Week 01&02

Class Description

Algebraic structures: Groups and Rings, Integers

Crystallography: Symmetries and 3D Geometry

F. Sorin (MX)

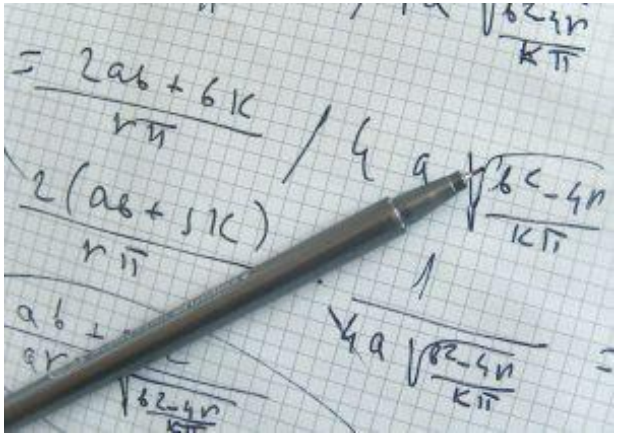
Ecole Polytechnique Fédérale de Lausanne

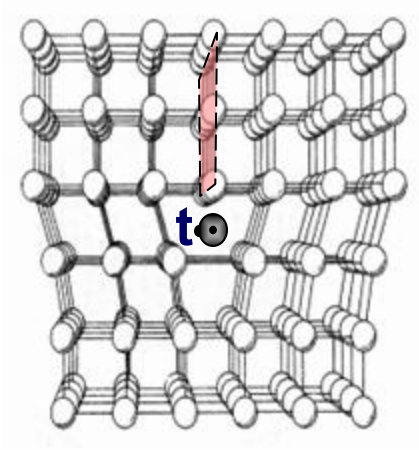
Overview

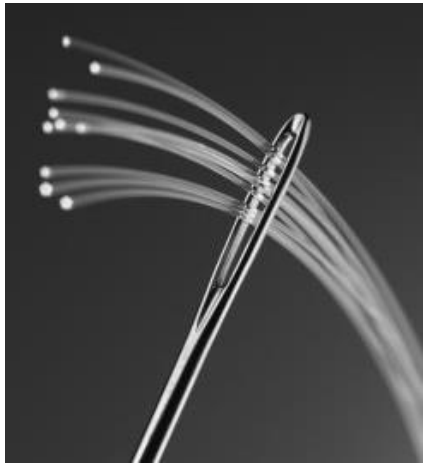
- Overview and structure of the class
- Algebraic structures: groups and Rings
- Point Group Symmetry in Crystallography
- Cells, Miller indices… (to be continued next week)

General Objectives

- To train you on applying theoretical concepts in mathematics learned at the bachelor level to Materials Science important concepts, and engineering problems more broadly.
- Review important Materials Science concepts via the lenses of the mathematics required to treat them.







- I am not a mathematician ! But well trained in applied mathematics… and Materials Science both theoretical and experimental.
- I will teach Materials Science with an emphasis on the applied mathematics
- Prof. Carter will show you examples via computational methods to visualize mathematical concepts and use them.

General Outline

Mathematical Concepts: ***a rough schedule***

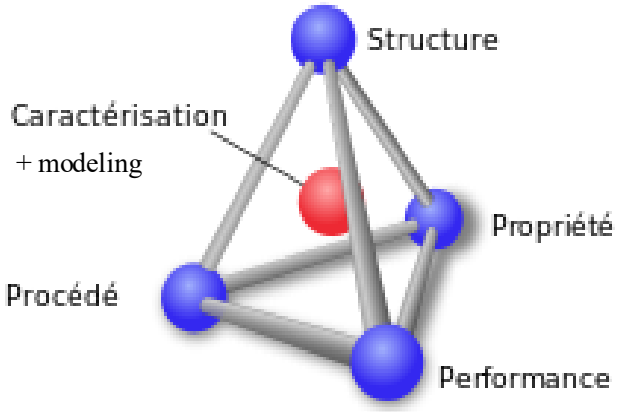
- *Weeks 1, 2 &3*: Foundations: Groups, Number theory and vectorial spaces
- *Week 3&4*: Real and Complex numbers
- *Week 4, 5 & 6*: Linear algebra;
- *Week 7 & 8*: Functions: important properties, main functions (e^x, log etc…) Integration and derivation
- Week 9: Fourier transform
- *Week 10*: Laplace transforms and ODEs
- *Week 11*: ODEs and PDEs
- *Week 12, 13 & 14*: Number theory (Combinatorial), Probability and Statistics

- This structure is aligned with the class on Solid State Materials of Prof. Marzari
- These notions should be familiar to you and we sometimes will use one or more in classes and exercises before having reached the class dedicated to them.

General Outline

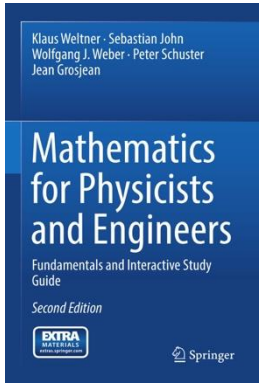
Important Materials Science Concepts:

- Structure of Materials: Crystallography
- Thermodynamics and Kinetics
- Phase diagrams and phase transformation
- Diffusion
- Mechanical properties
- Rheology and fluid dynamics
- Visco-elastic materials
- Optical properties and wave propagation
- Quantum Mechanics applied to solid states physics
- Statistical physics



Structure of the Class

- Typically, each concept will be spread over 1-2 weeks, with:
  - 2-3 hrs reminding basic concepts: 1-3 hrs applying the concepts to a Materials Science problem
  - 1-2hrs of Exercises
  - Classes will be mostly on Tuesdays. On Mondays we will finish the calss with exercise oriented development, followed by exercises.



- References:
  - Mathematics for Physicists and Engineers

K. Weltner et. al. – Springer (2nd edition)

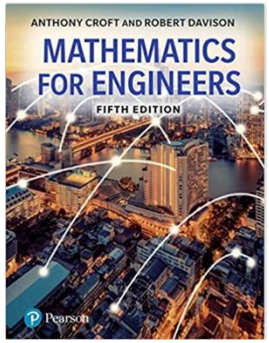
Availble online at the EPFL library: https://link.springer.com/book/10.1007/978-3-642-54124-7

A source of notes and exercises

  - Mathematics for Engineers

A. Croft and R. Davison – Pearson (5th edition)

  - "Algèbre Linéaire" et "Analyse", Gordon - Ellipse



Structure of the Class

- **2 PhD assistants**:
  - Stella Laperrousaz
  - Lucas Jourdan
- **The class will be held live**:
  - Tuesdays in MXF1, 09h15 – 11h00: Classes and Exercises
  - Mondays in CO123, 15h15-17h00: Classes and Exercises
- **Examples with Computational tutorials by Prof. Carter:**
  - 5-6 such sessions will be organized so you can visualize computationally concepts learned in class.
  - The first session next Monday
- **Some exceptions (travels etc..):**
  - Monday September 22nd: no class!
  - Will be announced in class and always check instructions also given on Moodle

Structure of the Class

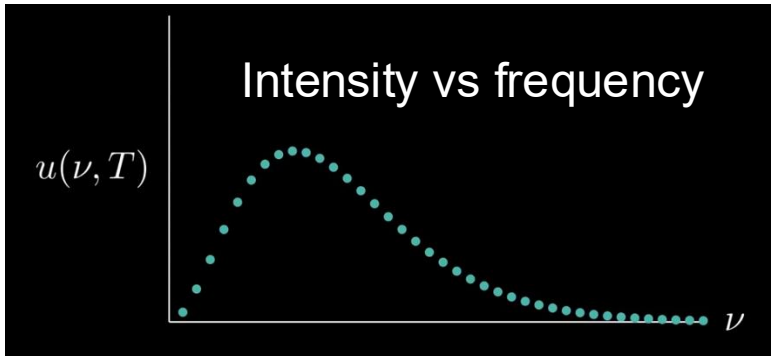
- **Exam**:
  - Written exam during the exam session in January/February 2026.

- It is essential to do the exercises (**learn by doing**):
  - More exercises than what can be done in 1 hour !
  - More exercises for more opportunities to learn: ask us for exercises of previous weeks at the exercise sessions if needed.
  - Some are purely mathematical, but most mix math and materials science.

- Tutorials taught by Prof. Carter from MIT:
  - Complement the classes to revisit the concepts from a numerical perspective;
  - Present other Materials Science concepts and associated math tools;

How Mathematics can shape discoveries

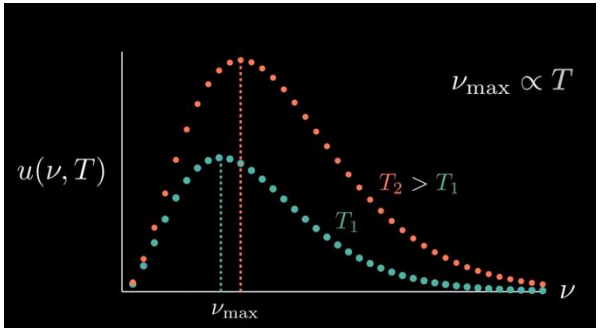
- Black body radiation
  - No clear understanding in the late 19th century.



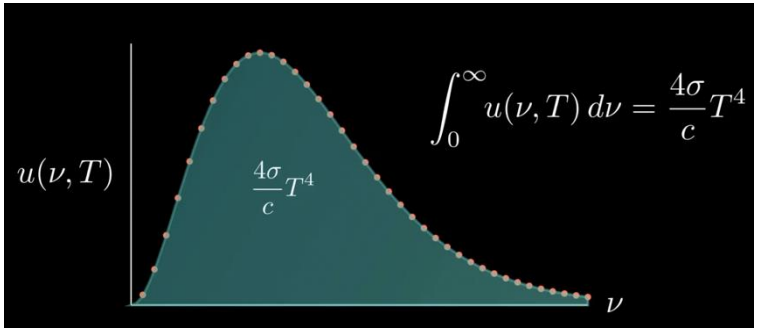
Vidéo of Dr. Jorge S. Diaz

  - Kircchof challenge (1860): find a mathematical expression that fits this curve and a physical meaning behind it.
  - By late 1800s, we knew that:

Wien's displacement law (1893)

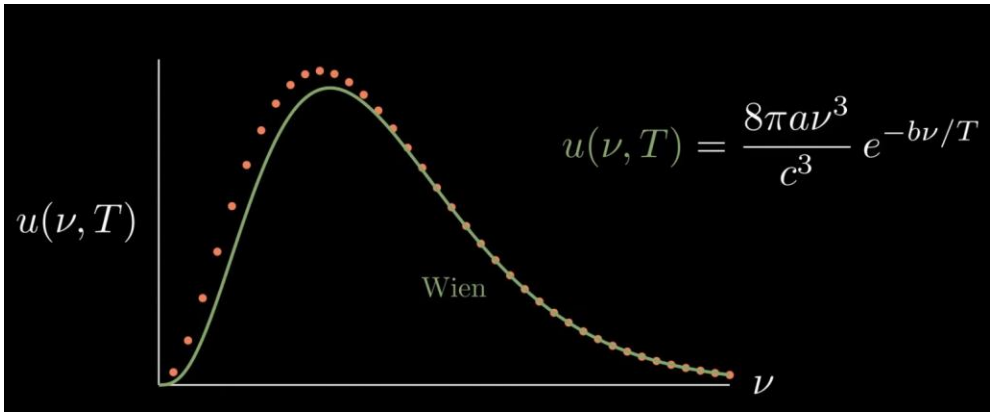


Stefan-Boltzmann law (1894)



How Mathematics can shape discoveries

- Black body radiation
  - By 1896, Wien came up with a law that fits pretty well with experimental data



  - Planck investigated the problem from a purely thermodynamics point of view.
    - A collection of oscillator in equilibrium with an electromagnetic field
    - $u(\nu, T) = \frac{8\pi\nu^2}{c^3} U(\nu, T)$ (we will study this further)

Density of states Internal Energy

    - From Wien's law, $U(\nu, T) = a\nu e^{-\frac{b\nu}{T}}$, or: $\frac{1}{T} = -\frac{1}{b\nu} \ln\left(\frac{U(\nu,T)}{a\nu}\right)$

How Mathematics can shape discoveries

- Fundamental result: $\frac{1}{T} = \frac{\partial S}{\partial U}$ (we will study this further)
- *R* number: $\frac{1}{R} = \frac{\partial^2 S}{\partial U^2}$
- Planck obtained an interesting relation: $R = -b\nu U$
- New and improved experimental results, that have driven most theoretical breakthroughs, refined the experimental results:
  - At low frequency, the intensity varies as ν^2 !

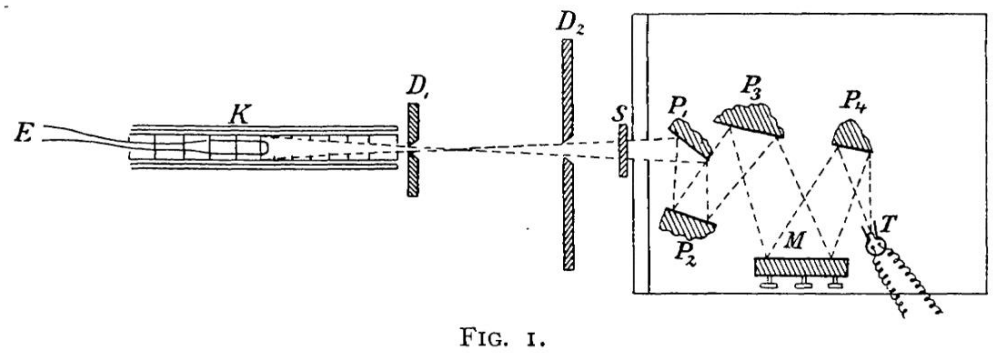
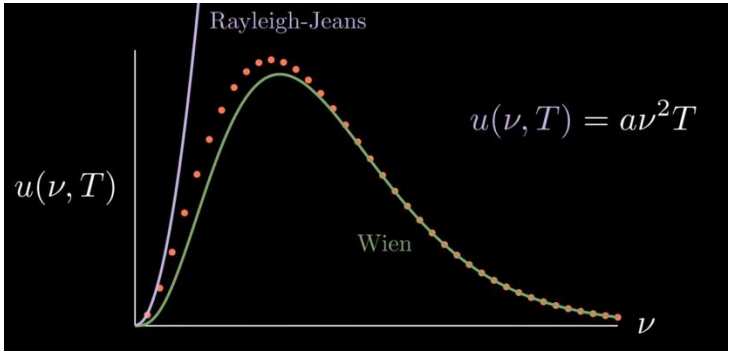


FIG. 1.



