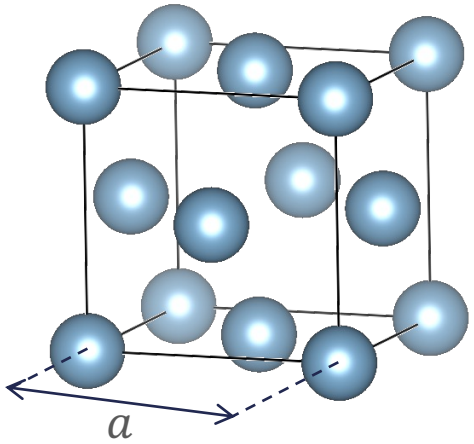
$$\eta = \frac{NV_{atom}}{V_{cell}} = \frac{\pi\sqrt{3}}{8} = 68\%$$

- **Coordination number**
  - Each atom is surrounded by 8 nearest neighbors.

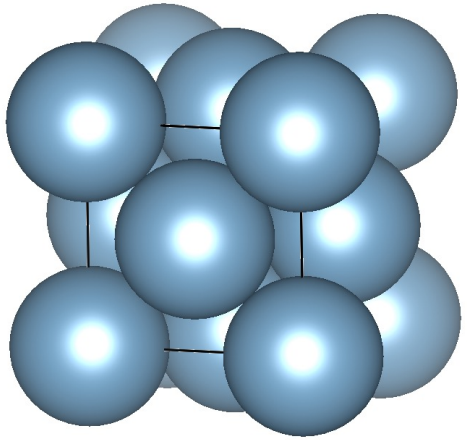
Face-Centered Cubic (FCC) – $Fm\bar{3}m$

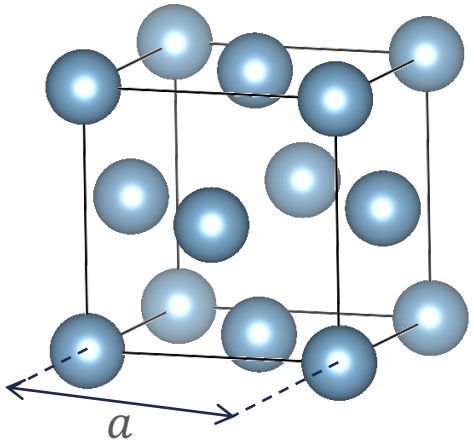


❖ **Geometrical description**



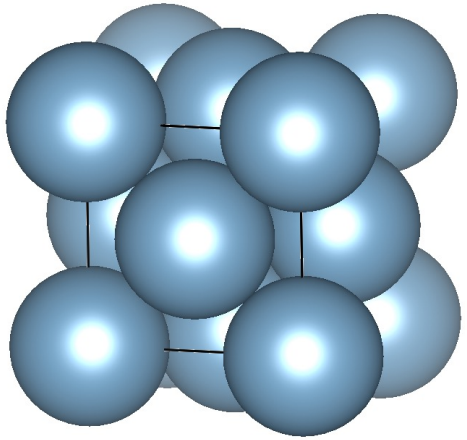
Face-Centered Cubic (FCC) – $Fm\bar{3}m$

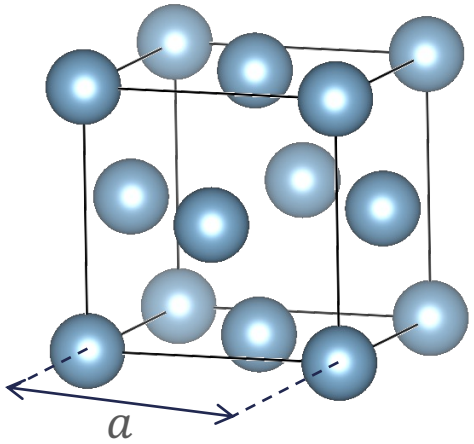




- **Geometrical description**
  - Atoms located at the 8 corners of the cube, plus 1 atom at the center of each of the 6 faces.
  - Each face-centered atom is shared between 2 adjacent unit cells.
- **Number of atoms per unit cell**

Face-Centered Cubic (FCC) – $Fm\bar{3}m$





- **Geometrical description**
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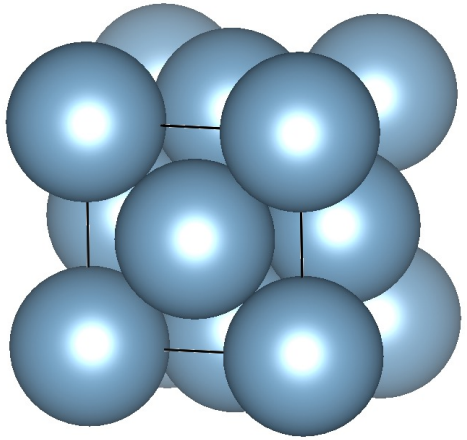
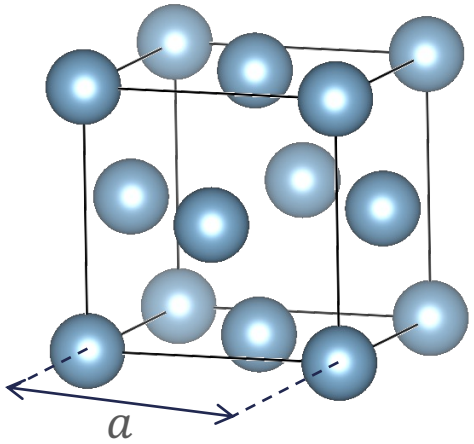
  - Each face-centered atom is shared between 2 adjacent unit cells.
- **Number of atoms per unit cell**

$$N = 8\times\frac{1}{8} + 6\times\frac{1}{2} = 4$$

- **Relationship between lattice parameter and atomic radius**

Face-Centered Cubic (FCC) – $Fm\bar{3}m$





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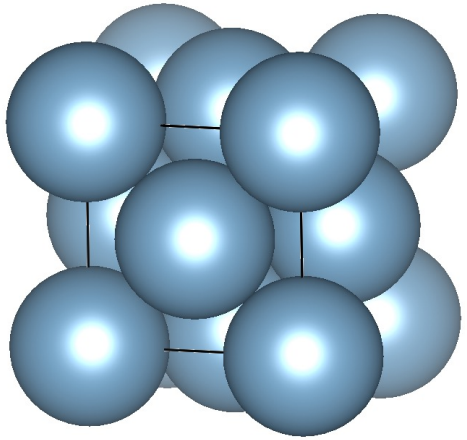
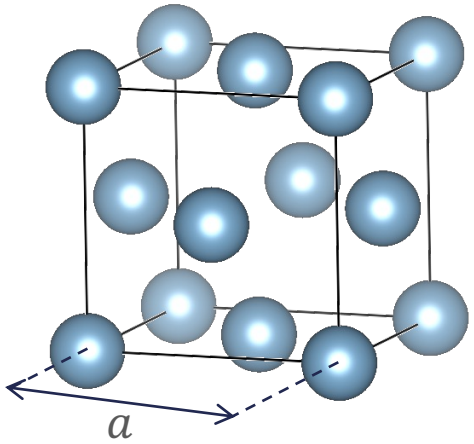
- **Relationship between lattice parameter and atomic radius**
  - Atoms touch along the face diagonal:

$$4R = a\sqrt{2}$$

- **Volume of one unit cell**

Face-Centered Cubic (FCC) – $Fm\bar{3}m$





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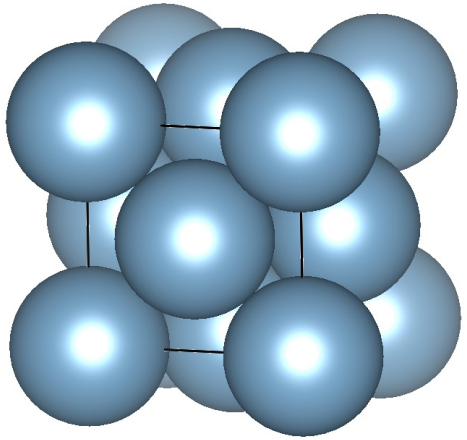
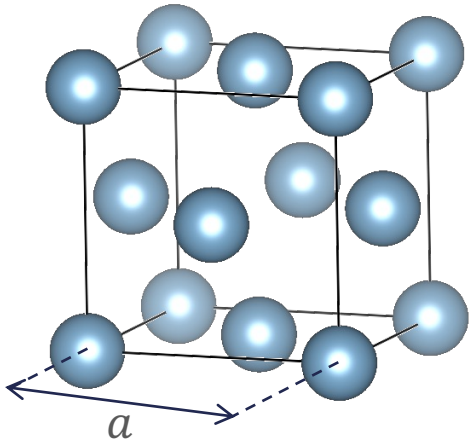
$$V_{cell} = a^3$$

- **Packing efficiency**

Face-Centered Cubic (FCC) – $Fm\bar{3}m$





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  - Each face-centered atom is shared between 2 adjacent unit cells.
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  - Atoms touch along the face diagonal:

$$4R = a\sqrt{2}$$

- **Volume of one unit cell**

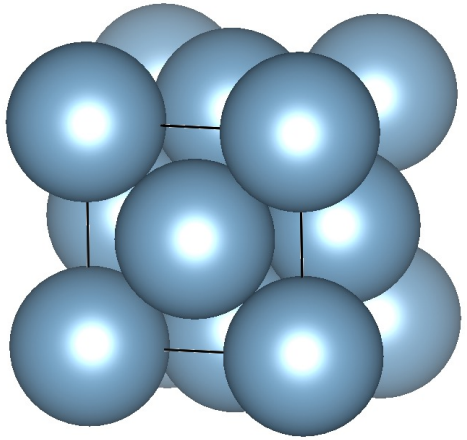
$$V_{cell} = a^3$$

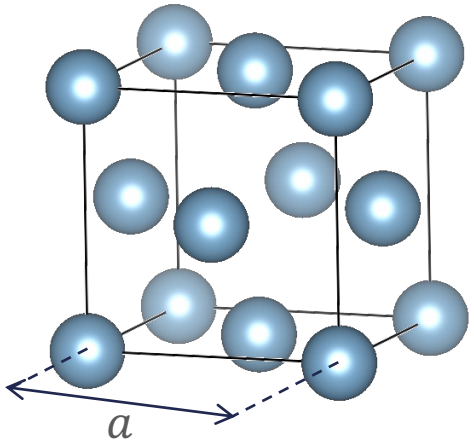
- **Packing efficiency**

$$\eta = \frac{NV_{atom}}{V_{cell}} = \frac{\pi\sqrt{2}}{6} = 74\%$$

- **Coordination number**

Face-Centered Cubic (FCC) – $Fm\bar{3}m$





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  - Atoms touch along the face diagonal:

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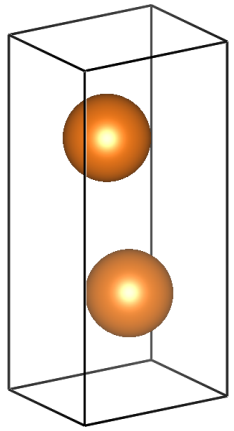
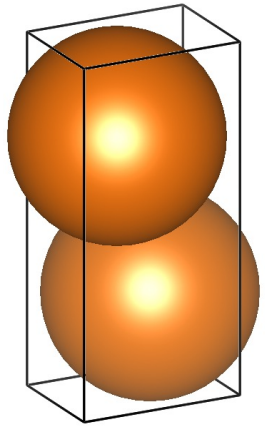
- **Packing efficiency**

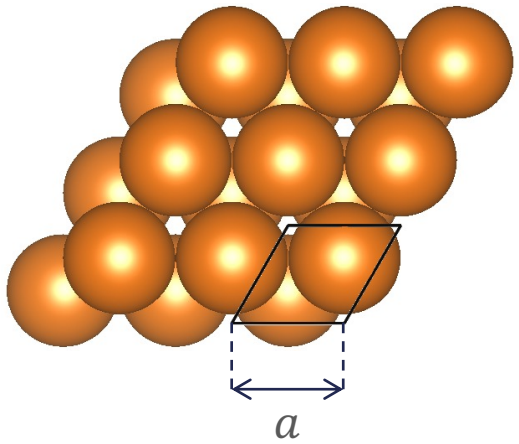
$$\eta = \frac{NV_{atom}}{V_{cell}} = \frac{\pi\sqrt{2}}{6} = 74\%$$

- **Coordination number**
  - Each atom is surrounded by 12 nearest neighbors.

Hexagonal Close Packed (HCP) – $P6_3/mmc$

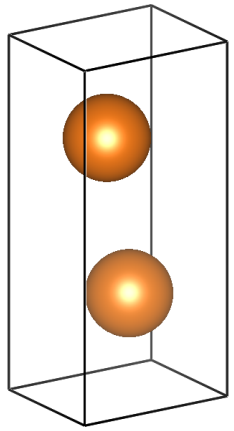


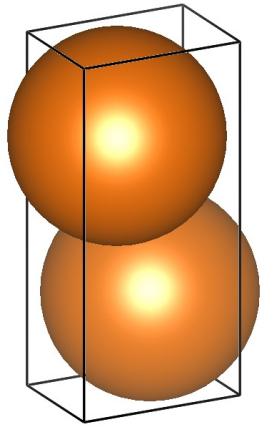


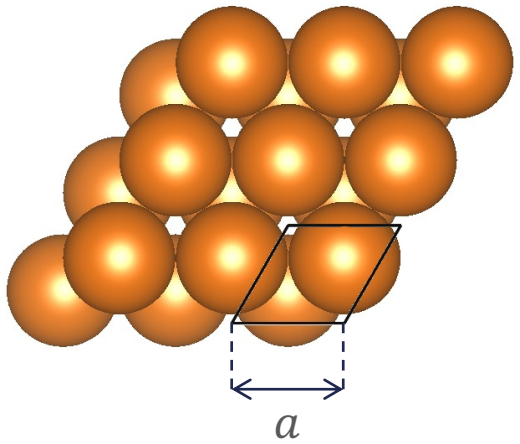


- **Geometrical description**

Hexagonal Close Packed (HCP) – $P6_3/mmc$

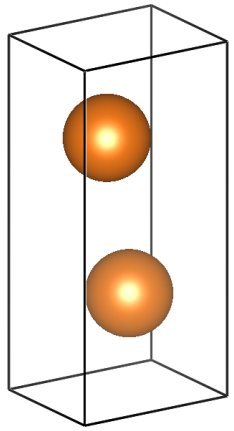


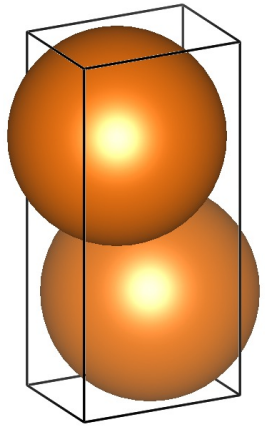


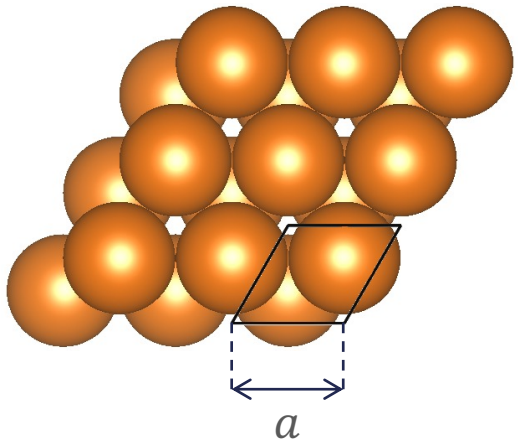


- **Geometrical description**
  - The unit cell is a right prism with a hexagonal base and contains 2 atoms.
  - The full hexagonal symmetry appears only when multiple cells are repeated.
- **Number of atoms per unit cell**