  - Rubens had diner with Planck early October to show him his results…
  - Question: which function $f(\nu, T)$ would work ? $\frac{8\pi\nu^2}{c^3} f(\nu, T)$

How Mathematics can shape discoveries

- Planck had to work fast and started from Thermodynamics….
  - He started from the expression of *R* and expanded it to higher powers of *U*…

$$R = -b\nu U - \frac{U^2}{k}$$

  - This leads to another differential equation

$$\frac{1}{R} = \frac{\partial}{\partial U}\left(\frac{1}{T}\right) = \frac{-1}{b\nu U + \frac{U^2}{k}} = \frac{-1}{b\nu}\left(\frac{1}{U} - \frac{1}{U + b\nu k}\right)$$

  - Leading to the correct expression: $u(\nu, T) = \frac{8\pi k b \nu^3}{c^3} \frac{1}{e^{+\frac{b\nu}{T}} - 1}$, with $b = \frac{h}{k}$
  - The same night, Rubens challenged the formula against his experimental results and found a very good match.
  - M. Planck (scientific Autobiography):

> *"So long as it had merely the standing of a law disclosed by lucky intuition, it could not be expected to possess more than a formal significance. For this reason, on the very day when I formulated this law, I began to devote myself to the task of investing it with a true physical meaning."*

Week 1 – Algebraic Structures

- Algebraic structures form the foundations of the mathematical objects on which are built what we use as scientists and engineers: real and complex numbers, functions, integrals, probability and statistics, linear algebra etc…

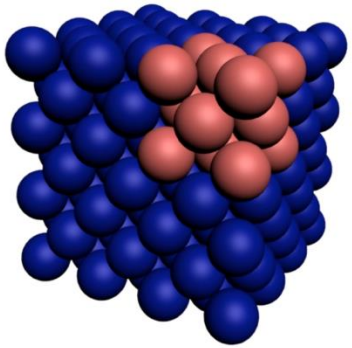
- In the first 2-3 weeks we will review these structures and introduce first examples of applications that relate to Materials Science problems.

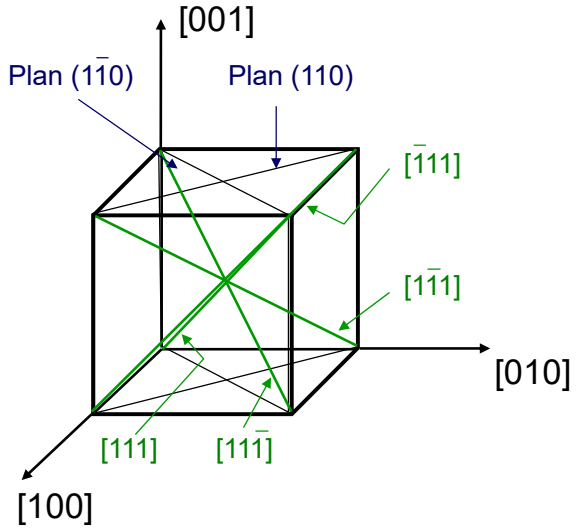
- It will establish the basis for all the classes, and we will get back to them particularly at the end of the semester when we review combinatorial with integers, probability and statistics.

- This first two classes are quite abstract and theoretical, this is just an intro, a deeper view of mathematical objects for your scientific culture. It is also an important foundation of the structure of Materials.

Relative Integers in Materials Science

- **Number theory** is the study of integers and integer-valued functions.
- It appears in the first introduction class of materials structure !





- *Notations:*
  - $\mathbb{N}$ is the ensemble of positive integers and $\mathbb{Z}$ the one for relative integers (positive and negative).
  - $\mathbb{Q}$, $\mathbb{R}$ and $\mathbb{C}$ are the ensemble of rational, real and complex numbers, respectively.
  - Number theory is quite important in Crystallography !

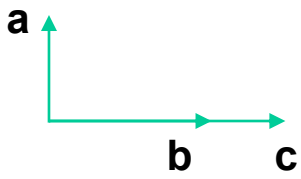
Algebraic structures – Groups and Rings

- **A *Group*** is a set G which is closed under an operation $*$, and satisfies the following properties:

- Closure: for any $x, y \in G$, $x * y \in G$
- Identity – There is an element e in G, such that for every $x \in G$, $e * x = x * e = x$
- Inverse – For every x in G there is an element $y \in G$ such that $x * y = y * x = e$
- Associativity – The following identity holds for every $x, y, z \in G$: $x * (y * z) = (x * y) * z$

A group is abelian if $*$ is commutative: for all $x, y \in G$, $x * y = y * x$

Examples: $(\mathbb{Z}, +)$ is an abelian group
$(\mathbb{Z}, x)$ is not a group.
$(\mathbb{R}^3, x)$ is not a group since the cross product x is not associative:



Other important notions: cardinal and order: number of elements in the group
Sub-groups

- **A *Ring*** is a set R which is closed under two operations + and × and satisfies the following properties:

- (R,+) is an abelian group.
- Associativity of × – For every a, b, c ∈ R, a × (b × c) = (a × b) × c
- Distributive Properties – For every a, b, c ∈ R the following identities hold: a × (b + c) = (a × b) + (a × c) and (b + c) × a = b × a + c × a
- R has an identity for x: there exists e ∈ R such that for all a ∈ R, a x e = e x a = a.

R is commutative if x is commutative.

Example: $(\mathbb{Z}, +, .)$ is a commutative Ring.

$\mathbb{N}$ and $\mathbb{Z}$

- Important notions we will use:
  - Order:

It is very intuitive, but the groups $\mathbb{N}$ and $\mathbb{Z}$ are fully ordered. Any finite sub-group admits a maximum and a minimum element (easy to show via proof by contradiction (also called the method of reductio ad absurdum)).

  - Recurrence relation:
    - An equation that expresses each element of a sequence as a function of the preceding ones.

  - Proof by induction (”Principe de récurence”)

For $n_0 \in \mathbb{N}$, for a proposition P(n) ($n \in \mathbb{N}$) to be true for all $n \geq n_0$, it is necessary and sufficient that:

- $P(n_0)$ is true
- For all $n \geq n_0$, if P(n) is true, then P(n+1) is also true.

  - Strong induction

It is equivalent to show that: if it is true for n_0, and for all integers < n, then P(n) is also true.

These are important notions that are very useful to demonstrate many formulae used in modeling various concepts in Materials Science:

- Toughness and the progression of a crack: in exercises
- Optical reflection of a thin layer
- etc..

$\mathbb{N}$ and $\mathbb{Z}$

- With Groups and Rings structures, one can already create the theoretical basis for number theory.

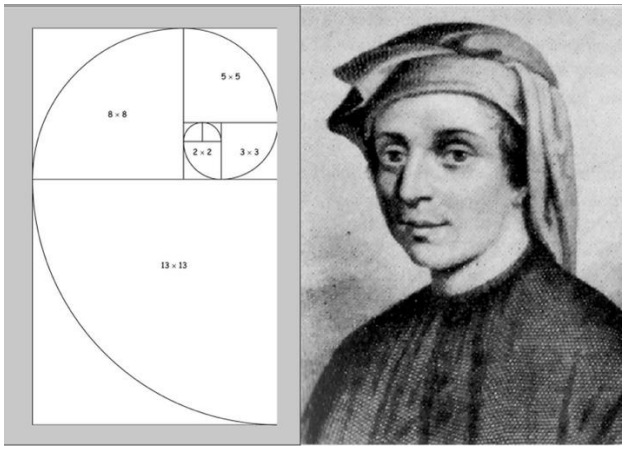
- Despite the seemingly simple nature of adding and multiplying integers (positive or negative), the complexity of problems is endless, the beauty of demonstrations and number structures are unimaginable, and the applications to materials Science problems already significant as we will see.

Examples:

- *Fermat last theorem*: for $(x, y, z, n) \in \mathbb{N}^*$ and $n \geq 3$, there is no solution to the relation: $x^n + y^n = z^n$

Envisioned by Fermat in 1637 or so, demonstrated by Andrew Wiles in 1994.

- *The Fibonacci sequence*: $F_n = F_{n-1} + F_{n-2}$

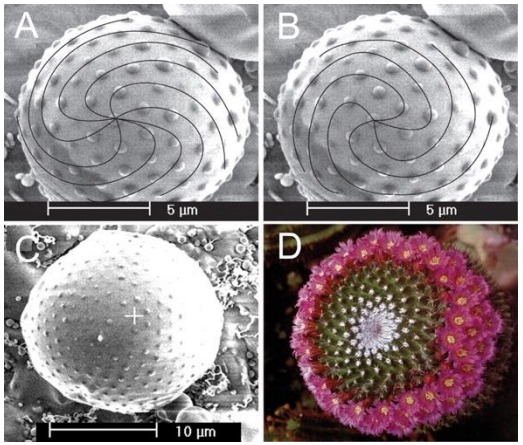


$$F_n = \frac{\varphi^n - \psi^n}{\sqrt{5}}$$

Golden ratio:

$$\varphi = \frac{1+\sqrt{5}}{2}$$

$$\psi = -\frac{1}{\varphi} = \frac{1-\sqrt{5}}{2}$$



Li et. al., Science 309, 909 (2005)

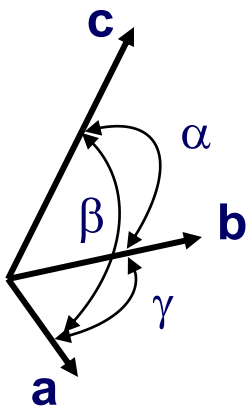
- Present in some patterns in nature, it also appears in some stress related phenomena in materials, but also in quantum computing, in resistor networks, in photonics, hydrogen bonds… interesting review: https://arxiv.org/ftp/arxiv/papers/1801/1801.01369.pdf

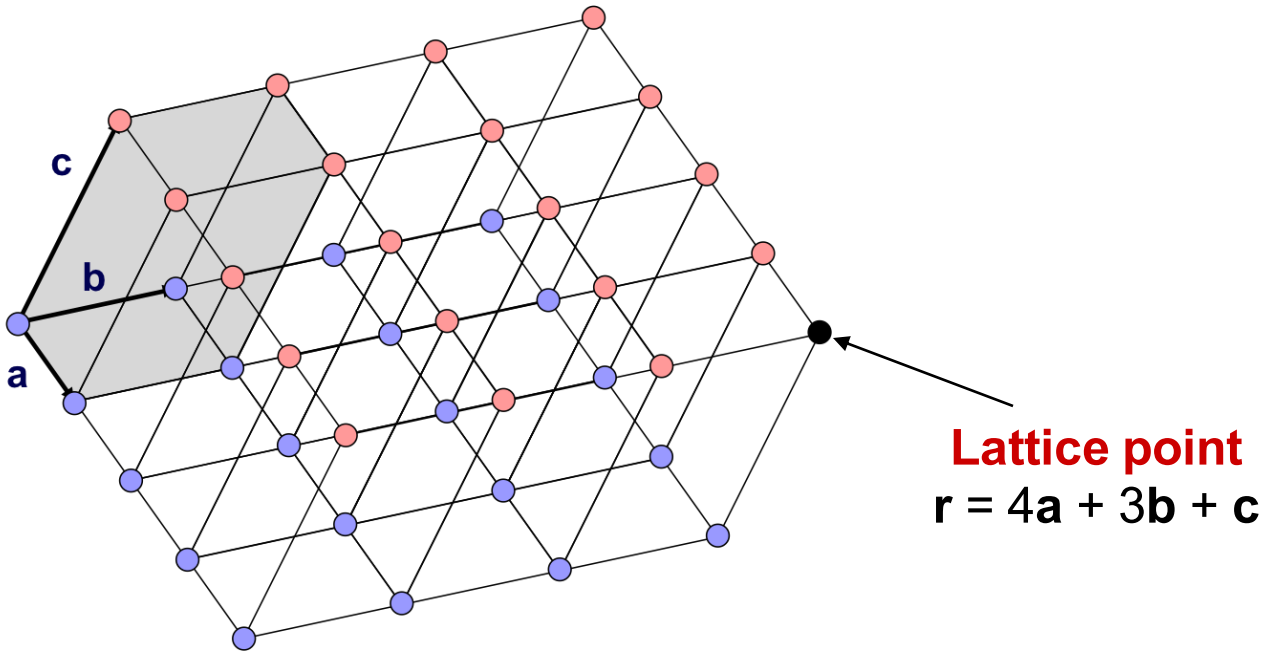
$\mathbb{N}$ and $\mathbb{Z}$: Fibonacci at EPFL

Crystalline state

Materials in a crystalline state are organized into ordered arrangements of atoms. The chemical composition of the material forms a **motif**, that is placed at prescribed positions on a lattice called the **Bravais Lattice**.

A set of 3 vectors for the basis for such a Bravais lattice, where every point is a linear combination with **relative integers** as coefficients.





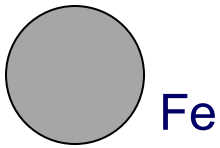
On each point of the lattice, the crystal appears identical: there is a translational symmetry along the vectors **a**, **b** and **c.**

Crystalline state

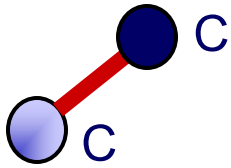
One can distinguish **7 crystal systems**, that reflect the symmetry of the crystal. **14 Bravais lattice** (see next slide).

Crystal = 1 Motif + 1 Bravais lattice

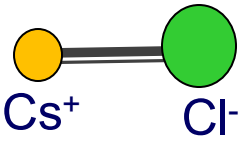
Motif: represents the nature of the materials, its chemical composition, that is repeated in space to form the crystal.