Hexagonal Close Packed (HCP) – $P6_3/mmc$





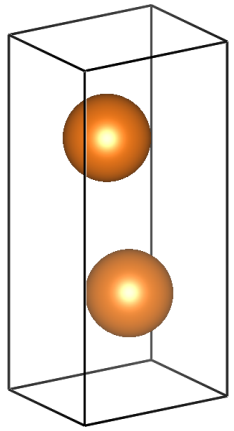


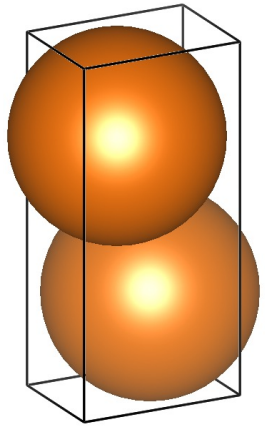
- **Geometrical description**
  - The unit cell is a right prism with a hexagonal base and contains 2 atoms.
  - The full hexagonal symmetry appears only when multiple cells are repeated.
- **Number of atoms per unit cell**

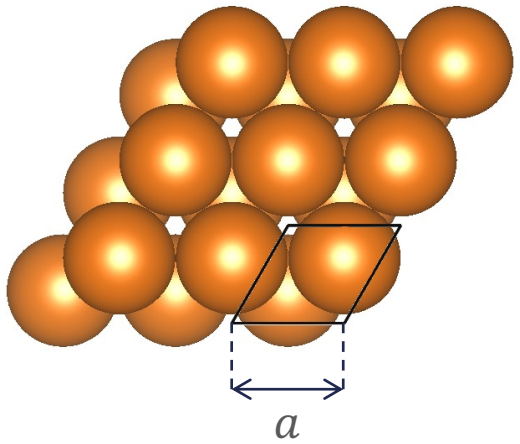
$$3N = 12\times\frac{1}{6} + 2\times\frac{1}{2} + 3 = 6 \Rightarrow N = 2$$

- **Relationship between lattice parameter and atomic radius**

Hexagonal Close Packed (HCP) – $P6_3/mmc$







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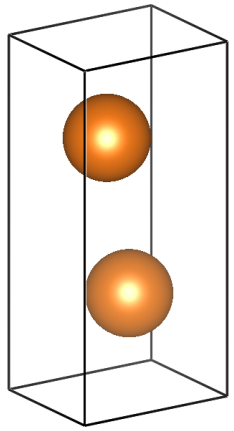
$$3N = 12\times\frac{1}{6} + 2\times\frac{1}{2} + 3 = 6 \Rightarrow N = 2$$

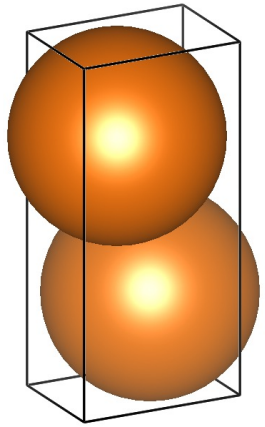
- **Relationship between lattice parameter and atomic radius**
  - Atoms touch along the edges of the hexagonal base:

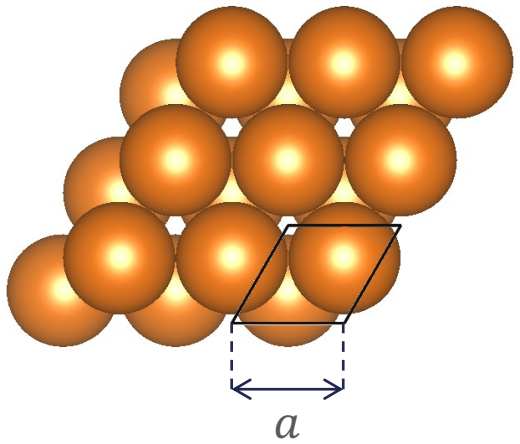
$$2R = a; c = a\sqrt{\frac{8}{3}}$$

- **Volume of one unit cell**

Hexagonal Close Packed (HCP) – $P6_3/mmc$







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$$3N = 12\times\frac{1}{6} + 2\times\frac{1}{2} + 3 = 6 \Rightarrow N = 2$$

- **Relationship between lattice parameter and atomic radius**
  - Atoms touch along the edges of the hexagonal base:

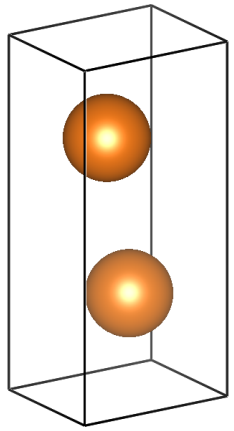
$$2R = a; c = a\sqrt{\frac{8}{3}}$$

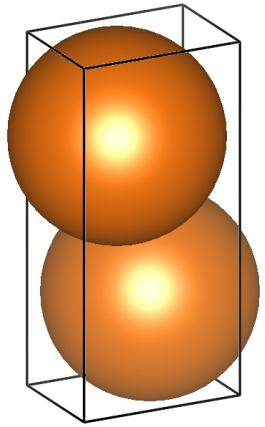
- **Volume of one unit cell**

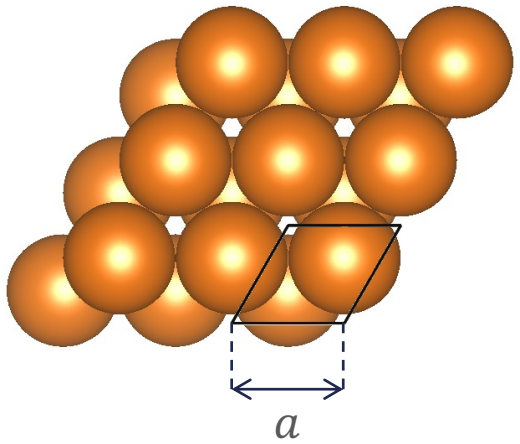
$$V_{cell} = \frac{\sqrt{3}}{2}a^2c$$

- **Packing efficiency**

Hexagonal Close Packed (HCP) – $P6_3/mmc$







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  - Atoms touch along the edges of the hexagonal base:

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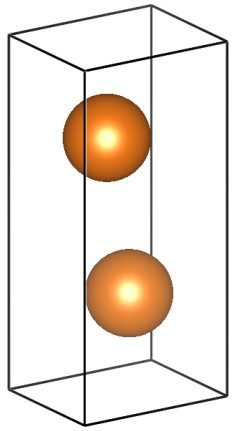
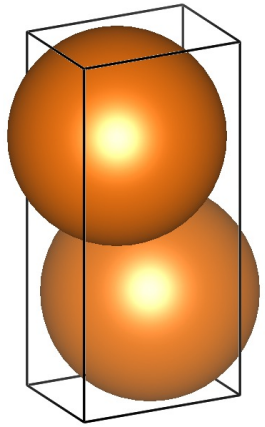
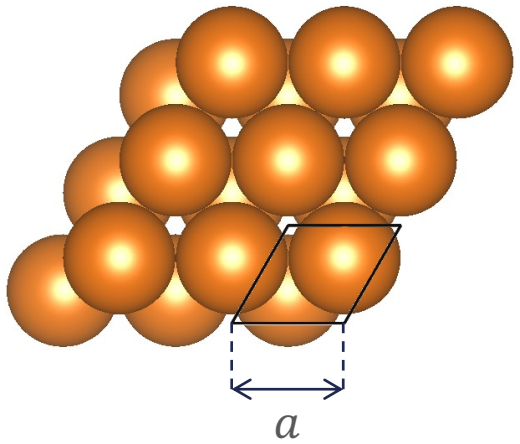
- **Coordination number**

Hexagonal Close Packed (HCP) – $P6_3/mmc$







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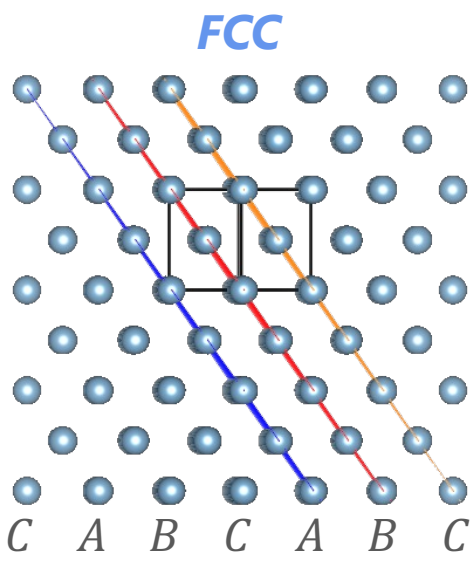
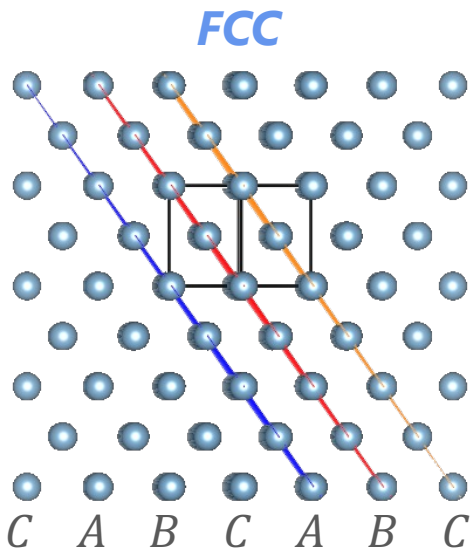
- **Coordination number**
  - Each atom is surrounded by 12 nearest neighbors.

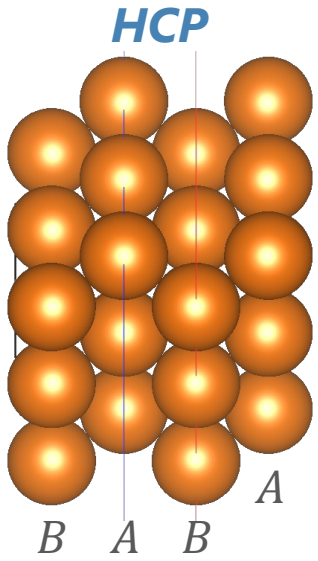
Atomic stacking sequence



- **FCC (Face-Centered Cubic):**
  - Atoms are stacked in a close-packed sequence.
  - Stacking follows an $ABCABCAB$ … pattern, when viewed along the close-packed direction,
  - Each layer is shifted relative to the one below.
  - High packing efficiency: 74%.

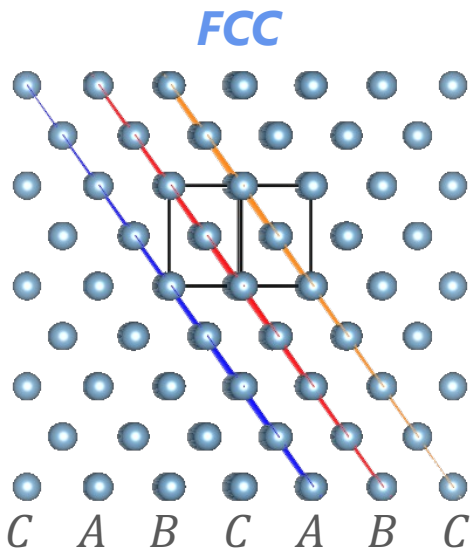
Atomic stacking sequence

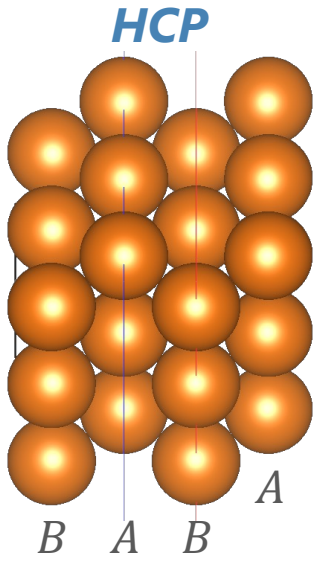




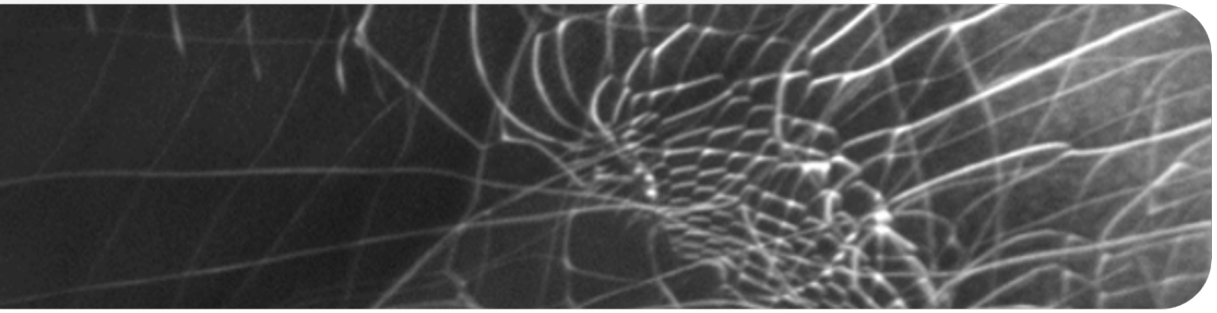
- **FCC (Face-Centered Cubic):**
  - Atoms are stacked in a close-packed sequence.
  - Stacking follows an $ABCABCAB$ … pattern, when viewed along the close-packed direction,
  - Each layer is shifted relative to the one below.
  - High packing efficiency: 74%.
- **HCP (Hexagonal Close-Packed):**
  - Also a close-packed structure.
  - Stacking follows an $ABABAB$ … pattern along the c-direction.
  - Alternate layers are identical.
  - High packing efficiency: 74%.