Metallic Bond



Covalent Bond



Ionic Bond

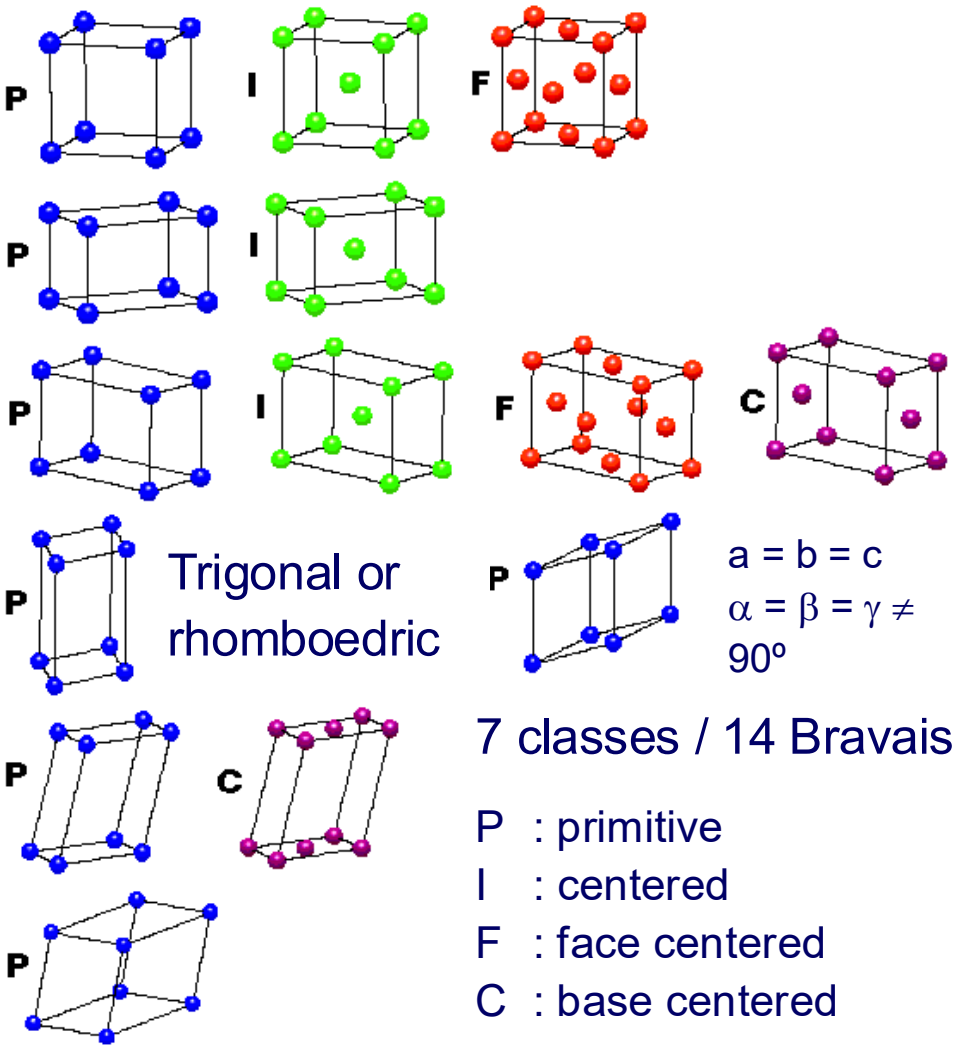
Bravais lattice: mathematical construction of an infinite set of points with translational symmetry along three axis that form a vector basis.

$$B\left(O,\vec{a},\vec{b},\vec{c}\right)=\left\{M/\overrightarrow{OM}=l\vec{a}+m\vec{b}+n\vec{c},(l,m,n)\in\mathbb{Z}^3\right\}$$

Crystalline state

One can distinguish **7 crystal systems**, that reflect the symmetry of the crystal. **14 Bravais lattice:**

Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^o$
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^o$
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^o$
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^o;\ \gamma = 120^o$
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^o \neq \beta$
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$



7 classes / 14 Bravais

P : primitive
I : centered
F : face centered
C : base centered

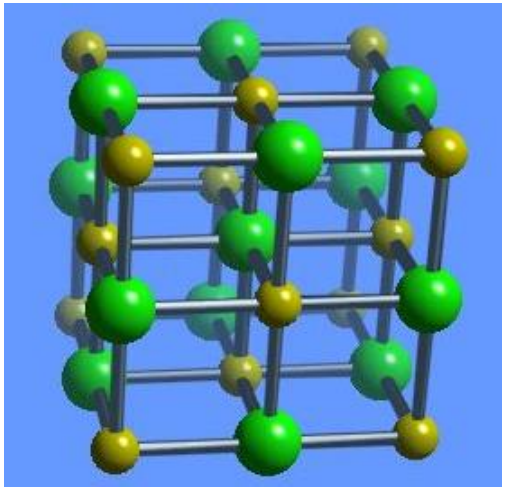
http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/lecture1/Bravais.gif

The cubic system

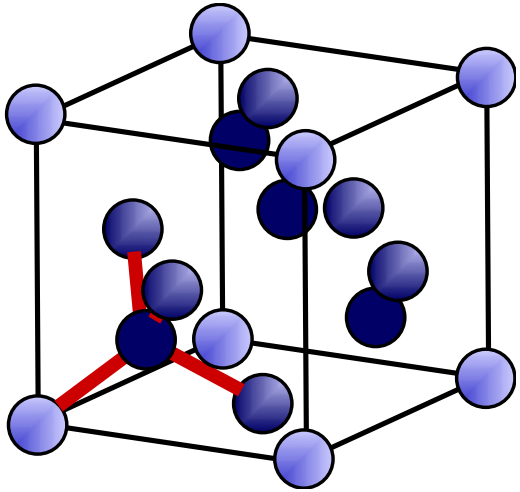
Examples:

Lattice:

Aluminium



NaCl

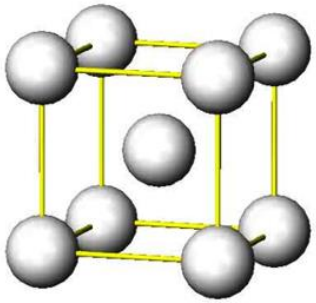


Diamond

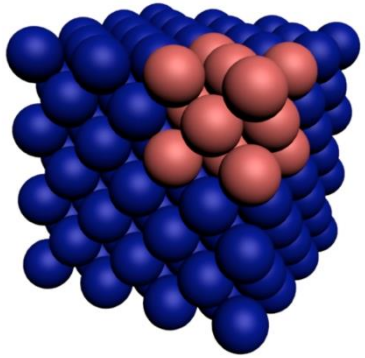
Motifs:

Crystalline state: examples

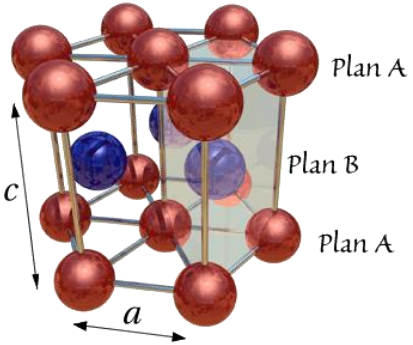
- Because of the nature of their bonds, metals tend to form highly compact structures such as body-centered and face-centered cubic or hexagonal compact:



Cr – Fe – Mo – V – W…

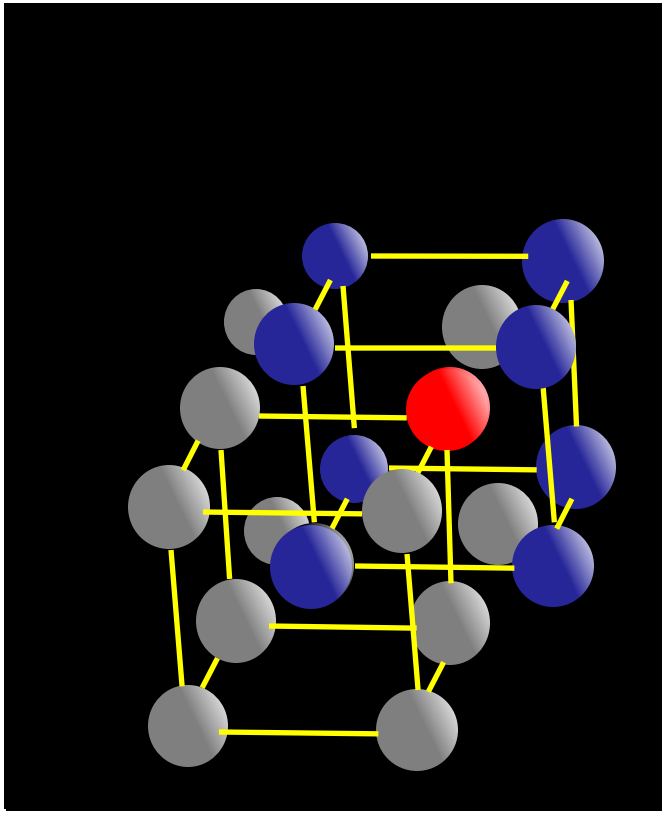


Al – Cu – Ni – Ag – Au …



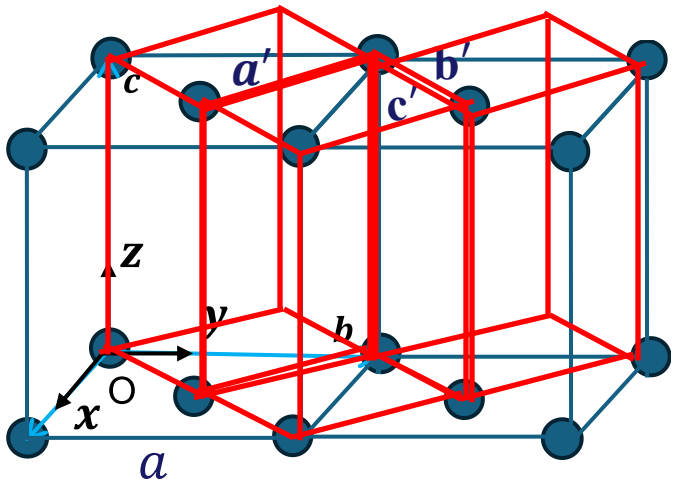
Zn – Mg – Ti – Zr …

- The configuration is the same on every lattice point:



Crystals and Symmetries

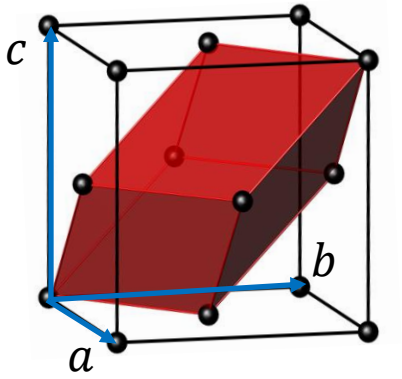
- Crystals can be first apprehended by their symmetry, which govern their classification in the different crystal classes and Bravais lattices.
  - Example: why not a base-centered cubic structure ?



  - It is a Primitive tetragonal !

$\|\boldsymbol{a}'\| = \|\boldsymbol{b}'\| = a\frac{\sqrt{2}}{2}$,
$\|\boldsymbol{c}'\| = a$
$\widehat{(\boldsymbol{a},\boldsymbol{b})} = \widehat{(\boldsymbol{a},\boldsymbol{c})} = \widehat{(\boldsymbol{b},\boldsymbol{c})} = \frac{\pi}{2}$

- However, one can show that the FCC is also another lattice, a rhombohedric structure !
  - And yet FCC is classified with its own Bravais Lattice…



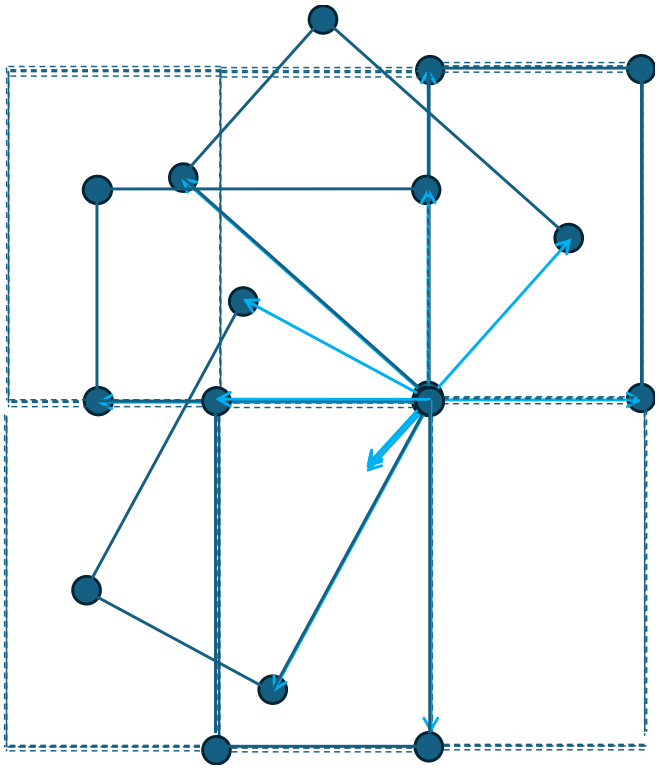
  - For the FCC, the Bravais lattice vectors are given by:

$\boldsymbol{a}' = \frac{1}{2}(\mathbf{b}+\mathbf{c})$; $\boldsymbol{b}' = \frac{1}{2}(\boldsymbol{a}+\boldsymbol{c})$; $\boldsymbol{c}' = \frac{1}{2}(\boldsymbol{a}+\boldsymbol{b})$

The primitive cell $\|\boldsymbol{a}'\| = \|\boldsymbol{b}'\| = \|\boldsymbol{c}'\| = a\frac{\sqrt{2}}{2}$,
$\widehat{(\boldsymbol{a},\boldsymbol{b})} = \widehat{(\boldsymbol{a},\boldsymbol{c})} = \widehat{(\boldsymbol{b},\boldsymbol{c})} = \frac{\pi}{3}$

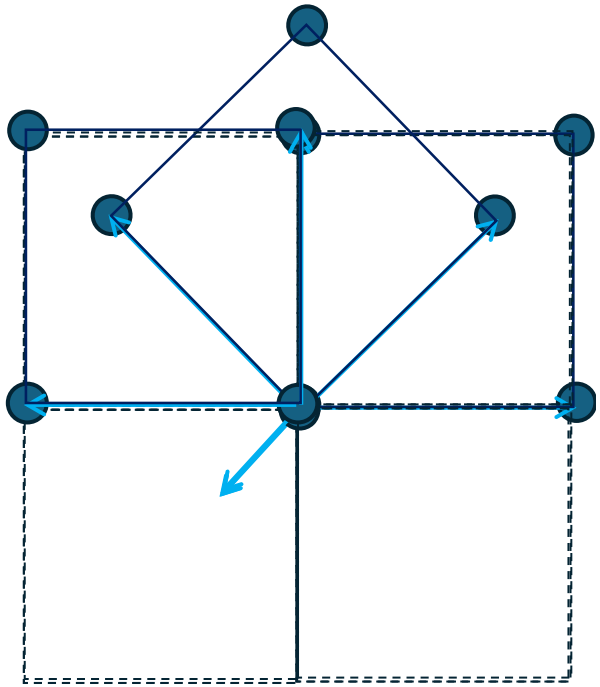
Crystals and Symmetries

- The classification is not about lattice parameter values, it classifies by level of symmetry.
  - A rhombohedric with a certain value of lattice parameters acquire novel symmetries that makes it have a specific Bravais lattice in the cubic structure system.
  - Other example: tetragonal vs cubic