Atomic stacking sequence



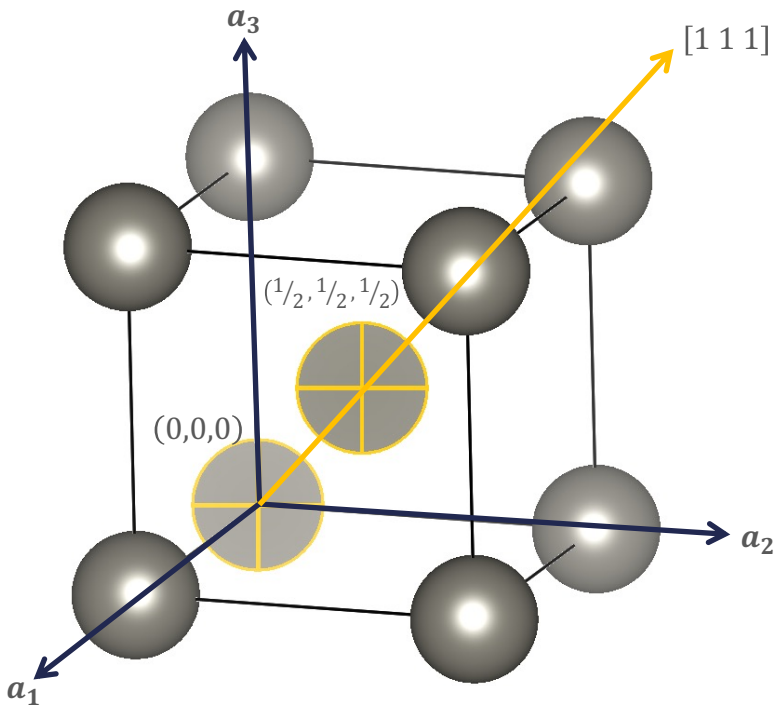


- **FCC (Face-Centered Cubic):**
  - Atoms are stacked in a close-packed sequence.
  - Stacking follows an $ABCABCAB$ … pattern, when viewed along the close-packed direction,
  - Each layer is shifted relative to the one below.
  - High packing efficiency: 74%.
- **HCP (Hexagonal Close-Packed):**
  - Also a close-packed structure.
  - Stacking follows an $ABABAB$ … pattern along the c-direction.
  - Alternate layers are identical.
  - High packing efficiency: 74%.
- **BCC (Body-Centered Cubic):**
  - Not a close-packed structure.
  - Atomic stacking is more open and irregular.
  - No clear ABC-type sequence.
  - Lower packing efficiency: 68%.



The miller notation

Crystallographic directions – $[u\ v\ w]$



❖ What is a crystallographic direction?

- A crystallographic direction is a vector expressed in terms of the unit cell basis, pointing from the origin to a specific lattice point.
- It is represented by a triplet of reduced integers $[u\ v\ w]$ in the direct lattice.

❖ Construction steps (to get $[u\ v\ w]$):

- Choose two points defining the direction, usually from the origin to a point (x, y, z) in units of the lattice
  - E.g.: from (0,0,0) to $(1/2, 1/2, 1/2)$
- Express the vector: $\boldsymbol{\mathcal{R} = x\boldsymbol{a_1} + y\boldsymbol{a_2} + z\boldsymbol{a_3}}$
  - E.g.: $\boldsymbol{\mathcal{R}} = 1/2 \times \boldsymbol{a_1} + 1/2 \times \boldsymbol{a_2} + 1/2 \times \boldsymbol{a_3}$
- Multiply the components by the smallest common factor to get integers (u, v, w)
  - E.g.: (1,1,1)
- Write the direction in square brackets: $[u\ v\ w]$
  - E.g.: [1 1 1]

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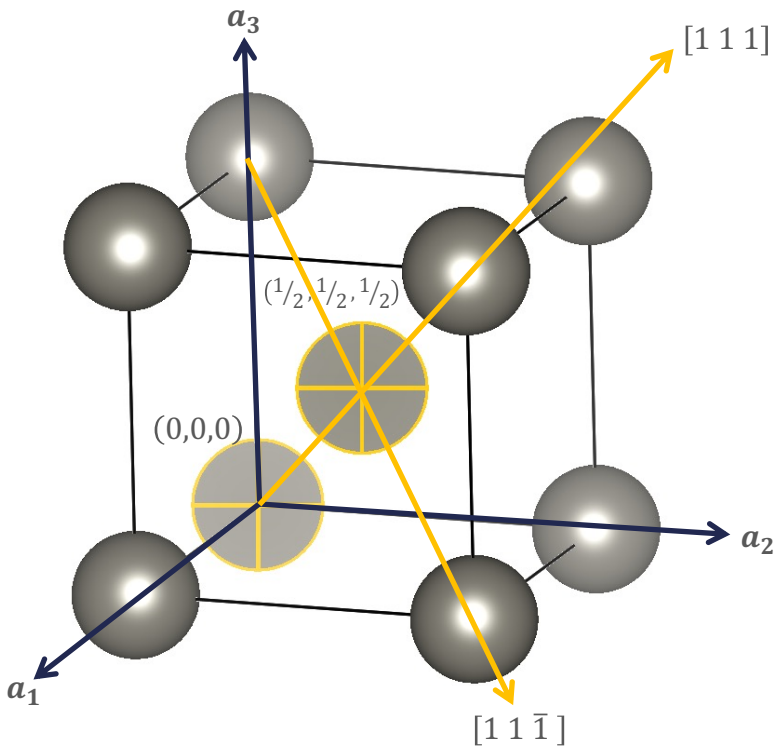

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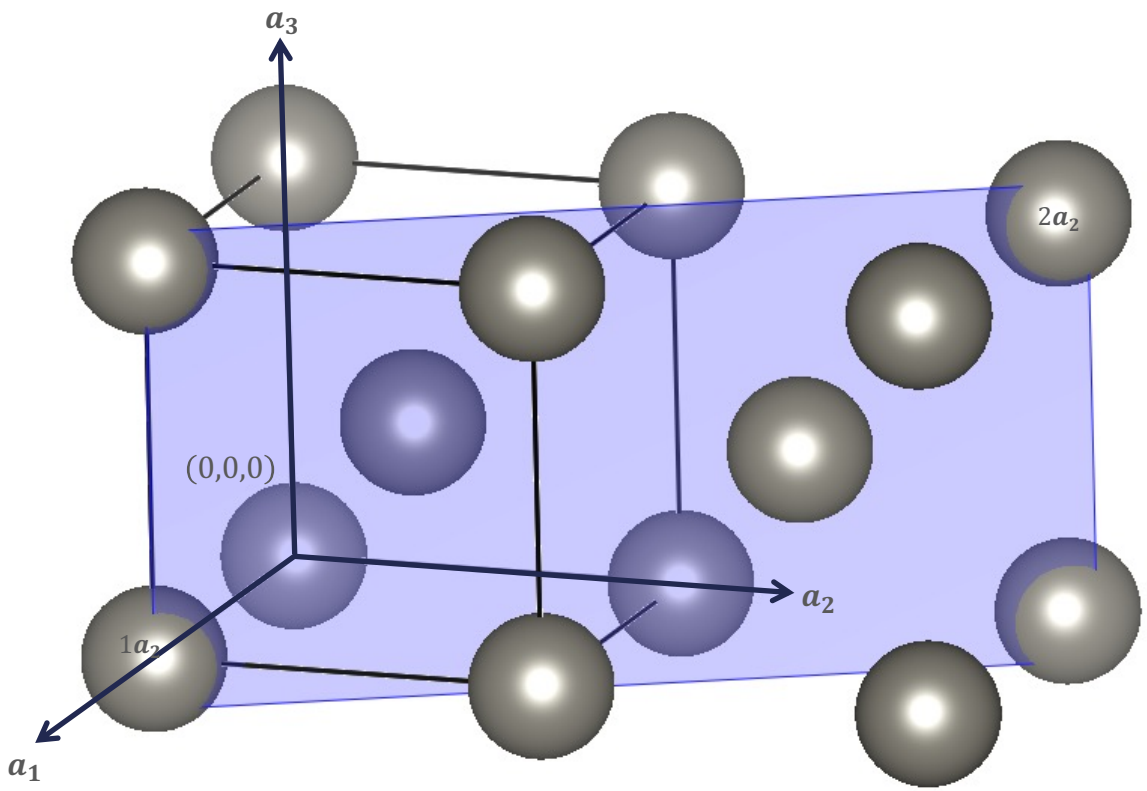
❖ Notation & conventions

- Negative numbers: use a bar ⇒ [1 0 $\bar{1}$]
- Equivalent directions (by symmetry) ⇒ $\langle u\ v\ w \rangle$
  - E.g.: $\langle 1\ 1\ 1 \rangle = \pm[1\ 1\ 1], \pm[\bar{1}\ 1\ 1], \pm[1\ \bar{1}\ 1], \pm[1\ 1\ \bar{1}]$

Crystallographic planes – $(h\ k\ l)$



❖ What is a crystallographic plane?

- It is a set of lattice points forming a flat surface within the crystal structure.
- It is represented by a triplet of Miller indices $(h\ k\ l)$ derived from the reciprocal of the intercepts with the unit cell axes.

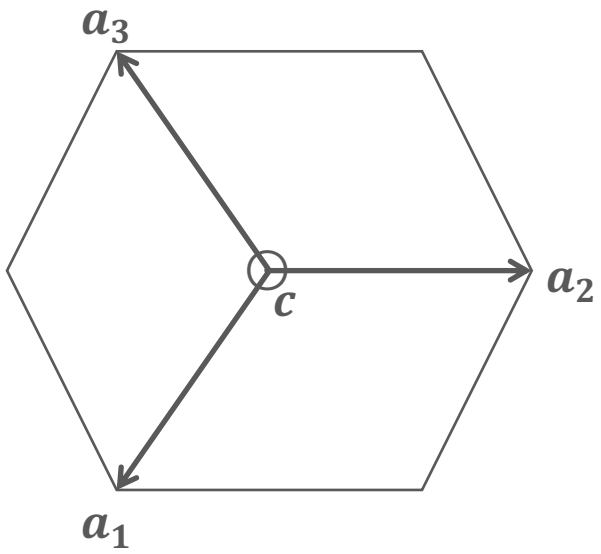
❖ Construction steps (to get $(h\ k\ l)$):

- Identify intercepts of the plane with the crystallographic axes, in lattice units.
  - E.g.: a plane cuts the axes at $(1, 2, \infty)$ intersects $\boldsymbol{a_1}$ at 1, $\boldsymbol{a_2}$ at 2 and parallel to $\boldsymbol{a_3}$.
- Take inverses of these intercepts.
  - E.g.: $(1,2,\infty) \rightarrow (1, {}^1/_2, 0)$
- Multiply by the smallest common factor to convert to the smallest set of integers.
  - E.g.: $(1, {}^1/_2, 0) \rightarrow (2,1,0)$
- Write in parentheses: $(h\ k\ l)$
  - E.g.: $(2\ 1\ 0)$

❖ Notation & conventions

- Negative numbers: use a bar ⇒ $(1\ 0\ \bar{2})$
- Equivalent directions (by symmetry) ⇒ $\{h\ k\ l\}$
  - E.g.:$\{2\ 0\ 1\} = (2\ 0\ 1), (\bar{2}\ 0\ 1), (1\ 2\ 0)$ ...

For hexagonal structure (Bravais-Miller)



❖ **Why Use 4 Indices?**

- Makes the 3-fold symmetry of the hexagonal lattice explicit.
- Equivalent planes like $(1\,\bar{1}\,0\,0)$, $(0\,1\,\bar{1}\,0)$, $(\bar{1}\,1\,0\,0)$ are clearly seen as symmetrical.
- In 3-index notation, this symmetry is hidden.

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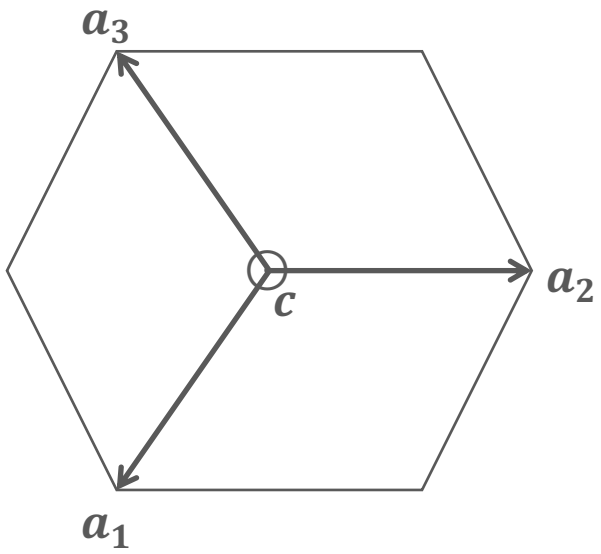

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- $(h\,k\,i)$ in the basal plane
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- Rule: $h + k + i = 0 \Rightarrow i = -(h + k)$

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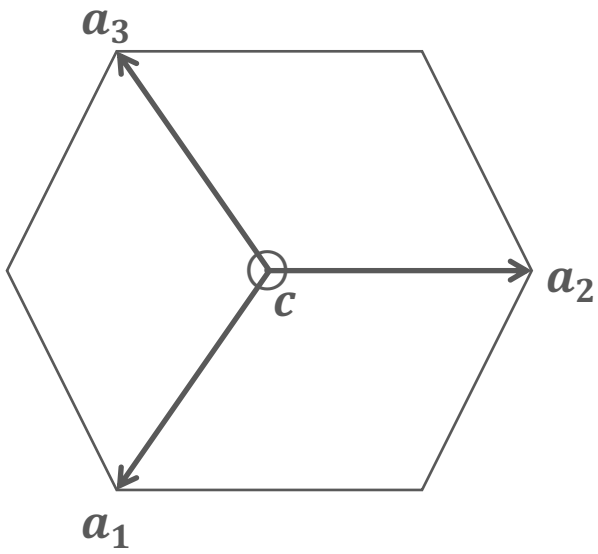

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- Plane: $(h\,k\,l) \rightarrow (h\,k\,i\,l)$ where $i = -(h + k)$
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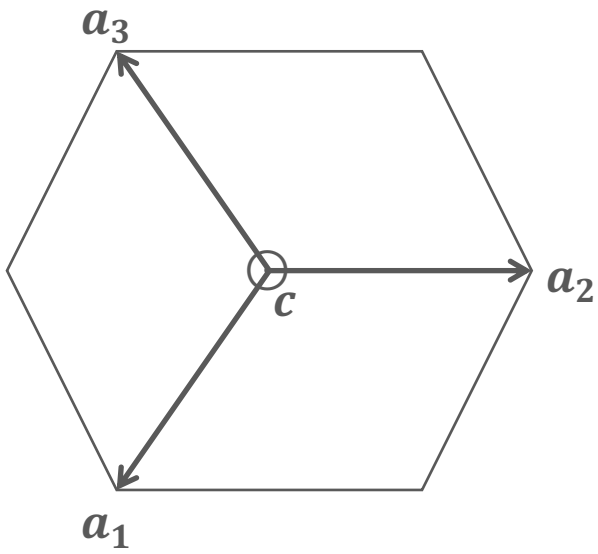

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❖ Be careful

- $(h\ k\ i\ l) \nLeftrightarrow (h\ k\ l\ i)$. There is no permutation involving the fourth index.