Tetragonal structure: $c > a$

2-fold rotational symmetry



Cubic structure: $c = a$

4-fold rotational symmetry

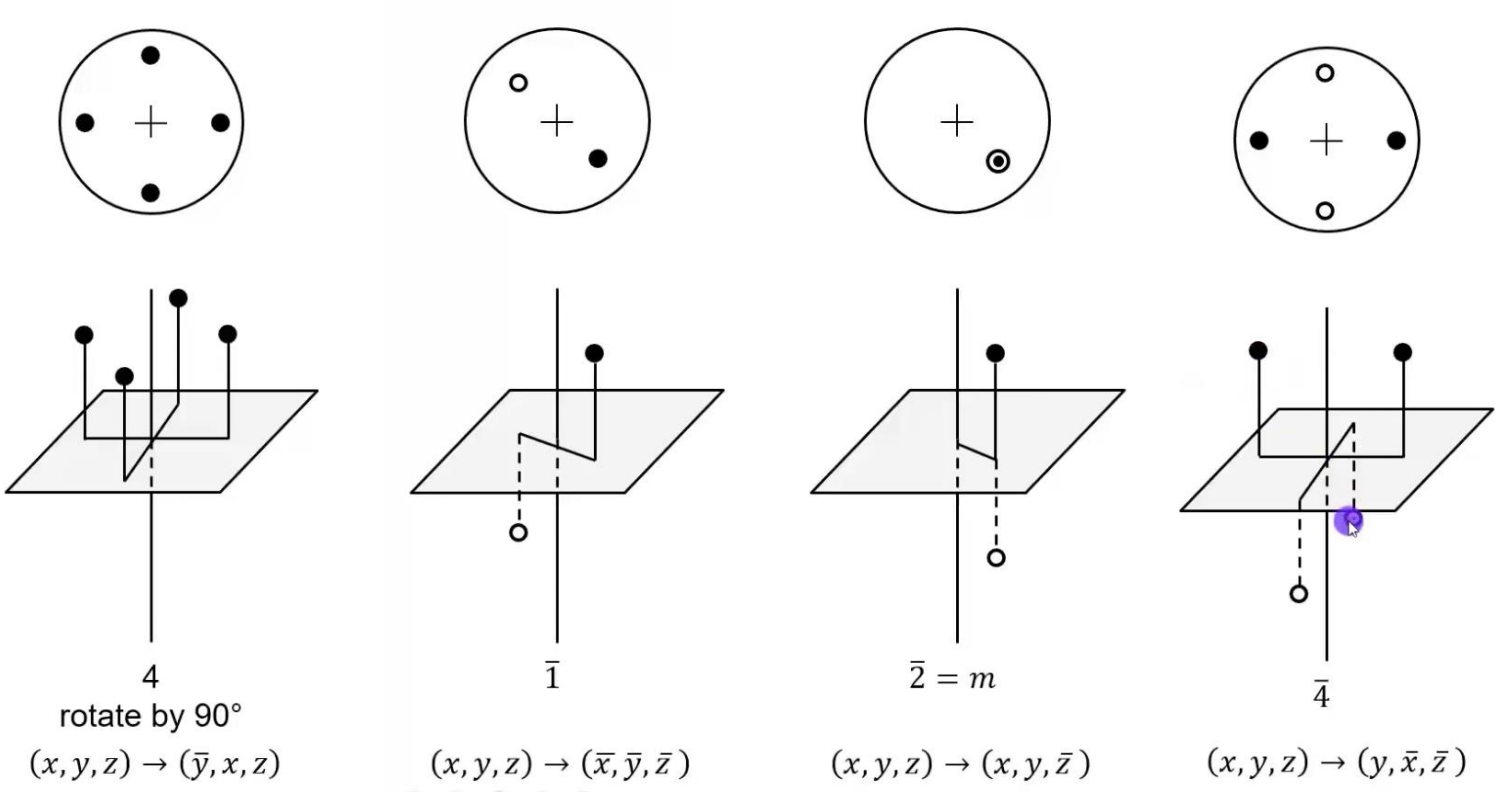
Symmetry Operations: Point symmetries

- **A symmetry operation** is an action that leaves an object unchanged.
- **Point symmetries** are operations that leaves at least one point of an object unchanged. The element unchanged (point, line, plane…) is called a **symmetry element**.
- There are different kinds of **Point symmetry operations** that can be reduced to the following:

  - **Identity (1)**
    - *Symmetry element*: entire object
  - **Inversion ($\bar{1}$)**
    - *Action*: inversion through a point
    - *Symmetry element*: a point
  - **Rotation (N)**
    - *Action*: N-fold rotation around an axis (360/N)
    - *Symmetry element*: a line
  - **Mirror plane or reflection (m)**
    - *Action*: Reflection through a plane
    - *Symmetry element:* a plane
  - **Roto-inversion ($\bar{N}$)**
    - *Action:* Rotation +Inversion
    - Symmetry element: a point

Symmetry Operations

- Exemples of symmetry operations in 3D:



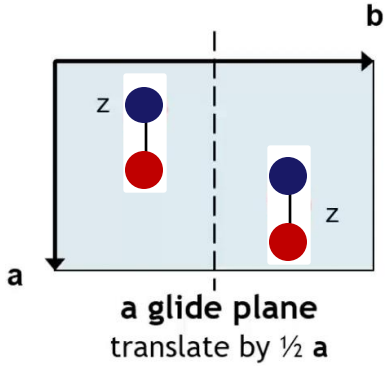
- In 2D:
  - A rotation is always around an axis perpandicular to the 2D plane, so an inversion is a rotation by 180°.
  - There is hence no roto-inversion, as they are just another rotation.

Symmetry Operations

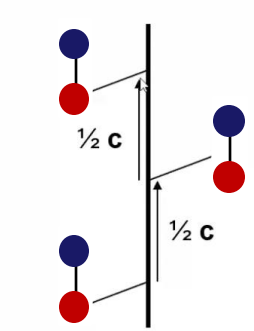
- The Bravais lattice is an infinite object with translational symmetry: this brings new symmetry operations that can leave no point unchanged !

- **Travel symmetry operations**:

  - **Glide plane**
    - *Action:* Reflect through a plane then translate parallel to it



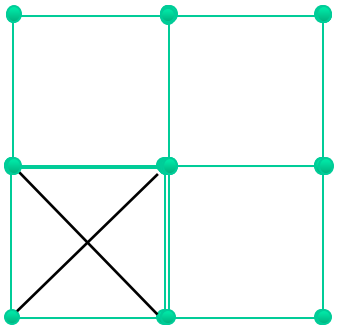
  - **Screw axis**
    - *Action*: Rotation by 360/N around an axis and translation along the axis

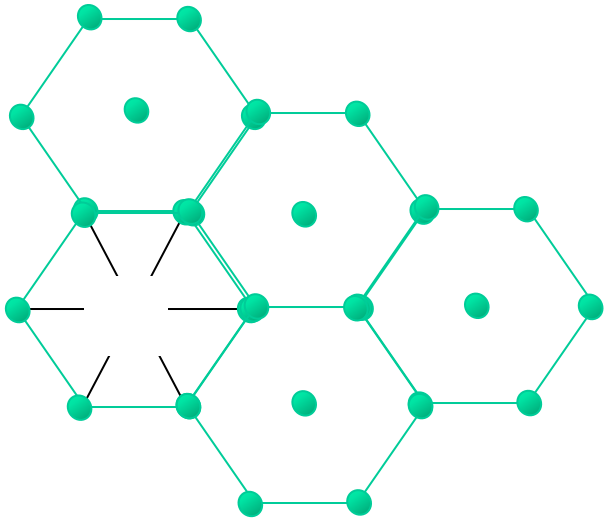


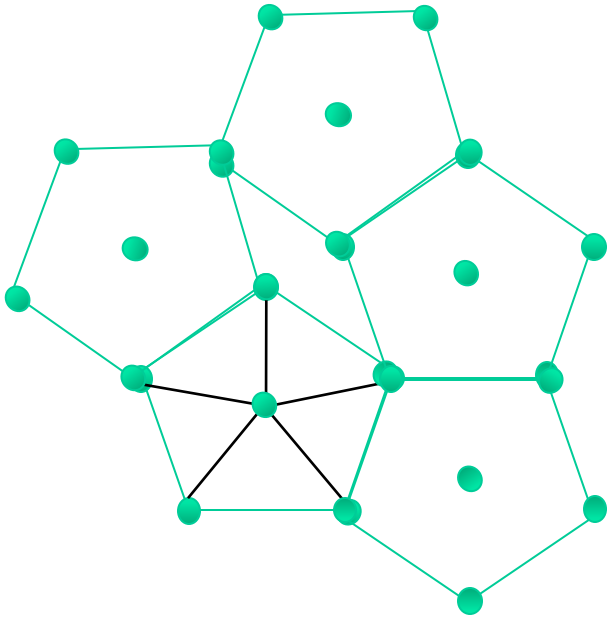
- In 2D:
  - There is only glide plane operations

Crystals and Symmetries

- There are an infinite possibilities of Bravais lattices as the lattice parameters (vector norms and angles) can be chosen arbitrarily.
- For certain values however, symmetries appear: why only certain rotations allowed ?
  - For discrete objects, rotational symmetries can only be discrete: $\frac{2\pi}{n}, n \in \mathbb{N}$
- Possible cells in 2D
  - Need to fill the space without void (translational symmetry of the Bravais Lattice);
  - This restricts the possible rotational symmetries.

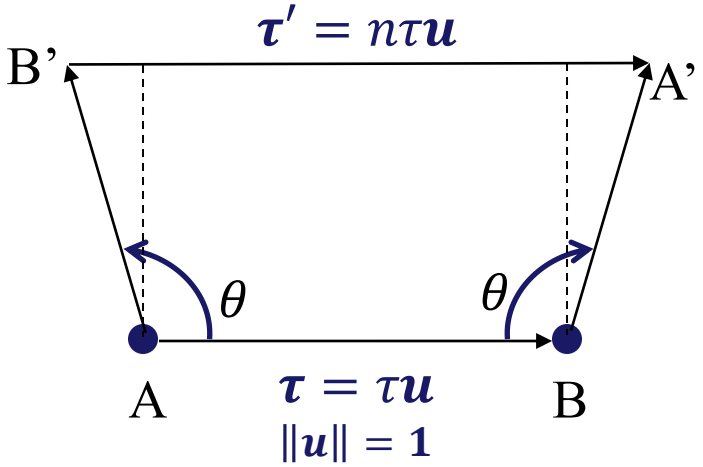






Possible Rotational Symmetries

- This fact reveals the interplay between translational symmetry and a rotational symmetry.
- For a rotational symmetry of angle θ to exist, translational symmetry indeed brings severe restrictions:



$$n\tau = \tau - 2\tau\cos(\theta), n \in \mathbb{Z}$$

Or: $n = 1 - 2\cos(\theta)$

$$\rightarrow \cos(\theta) = \frac{1-n}{2}$$

Which has real solutions only for: $n = -1, 0, 1, 2, 3$

With corresponding possible angles:

$$\frac{2\pi}{1}, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$$

- So, only 1-, 2-, 3-, 4- and 6-fold rotations are allowed.
  - 1-fold is the identity. Triclinic only has this symmetry (with an inversion symmetry ($\bar{1}$).
  - 6-fold only found in hexagonal structure;
  - 3-fold found in Trigonal and cubic;
  - 4-fold found in tetragonal and square;
  - 2-fold is found in all structures except Triclinic.

Building Point Groups

- Point groups: a set of point symmetries that apply to a given object, the motif or the lattice, that form a group.

- In crystallography, we will only look for point groups with the restricted rotational symmetries.

- A *Group* is a set G which is **closed under an operation** $*$ (that is, for any x, y $\in$ G, x $*$ y $\in$ G) and satisfies the following properties:

- Identity (fixed point) – There is an element e in G, such that for every x $\in$ G, e $*$ x = x $*$ e = x
- Inverse – For every x in G there is an element y $\in$ G such that x $*$ y = y $*$ x = e
- Associativity – The following identity holds for every x, y, z $\in$ G: x $*$ (y $*$ z) = (x $*$ y) $*$ z

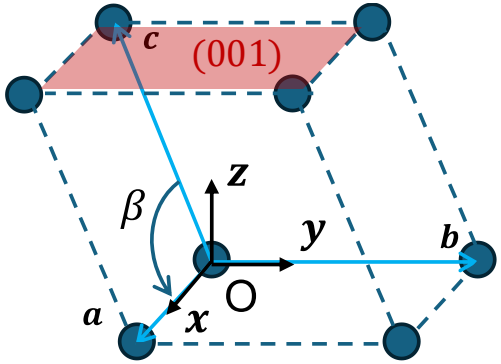
- Point Group Symmetry
  - Closure: The combination of symmetry operators is a symmetry operator in the group.
  - All symmetry operators have an inverse, some are their own inverse.
  - Identity is part of all the Point group symmetry.
  - Associativity is respected

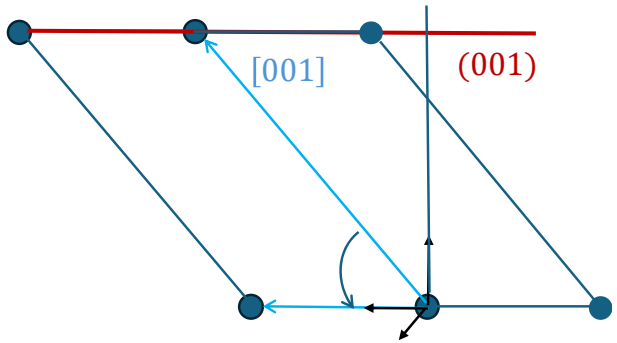
- Examples: Can we create a point group with the 2-fold or 4-fold rotation ?
  - Point Group 2
    - It contains the identity (1 - 2π rotation) and the 2-fold rotation 2.
    - The 2-fold identity is its on inverse: $2o2 = 1$

  - Point Group 4

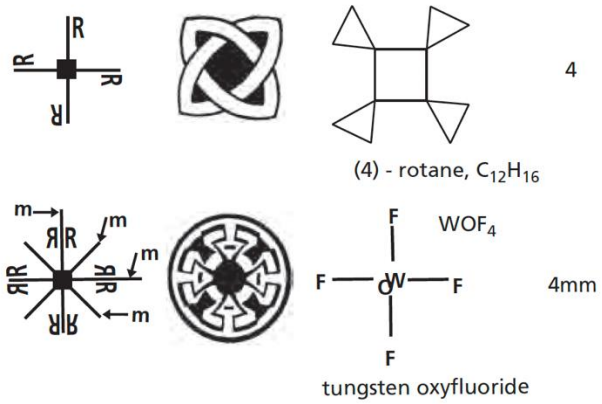
Building Point Groups

- Let's consider the Monoclinic structure and build a point symmetry group for this discrete object.
- We can visualize a group called 2/m (see exercise for solving this with calculus)





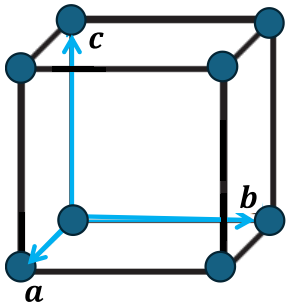
- Another example are the Group 4 in 2D



- A motif with a 4-fold symmetry doesn't have necessarily a mirror symmetry
- A motif with a 4-fold symmetry plus mirror symmetries, with some planes perpendicular.