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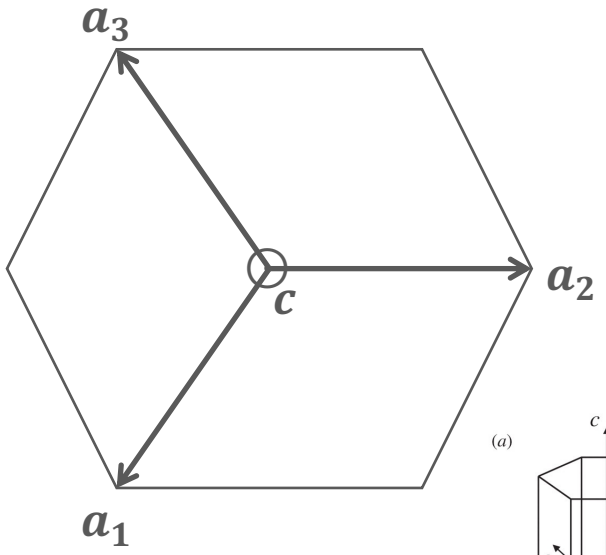

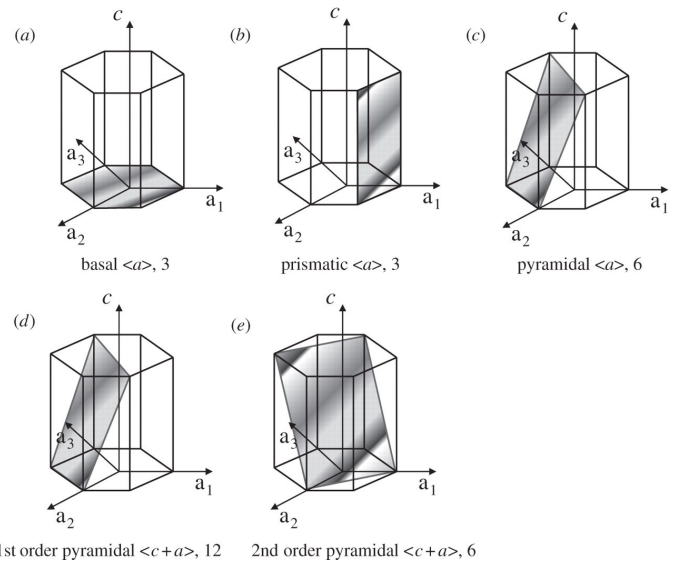

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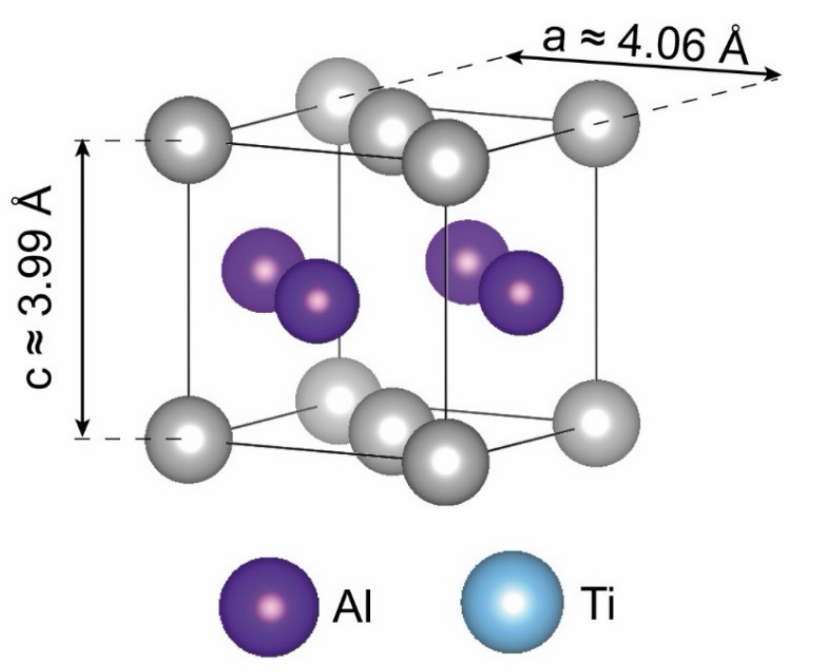
Hybrid notation



- **The γ-TiAl:**
  - $P4/mmm$: tetragonal $\Rightarrow a = b \neq c$
  - Since $^{c}/_{a} = 1.02 \Rightarrow a = b \approx c$
  - Similar to FCC but with alternating planes of Ti and Al along $[0\ 0\ 1]$
- **Why use $\langle u\ v\ w]$?**
  - In FCC, $\langle 0\ 0\ 1\rangle$ are crystallographically equivalent
  - Here, alternating planes of Ti and Al along the $[0\ 0\ 1]$ direction
  - This breaks cubic symmetry and permutations:
    - $[0\ 0\ 1] \neq [1\ 0\ 0]$, $[0\ 0\ 1] \neq [0\ 1\ 0]$
    - $[1\ 0\ 0] = [0\ 1\ 0]$

Some calculations

- Let $\boldsymbol{u} = [u_1\ u_2\ u_3]$ and $\boldsymbol{v} = [v_1\ v_2\ v_3]$, two directions expressed in $\boldsymbol{\mathcal{C} = (a_1, a_2, a_3)}$
- The metric tensor $\boldsymbol{\mathcal{G}}$

$$\mathcal{G}_{i,j} = \boldsymbol{a_i} \cdot \boldsymbol{a_j} = \mathcal{G}_{j,i} \Rightarrow \boldsymbol{\mathcal{G}} = \begin{pmatrix} \boldsymbol{a_1 \cdot a_1} & \boldsymbol{a_1 \cdot a_2} & \boldsymbol{a_1 \cdot a_3} \\ \cdot & \boldsymbol{a_2 \cdot a_2} & \boldsymbol{a_2 \cdot a_3} \\ \cdot & \cdot & \boldsymbol{a_3 \cdot a_3} \end{pmatrix}$$

- The dot product:

$$\boldsymbol{u \cdot v} = \boldsymbol{u^T \cdot \mathcal{G} \cdot v} \overset{cubic}{\Longrightarrow} \boldsymbol{u \cdot v} = u_1 v_1 + u_2 v_2 + u_3 v_3$$

- Norm of $\boldsymbol{u}$:

$$\|\boldsymbol{u}\| = \sqrt{\boldsymbol{u^T \cdot \mathcal{G} \cdot u}} \overset{cubic}{\Longrightarrow} \|\boldsymbol{u}\| = \sqrt{u_1^2 + u_2^2 + u_3^2}$$

- Angle between $\boldsymbol{u}$ and $\boldsymbol{v}$:

$$\cos\theta = \frac{\boldsymbol{u^T \cdot \mathcal{G} \cdot v}}{\sqrt{\boldsymbol{u^T \cdot \mathcal{G} \cdot u}}\sqrt{\boldsymbol{v^T \cdot \mathcal{G} \cdot v}}} \overset{cubic}{\Longrightarrow} \cos\theta = \frac{u_1 v_1 + u_2 v_2 + u_3 v_3}{\sqrt{u_1^2 + u_2^2 + u_3^2}\sqrt{v_1^2 + v_2^2 + v_3^2}}$$

- Interplanar distance d_{hkl} (for orthorhombic system):

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

Linear and planar densities

❖ **Linear density (LD)**

$$LD = \frac{\text{number of atoms centered on the direction vector}}{\text{Length of the direction vector}}$$

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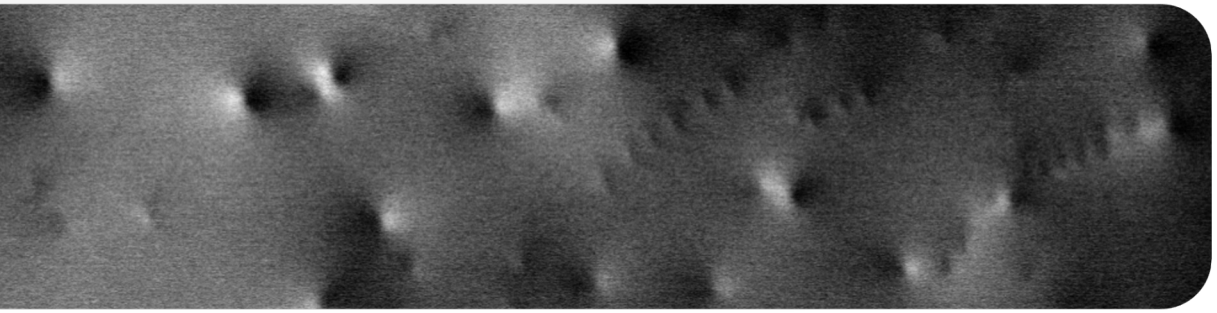
Structure	Direction	LD	Plane	PD
FCC	$\langle 110 \rangle$	$\frac{2}{a\sqrt{2}}$	$\{111\}$	$\frac{4}{a^2\sqrt{3}}$
BCC	$\langle 111 \rangle$	$\frac{2}{a\sqrt{3}}$	$\{110\}$	$\frac{2}{a^2\sqrt{2}}$
HCP	$\langle 11\bar{2}0 \rangle$	$\frac{1}{a}$	(0001)	$\frac{2}{a^2\sqrt{3}}$

↳ The most densely packed planes and directions are the most physically relevant crystallographic elements.



“Practical” crystallography

How to use a crystallography software?

❖ **Wyckoff Positions:**

- Unique atomic sites allowed by the symmetry of a space group.
- Each is labeled with a letter $(a, b, c, \dots)$.

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- **How to use them in software (e.g. VESTA, CIF files):**
  - Enter only one Wyckoff site (e.g. W at $2a$ $(0,0,0)$ in $Im\bar{3}m$).
  - The software automatically generates all symmetry-equivalent positions (e.g. adds $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ⇒ BCC).
  - This keeps structural data compact and avoids duplication.

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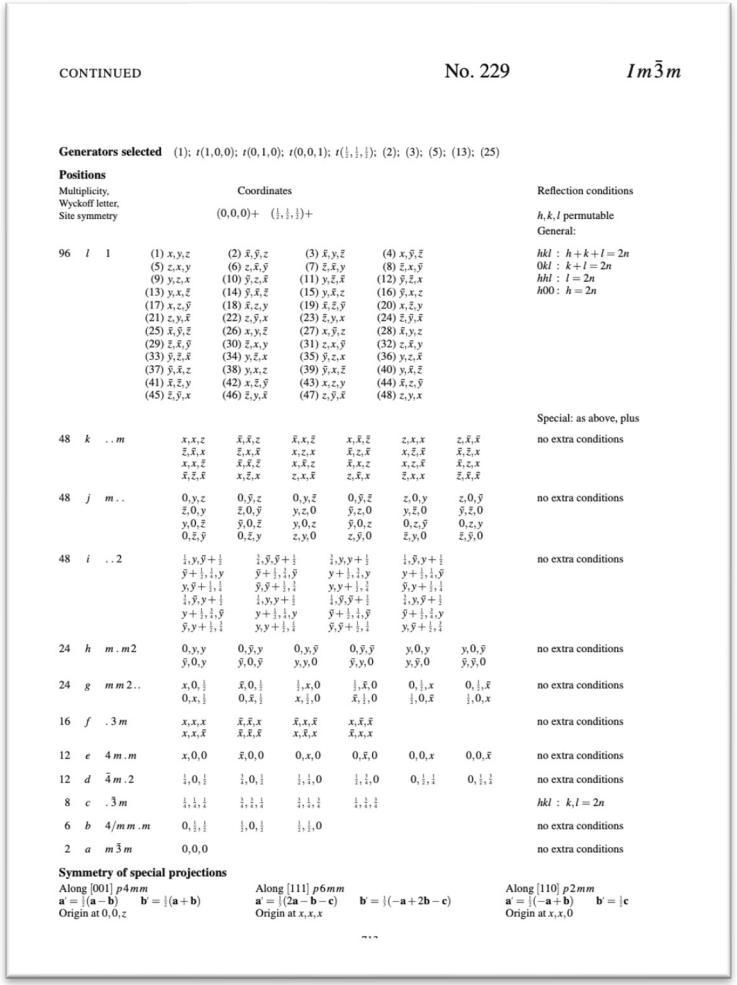
↳ Work smart: choose the right Wyckoff position and let symmetry build the crystal for you..



CONTINUED No. 229 $Im\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

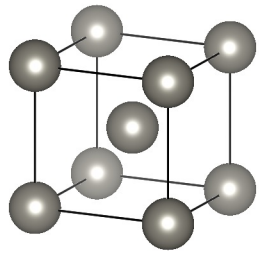
Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+	Reflection conditions
		h,k,l permutable
		General:
96 *l* 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$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

Symmetry of special projections

Along [001] $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$ Origin at $0,0,z$

Along [111] $p6mm$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$ Origin at x,x,x

Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$ Origin at $x,x,0$



Some examples

- **α-Fe**
  - Space group: $Im\bar{3}m$ n°: 229 (BCC)
  - Atom positions:
    - Fe atoms in $2a$
  - Lattice parameters:
    - $a = 0.2866$ nm
    - $\alpha = \beta = \gamma = 90°$

Some examples

- **α-Fe**
  - Space group: $Im\bar{3}m$ n°: 229 (BCC)
  - Atom positions:
    - Fe atoms in $2a$
  - Lattice parameters:
    - $a = 0.2866$ nm
    - $\alpha = \beta = \gamma = 90°$

- **AsGa**
  - Space group: $F\bar{4}3m$ n°: 216 (FCC)
  - Atom positions:
    - Ga atoms in $4a$
    - As atoms in $4c$
  - Lattice parameters:
    - $a = 0.5653$ nm
    - $\alpha = \beta = \gamma = 90°$

Some examples

- **α-Fe**
  - Space group: $Im\bar{3}m$ n°: 229 (BCC)
  - Atom positions:
    - Fe atoms in $2a$
  - Lattice parameters:
    - $a = 0.2866$ nm
    - $\alpha = \beta = \gamma = 90°$

- **AsGa**
  - Space group: $F\bar{4}3m$ n°: 216 (FCC)
  - Atom positions:
    - Ga atoms in $4a$
    - As atoms in $4c$
  - Lattice parameters:
    - $a = 0.5653$ nm
    - $\alpha = \beta = \gamma = 90°$

- **GaN**
  - Space group: $P6_3mc$ n°: 186 (Hex)
  - Atom positions:
    - Ga atoms in $2b$
    - N atoms in $2b$
  - Lattice parameters:
    - $a = 0.3189$ nm; $c = 0.5185$ nm
    - $\alpha = \beta = 90°; \gamma = 120°$
    - $z = 0.337$

Some examples

❖ α-Fe

- Space group: $Im\bar{3}m$ n°: 229 (BCC)
- Atom positions:
  - Fe atoms in $2a$
- Lattice parameters:
  - $a = 0.2866$ nm
  - $\alpha = \beta = \gamma = 90°$

❖ AsGa

- Space group: $F\bar{4}3m$ n°: 216 (FCC)
- Atom positions:
  - Ga atoms in $4a$
  - As atoms in $4c$
- Lattice parameters:
  - $a = 0.5653$ nm
  - $\alpha = \beta = \gamma = 90°$

❖ GaN

- Space group: $P6_3mc$ n°: 186 (Hex)
- Atom positions:
  - Ga atoms in $2b$
  - N atoms in $2b$
- Lattice parameters:
  - $a = 0.3189$ nm; $c = 0.5185$ nm
  - $\alpha = \beta = 90°; \gamma = 120°$
  - $z = 0.337$

❖ Ti_2AlN

- Space group: $P6_3/mmc$ n°: 194 (Hex)
- Atom positions:
  - Ti atoms in $4f$
  - Al atoms in $2d$
  - N atoms in $2a$
- Lattice parameters:
  - $a = 0.298$ nm; $c = 1.357$ nm
  - $\alpha = \beta = 90°; \gamma = 120°$
  - $z_{Ti} = 0.083$

Thanks for your listening!

If you need further information:

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LEM3 LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

UNIVERSITÉ DE LORRAINE

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