Point Groups

- Examples: point group of the cube.



- A cube, or a motif formed by four points at the corners, have the highest symmetry, with a point group of order 48, i.e. with 48 symmetries.
- Order of a group: its cardinal, or number of elements in the group.

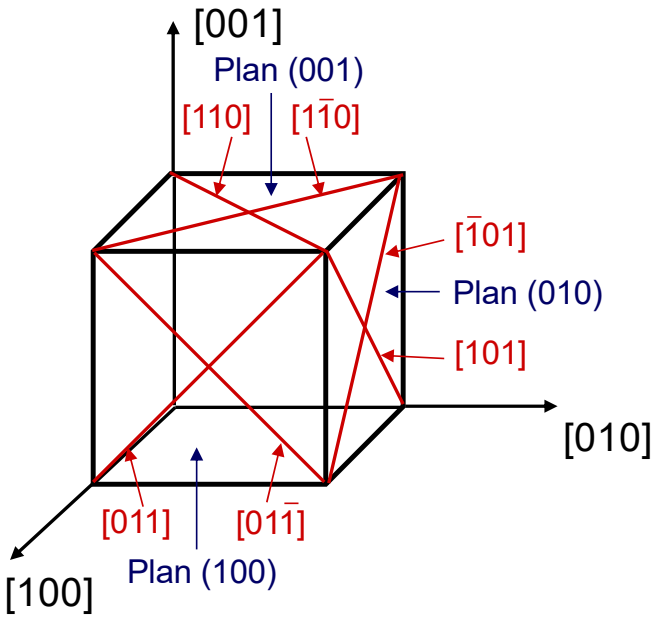
Symmetry operations

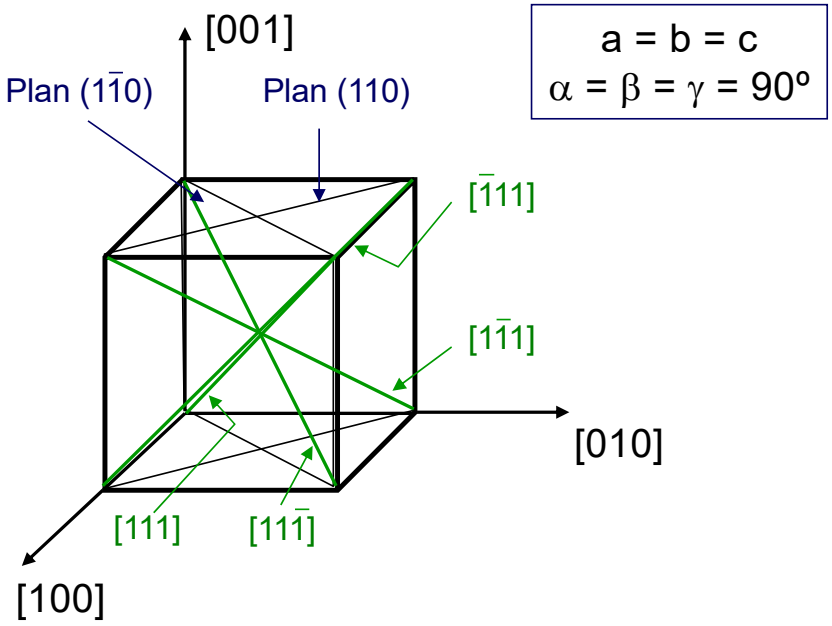
(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^- $0,0,z$	(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$	(22) 2 $x,0,x$	(23) 4^- $0,y,0$	(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$	(26) m $x,y,0$	(27) m $x,0,z$	(28) m $0,y,z$
(29) $\bar{3}^+$ $x,x,x;$ $0,0,0$	(30) $\bar{3}^+$ $\bar{x},x,\bar{x};$ $0,0,0$	(31) $\bar{3}^+$ $x,\bar{x},\bar{x};$ $0,0,0$	(32) $\bar{3}^+$ $\bar{x},\bar{x},x;$ $0,0,0$
(33) $\bar{3}^-$ $x,x,x;$ $0,0,0$	(34) $\bar{3}^-$ $x,\bar{x},\bar{x};$ $0,0,0$	(35) $\bar{3}^-$ $\bar{x},\bar{x},x;$ $0,0,0$	(36) $\bar{3}^-$ $\bar{x},x,\bar{x};$ $0,0,0$
(37) m $x,\bar{x},z$	(38) m x,x,z	(39) $\bar{4}^-$ $0,0,z;$ $0,0,0$	(40) $\bar{4}^+$ $0,0,z;$ $0,0,0$
(41) $\bar{4}^-$ $x,0,0;$ $0,0,0$	(42) m $x,y,\bar{y}$	(43) m x,y,y	(44) $\bar{4}^+$ $x,0,0;$ $0,0,0$
(45) $\bar{4}^+$ $0,y,0;$ $0,0,0$	(46) m $\bar{x},y,x$	(47) $\bar{4}^-$ $0,y,0;$ $0,0,0$	(48) m x,y,x

- The n-fold rotations have the coordinates of the rotation axis.
- The mirror symmetry (m) have the plane of symmetry indicated.
- We see the presence of roto-inversion symmetries.

Miller Indices and Symmetries

- The point groups shows have all the symmetries around axis we described before (see next slide). Many other elements are present that ensures the closure property of the group.
  - 1 and $\bar{1}$
  - The counter clockwise 3 and 4-fold
  - The roto-inversion $\bar{3}$ and $\bar{4}$ (not $\bar{2}$ because it is equivalent to a mirror symmetry)
  - 2-fold symmetries around the edges that are the composition of two 4-fold symmetries.





3 directions <100>, symmetry 4
6 directions <110>, symmetry 2
3 plans {100} of symmetry

4 directions <111>, symmetry 3
6 plans {110} of symmetry

Crystals and Symmetries

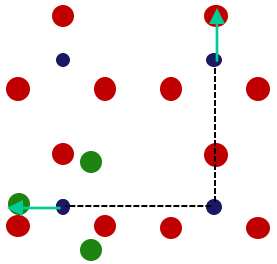
- Each point group must be associated to a certain Bravais Lattice, but all kind of new symmetries can come from merging a Motif in a Lattice

Crystal System	Lattice	Required symmetry	Point groups
Cubic	Cubic	3-fold axes along body diagonals	$23, m\bar{3}, \bar{4}3m, 432, m\bar{3}m$
Tetragonal	Tetragonal	4-fold axis	$4, \bar{4}, 4/m, 422, 4mm, \bar{4}m2, 4/mmm$
Hexagonal	Hexagonal	6-fold axis	$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/mmm$
Trigonal	Hexagonal or Rhombohedral	3-fold axis	$3, \bar{3}, 32, 3m, \bar{3}m$
Orthorhombic	Orthorhombic	Three mutually perpendicular 2-fold axes or mirror planes	$222, 2mm, mmm$
Monoclinic	Monoclinic	2-fold axis or mirror plane	$2, m, 2/m$
Triclinic	Triclinic	none	$1, \bar{1}$

From Point Groups to Space Groups

- Considering now the lattice and the motif together, new restrictions appears when looking at the symmetry of the crystal.

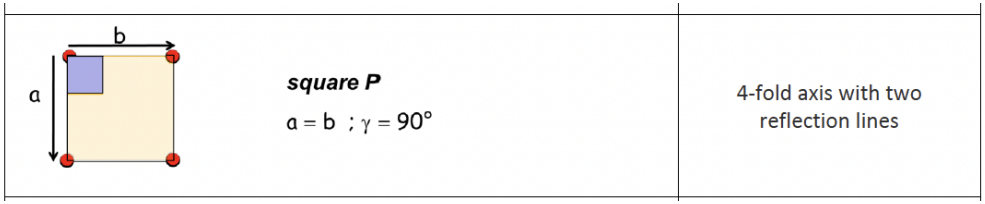
- Since we are limited to 1,2,3,4 and 6 fold rotations because of translational symmetry, we will not be able to construct a crystal with a motif that has a different rotational symmetry element.

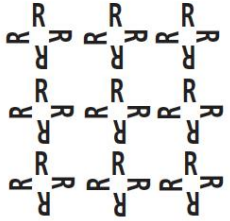


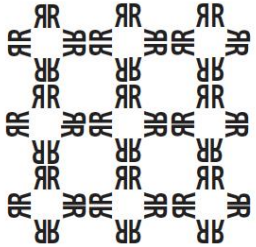
- When we want to merge the symmetry of the motif and the one of the Bravais lattice, restrictions occur and the symmetry of the crystal will result of this analysis.
  - The rotational symmetry of the motif must coincide with the one of the Lattice;
  - So each point group can be associated to a certain Bravais Lattice, but all kind of new symmetries can come from merging a Motif in a Lattice.

Symmetries in 2D: Plane Groups

- Exemple: 4 fold symmetry will only be associated to the square lattice.

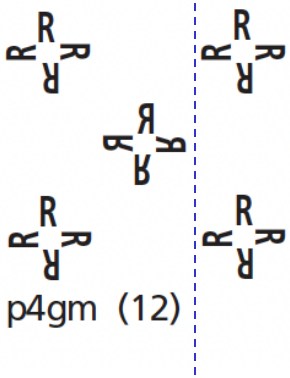



p4 (10)


p4mm (11)

- One could think that there is only 2 plane groups (like space groups but in 2D) associated with the 2 point groups noted 4 and 4mm.

- There is however a third one ! Associated to a glide plane symmetry noted g.
- Adding glide and screw symmetries create a new class of group of symmetries called space group in 3D.


p4gm (12)

Symmetries in 3D: Space Groups

- The construction of the space groups associated to the 3D 14 Bravais lattices, from the 32 3D point groups, proceed similarly, with noticeable differences:
  - 3D has 32 point groups and not 10, because of extra possible symmetry operations: inversion and roto-inversion.
  - For glide planes, the glide can happens along different directions in 3D;
  - Screw axis operations also occur: n_m is a n-fold rotation followed by a translation

- The first letter is a capital letter indicating the Bravais lattice, and many different types occur: P, I, F, and other letters depending on the base-centered plane.

- Glides bring several new types of symmetries and notations:
  - a,b,c: glide translation along half the lattice vector of this face;
  - N,d: glide translation along half and a quarter respectively, along the face diagonal
  - e: two glides with the same glide plane and translation along two half-lattice vectors.

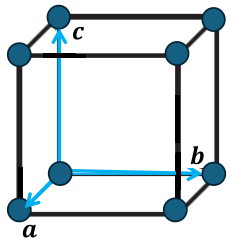
- There are 230 space groups that can be built from the 32 point group in 3D.

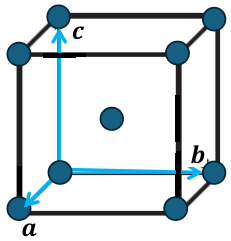
- A list of all the space groups can be found here: https://en.wikipedia.org/wiki/List_of_space_groups

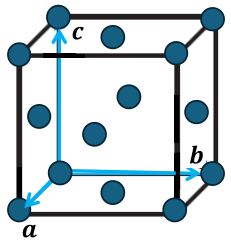
- A more concise one: https://en.wikipedia.org/wiki/Space_group

- You can find them all here: https://onlinelibrary.wiley.com/iucr/itc/Ac/contents/

Symmetries in 3D: Space Groups

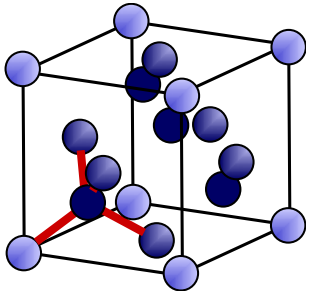




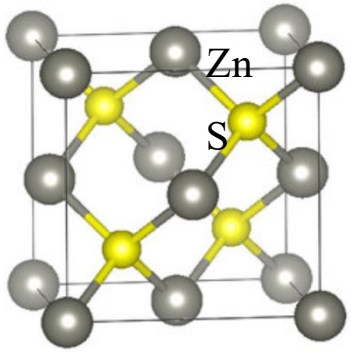


- For the cubic Bravais Lattice, the BCC and FCC structures add atoms that do not change the symmetry operations !
- Space groups are then $P4/m\bar{3}2/m$, $\mathrm{I}4/m\bar{3}2/m$ and $\mathrm{F}4/m\bar{3}2/m$ respectively.

- What happens when we change the motif ? Diamond structure:
  - The extra atom in this case changes the possible symmetries
  - Space group: $\mathrm{Fd}\bar{3}m$ (#227): apparition of a glide symmetry.
  - Also highly symmetric, order of the group 48 !



- As the motif is more complex, the symmetry of the resulting crystal tends to be lower.
  - Space group $\mathrm{F}\bar{4}3m$ (#216): less symmetries ! Order of the group 24

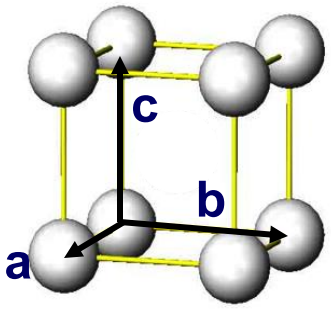


The cubic system

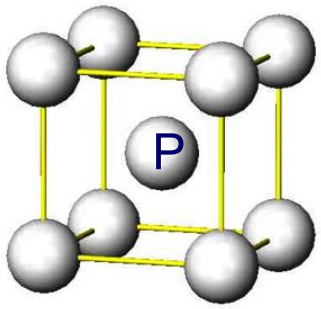
- Symmetry is an important way to approach the crystalline state. However, it is equally important and very useful to describe crystals in a more geometric way.
- This approach leads to deeper understanding of crystal orientations, X-ray diffractions and reciprocal spaces.
- To represent crystals, we use different types of unit cells. The conventional unit cell is the most commonly used as it exhibits the symmetry of the crystal. They can however contain several motifs.
- Primitive unit cells are cells with one motif.

- In this approach, number theory and Euclidean geometry find profound usefulness.

- (**a**,**b**,**c**) is not a basis for the BCC, as P has the coordinates (½, ½, ½).



Primitive cubic
basis: (**a**,**b**,**c**)



$$\vec{a}' = \frac{1}{2}(-\vec{a} + \vec{b} + \vec{c})$$

$$\vec{b}' = \frac{1}{2}(\vec{a} - \vec{b} + \vec{c})$$

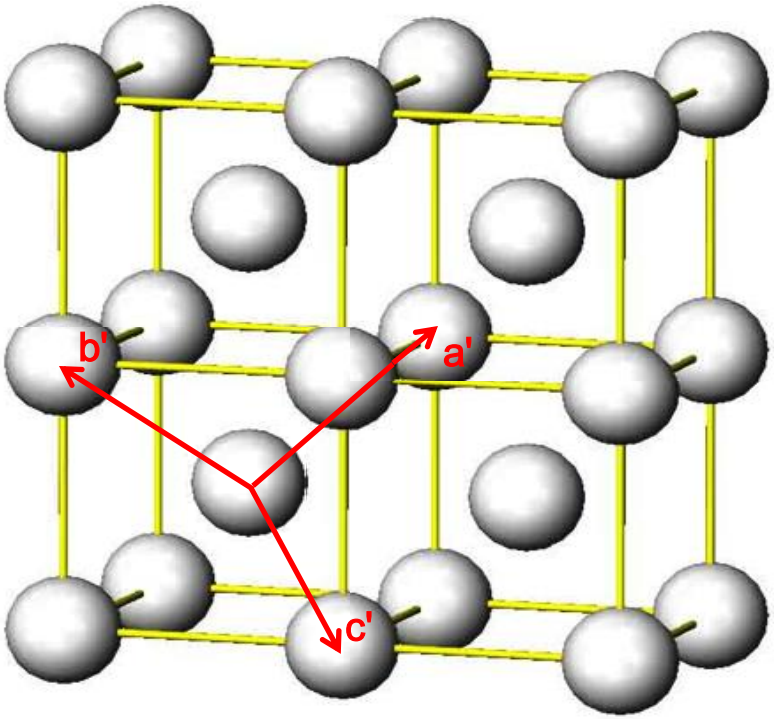
$$\vec{c}' = \frac{1}{2}(\vec{a} + \vec{b} - \vec{c})$$

Body-centered cubic
basis: (**a'**,**b'**,**c'**)

The cubic system

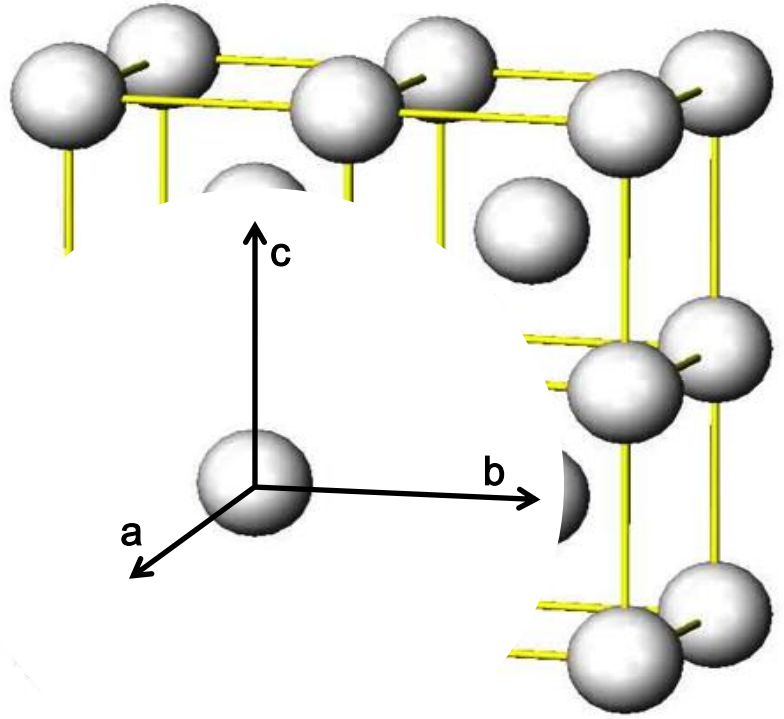
Primitive cell

- Find the motif;
- Translate it along the BCC lattice;



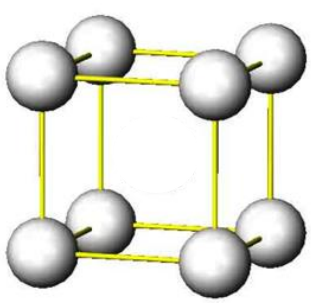
Conventionnal cell

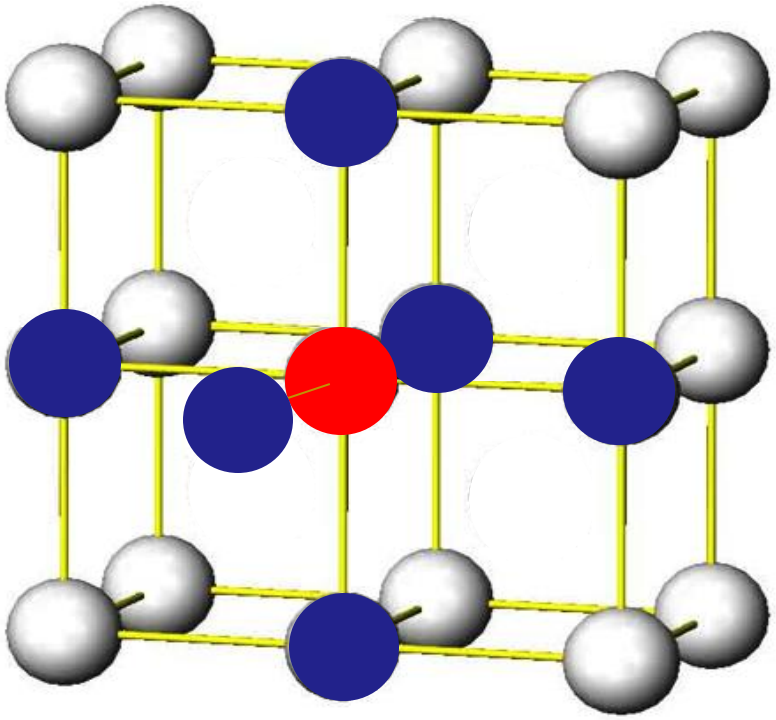
- Find the motif;
- Place it within the Conventional cell;
- Translate the cell along the orthonormal basis **a**, **b** and **c** of the cubic system;



Coordination

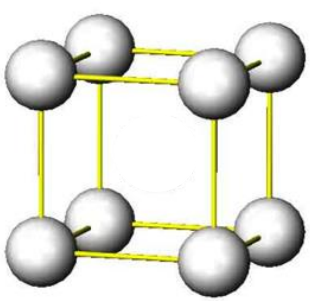
- One can represent atoms as rigid spheres to give some insights about the atomic arrangement and resulting properties.
- A first important notion is the coordination number: number of closest neighbors, ie when spheres are in contact.
- For primitive cubic:



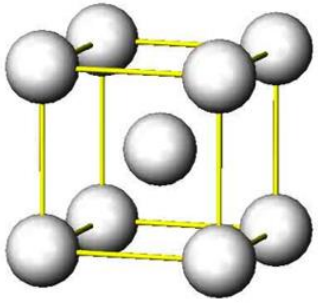


Coordination

- Coordination number:



6



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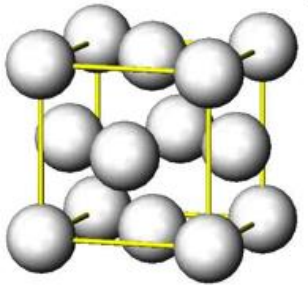
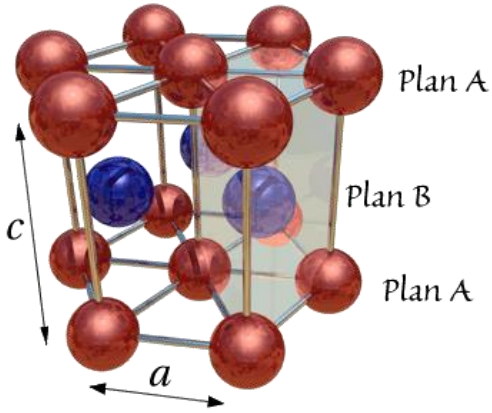


12

- Close-packed planes



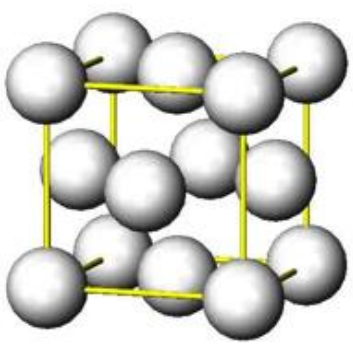
Hexagonal close-packed :

-Coordination: 12

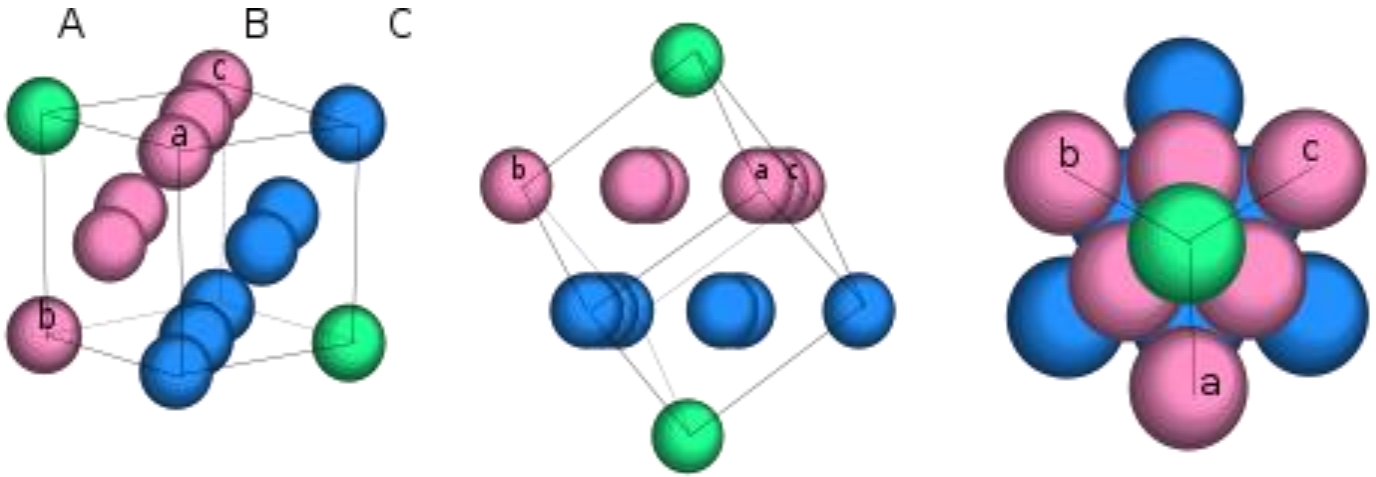
-Close-packed plans are the (1000)

Coordination

- Face-centered Cubic:



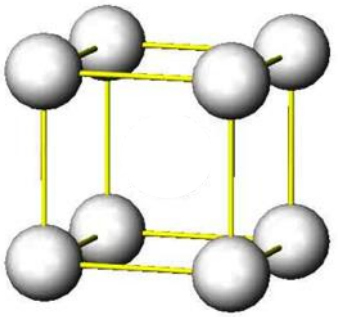
- Coordination: 12
- Close-packed plans (111)



Empilement compact Cubique Faces Centrées
(cubic close- pack CCP, ABC)

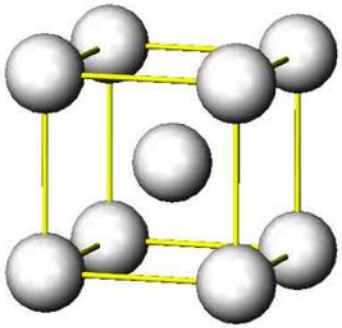
The hard sphere model

- What do we mean by densely packed ?



Simple Cubic structure (sc)

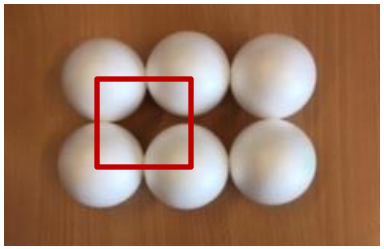
- Is this the denser packing that can be done ?

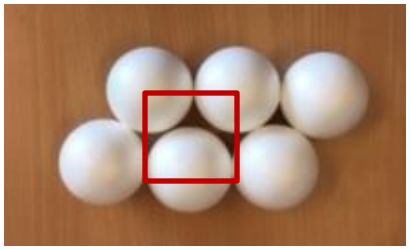


Boddy-centered Cubic structure (bcc)

The hard sphere model

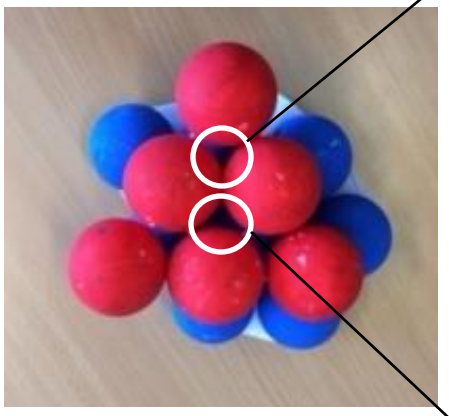
- 2D configuration:

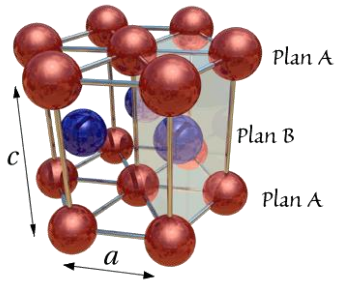




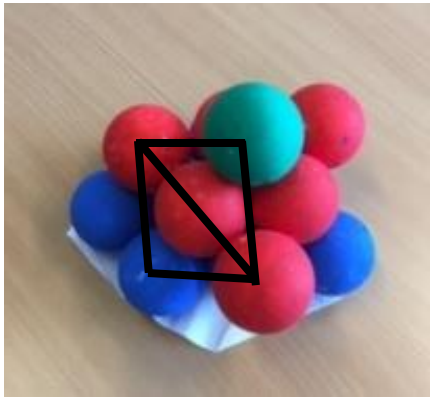
- 3D configuration:

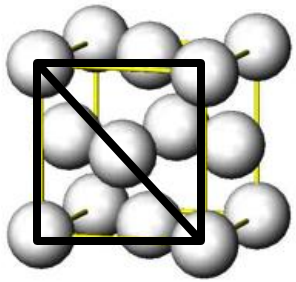
2 possibilities:





Hexagonal Compact



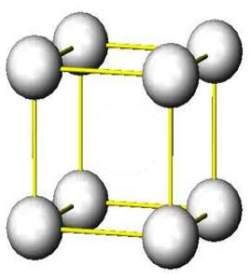


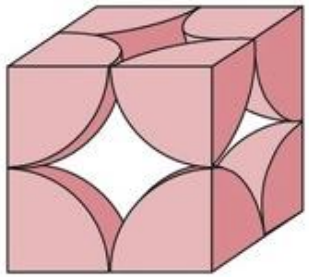
Face-centered Cubic

Number of atoms per unit cell

- Primitive cubic:

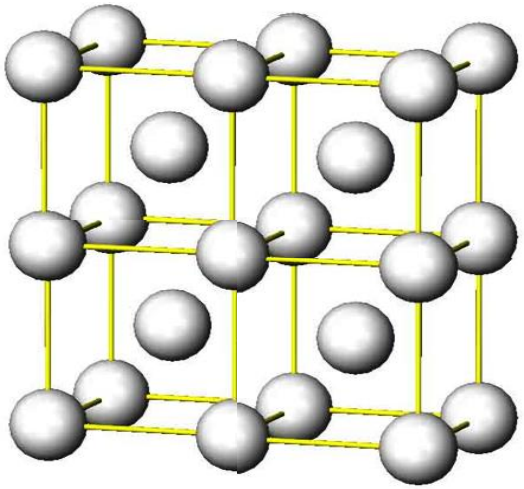
  - Motifs at the corners of the cube count for 1/8
  - The primitive cell has as expected 1 motif.





- Body-centered conventional cell:

  - Motifs at the corners of the cube count for 1/8
  - The motif inside the cell count for 1.
  - Hence the BCC conventional unit cell has 2 motifs.



Density and Free volume

From basic geomtric and vectorial consideration of the unit cell, one call calculate key properties of materials such as density and free volume.

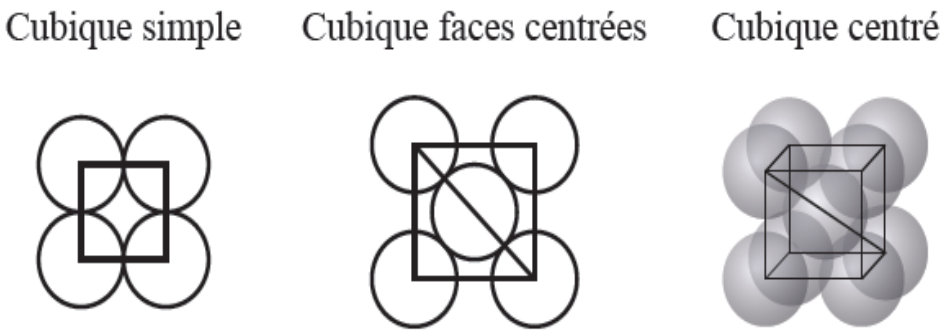
- Density: $\rho = \frac{N_{atoms\ per\ unit\ cell} \times m_{atoms}}{V_{unit\ cell}}$

$$\rho = \frac{N_{atomes\ par\ mailles} \times m_{atome}}{V_{maille}}$$

-Packing fraction:

$$c = \frac{N_{atomes\ par\ mailles} \times V_{atome}}{V_{maille}}$$

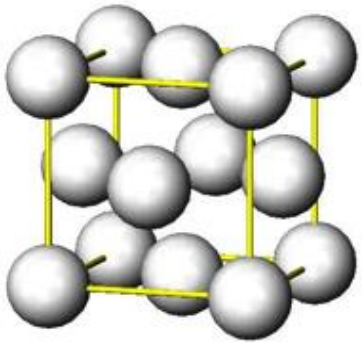
-Direction and planes of high density



Structure of Metals

- Most metals crystalize in the BCC or FCC structure:

Face-centered Cubic (FCC)

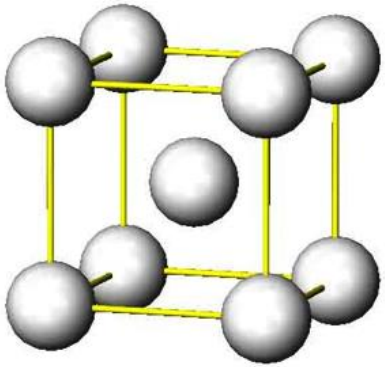


Al – Cu – Ni – Ag – Au – Fe …

Free volume : **26%**

Iron exhibits polymorphism, ie has different equilibrium structures at different temperatures:

Body-centered Cubic (BCC)



Cr – Fe – Mo – V – W – Ta …

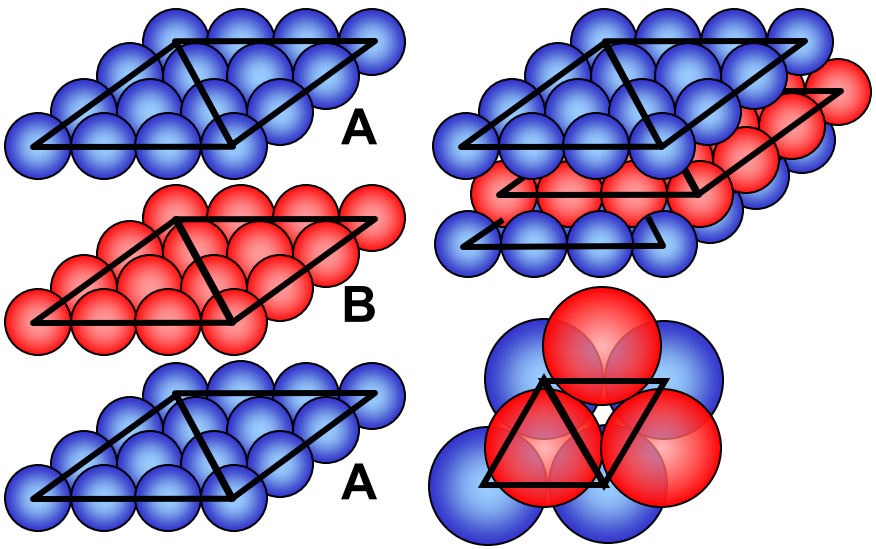
Fe: bcc for T > 1403ºC and T < 910ºC

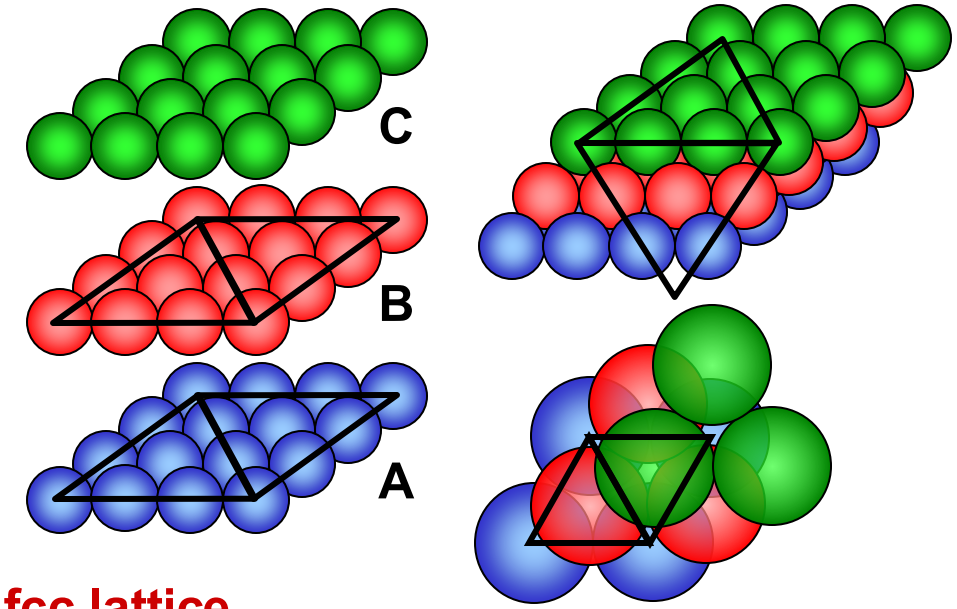
fcc for 910ºC < T < 1403ºC

Free volume : **32%**

Hexagonal compact vs. FCC

- The FCC and the hexagonal compact structures are constructed from very similar atomic arrangements.





hc lattice

Atoms in the basal plan (0001) stack in a sequence: **A – B – A – B – A – B …**

Zn – Mg – Ti – Zr …

fcc lattice

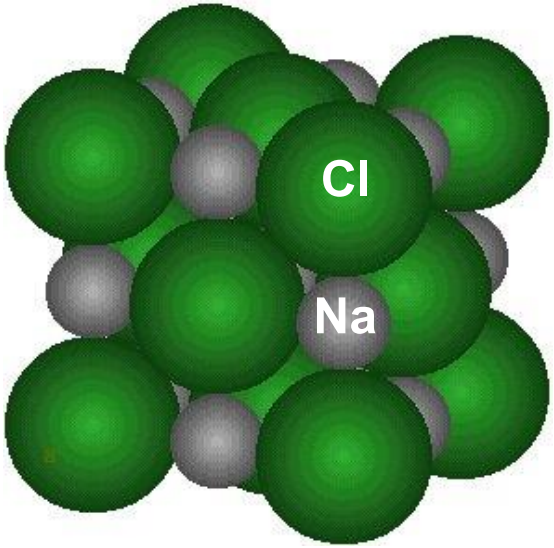
Atoms in the plan (111) stack with the sequence:

A – B – C – A – B – C – A …

Al – Cu – Ni – Ag – Au – Fe …

Structure of Ceramics

- Ceramics possess ionic or covalent (or polar) bonds that are very strong.
- The structure can be compact like metals but more complex, as it depends on the ionic radius of the different atoms, and their valence.
- As a result, the crystallographic arrangements can be quite complex and they have a higher ability to be quenched into an amorphous structure.
- Some simple cases where the structure mostly depends on the ratio of the atomic radius:

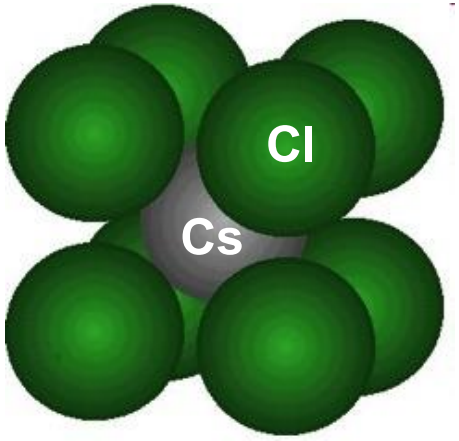


NaCl

R_{Na+} = 1.02 Å

R_{Cl-} = 1.81 Å

6	Coordination	8
0.56	Rapport R_c/R_a	0.92



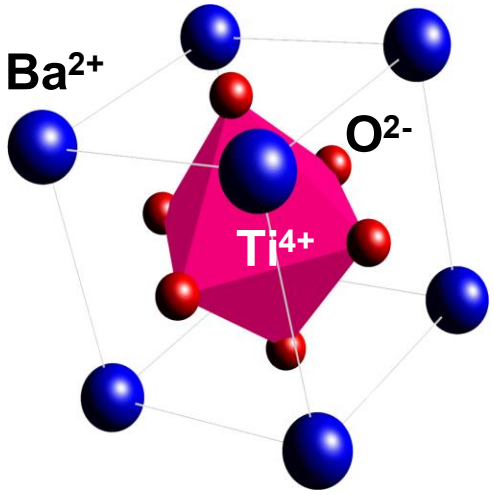
CsCl

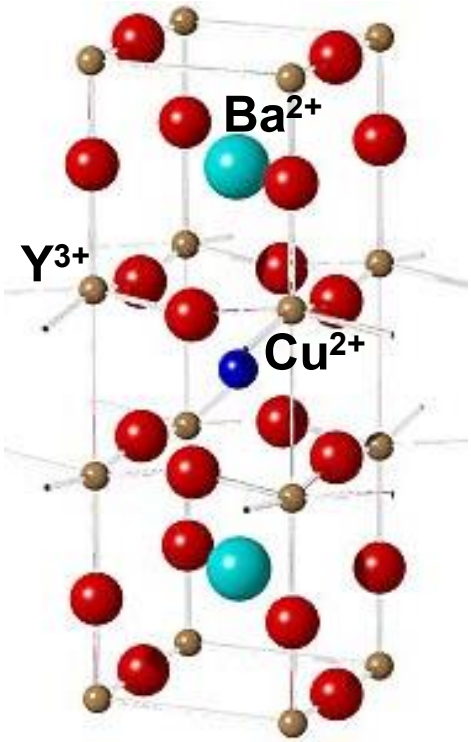
R_{Cs+} = 1.67 Å

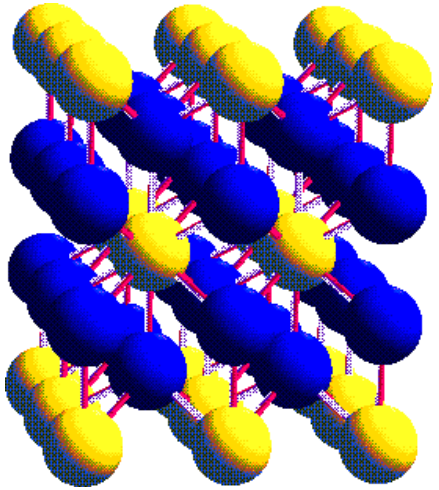
R_{Cl-} = 1.81 Å

Structure of Ceramics

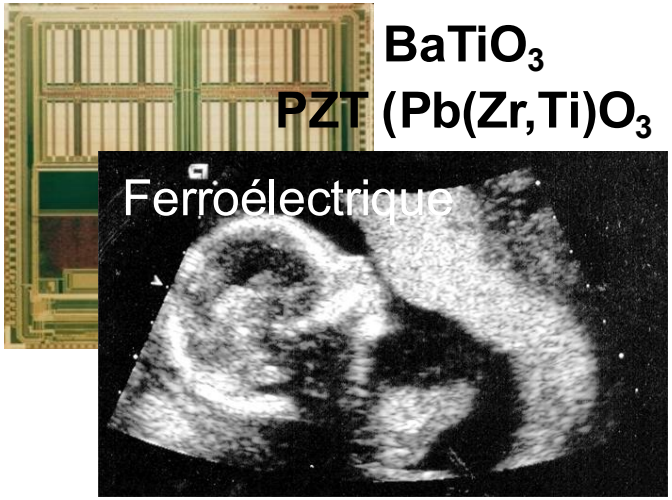
- A few "high tech" ceramics with more complex structures:





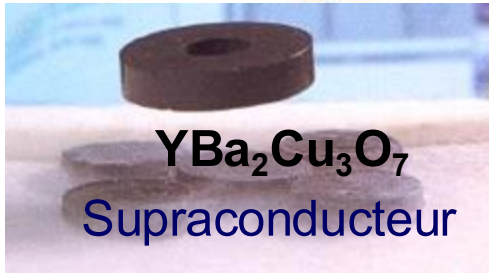


$MoSi_2$



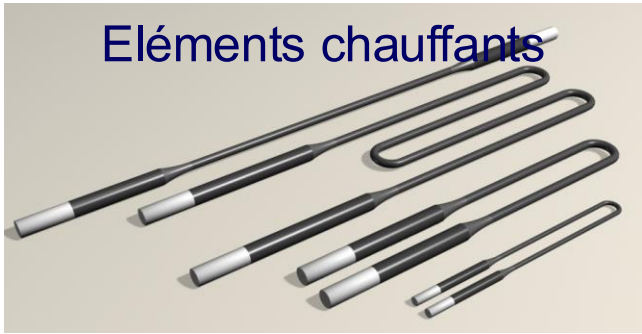
$BaTiO_3$

PZT $(Pb(Zr,Ti)O_3$



$YBa_2Cu_3O_7$

Supraconducteur



Structure of Ceramics

Argile (kaolin)

$(Si_2O_5)Al_2(OH)_4$

Concrete

gravier + quartz + ciment

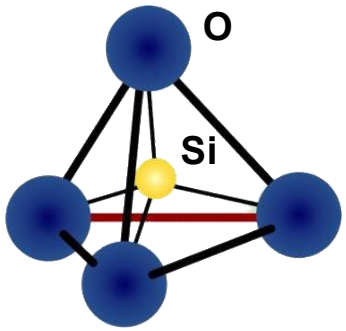
Ciment is a mix of:

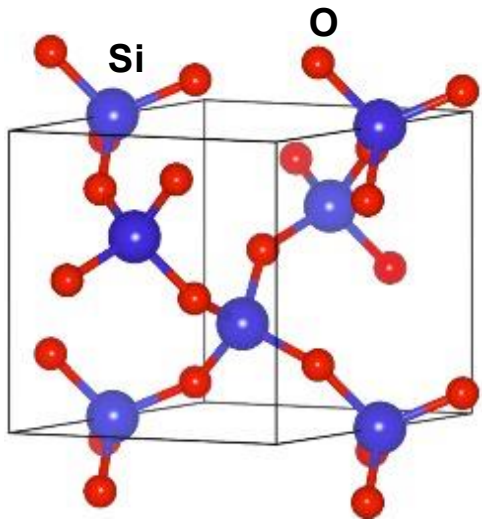
$(CaO)_2SiO_2$ - $(CaO)_3SiO_2$

$(CaO)_3Al_2O_3$ - $(CaO)_4Al_2O_3Fe_2O_3$

Quartz

Tétraèdre $(SiO_4)^{4-}$



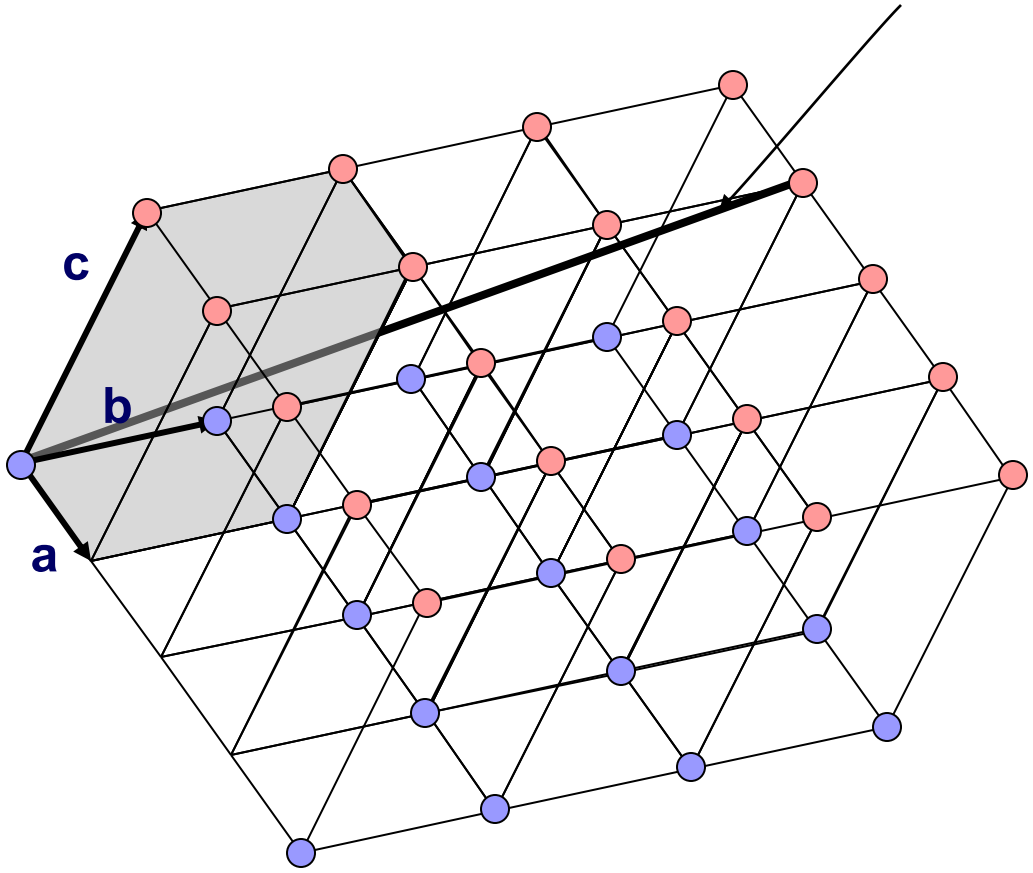


Crystal directions

- Crystal directions are lines that pass through at least two lattice points.
- The direction can be defined by an origin (all lattice point can be an origin) and the coordinate of the other point in the lattice basis.
- The coordinates, which are relative integers, represent the Miller indices.

Crystal Direction : **r** = λ(**1a** + **3b** + **1c**)

[1 3 1]



Basics of Euclidean Geometry

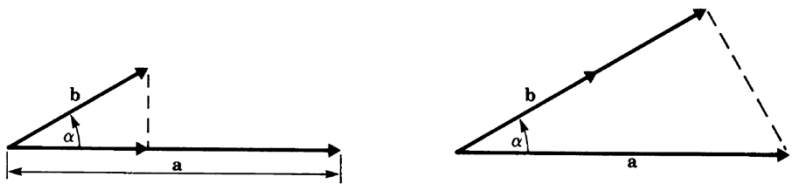
- If we define an origin (0,0,0), all vectors are generated by the linear combination of (1,0,0), (0,1,0) and (0,0,1), that in engineering are often referred to as $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$.
- A vector $\boldsymbol{a}$ is then a linear combination: $\exists (a_x, a_y, a_z) \in \mathbb{R}^3$: $\boldsymbol{a} = a_x \boldsymbol{i} + a_y \boldsymbol{j} + a_z \boldsymbol{k}$
- The following notation will be used: $\boldsymbol{a} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}$
- Reminders:
  - The magnitude (or norm) of a vector: $\|\boldsymbol{a}\| = \sqrt{{a_x}^2 + {a_y}^2 + {a_z}^2}$
  - The scalar (or dot) product: an algebraic operation that provides the $\mathbb{R}$-vector space with an inner product. In cartesian coordinates, for two vectors in the **orthonormal basis** $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$, we have:

$$\boldsymbol{a}.\boldsymbol{b} = a_x b_x + a_y b_y + a_z b_z$$

  - The dot product brings forward the notions of length, angle and orthogonality. A geometric definition for two vectors that form an angle α is:

  - With $a = \|\boldsymbol{a}\|$ and $b = \|\boldsymbol{b}\|$. It is the projection of $\boldsymbol{a}$ on $\boldsymbol{b}$, or of $\boldsymbol{b}$ on $\boldsymbol{a}$.
  - If $\boldsymbol{a}$ and $\boldsymbol{b}$ are orthogonal, then $\boldsymbol{a}.\boldsymbol{b} = 0$.

$$\boldsymbol{a} \cdot \boldsymbol{b} = ab\cos\alpha$$



Basics of Euclidean Geometry

Cross product

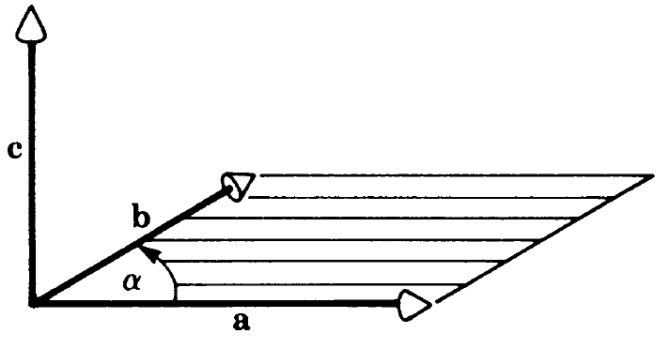
- The cross product of two vectors forming an angle α is a vector perpendicular to these vectors, with the magnitude:

$$\|\boldsymbol{a} \times \boldsymbol{b}\| = ab\sin\alpha$$

- In an orthonormal basis (***i,j,k***), the Cross product of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is:

$$\boldsymbol{a} \times \boldsymbol{b} = (a_y b_z - a_z b_y)\boldsymbol{i} + (a_z b_x - a_x b_z)\boldsymbol{j} + (a_x b_y - a_y b_x)\boldsymbol{k}$$

- Examples: Torques and the Lorentz force.



- $\boldsymbol{a} \times \boldsymbol{b} = -\boldsymbol{b} \times \boldsymbol{a}$
- $\boldsymbol{i} \times \boldsymbol{j} = \boldsymbol{k}$
- Two parallel vectors have a zero cross product.
- See exercices in chapter 1&2 of the book.

- Calculation methods:
  - Determinant:

$$\boldsymbol{a} \times \boldsymbol{b} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix}$$

  - Practical way: :

$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \times \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \times \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} \boldsymbol{i} - \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \times \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} \boldsymbol{j} + \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \times \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} \boldsymbol{k}$$

Basics of Euclidean Geometry

- **Line**:
  - A line is defined by 2 points $A = \begin{pmatrix} x_A \\ y_A \\ z_A \end{pmatrix}$ and $\mathrm{B} = \begin{pmatrix} x_B \\ y_B \\ z_B \end{pmatrix}$ or a point A and a direction $\boldsymbol{AB} = \begin{pmatrix} x_B - x_A \\ y_B - y_A \\ z_B - z_A \end{pmatrix}$:
  - This can be expressed in two ways:
    - Parametric equation: $D = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \; \exists \lambda \in \mathbb{R}, \boldsymbol{AM} = \lambda \boldsymbol{AB} \right\}$

      which we can write:

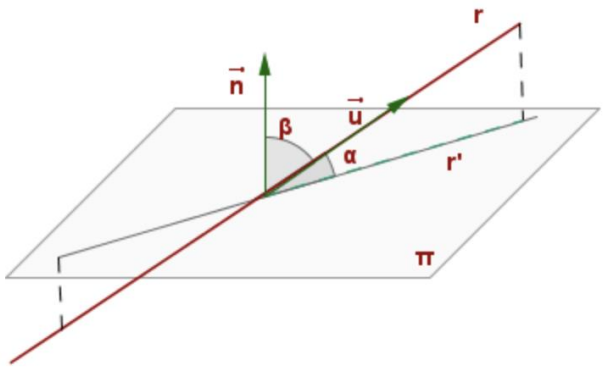
$$\begin{cases} x = x_A + \lambda (x_B - x_A) \\ y = y_A + \lambda (y_B - y_A) \\ z = z_A + \lambda (z_B - z_A) \end{cases}$$

    - A set of linear equations: $D = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \; with \; \begin{matrix} a_1 x + b_1 y + c_1 z - d_1 = 0 \\ a_2 x + b_2 y + c_2 z - d_2 = 0 \end{matrix} \right\}$
- **Plane**:
  - A plane is defined by 3 points $A = \begin{pmatrix} x_A \\ y_A \\ z_A \end{pmatrix}$, $\mathrm{B} = \begin{pmatrix} x_B \\ y_B \\ z_B \end{pmatrix}$ and $\mathrm{C} = \begin{pmatrix} x_C \\ y_C \\ z_C \end{pmatrix}$ or a point A and a normal $\boldsymbol{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$
  - This can be expressed in a simple way as: $P = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \boldsymbol{AM}.\boldsymbol{n} = 0 \right\}$
  - One can extract the linear equation: for $(a, b, c, d) \in \mathbb{R}^4, P = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, ax + by + cz - d = 0 \right\}$
  - Note that a line is the intersection of two planes !

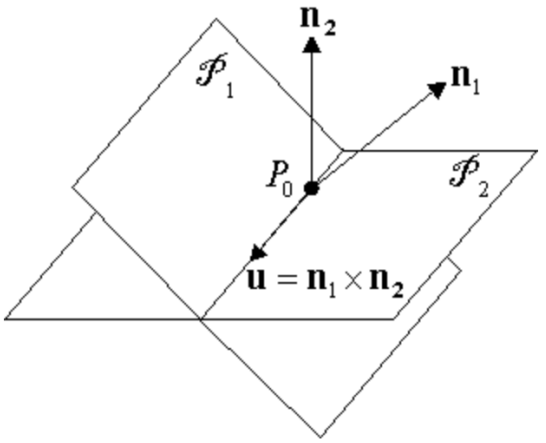
Basics of Euclidean Geometry

- **Angles**
  - The angle between two vectors can be calcluated from the dot or the scalar products.

- Angle between a line and a plane:
Complementary of the angle between the line direction and the normal of the plan

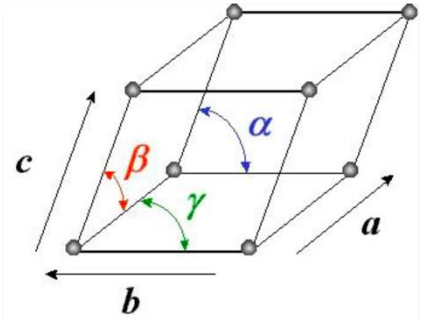


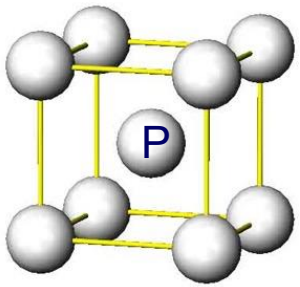
- Angle between two planes:
Angle between their normals:



- **Volume**

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

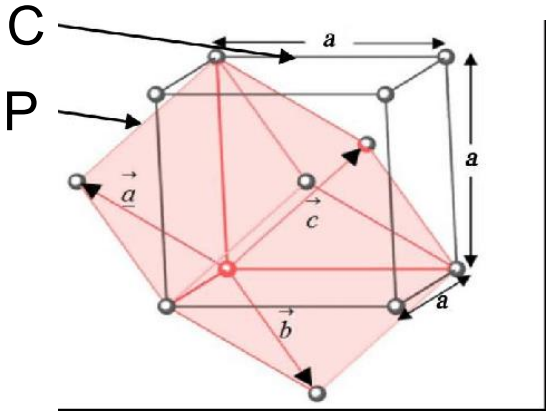




$$a' = \frac{1}{2}(-a + \vec{b} + \vec{c})$$

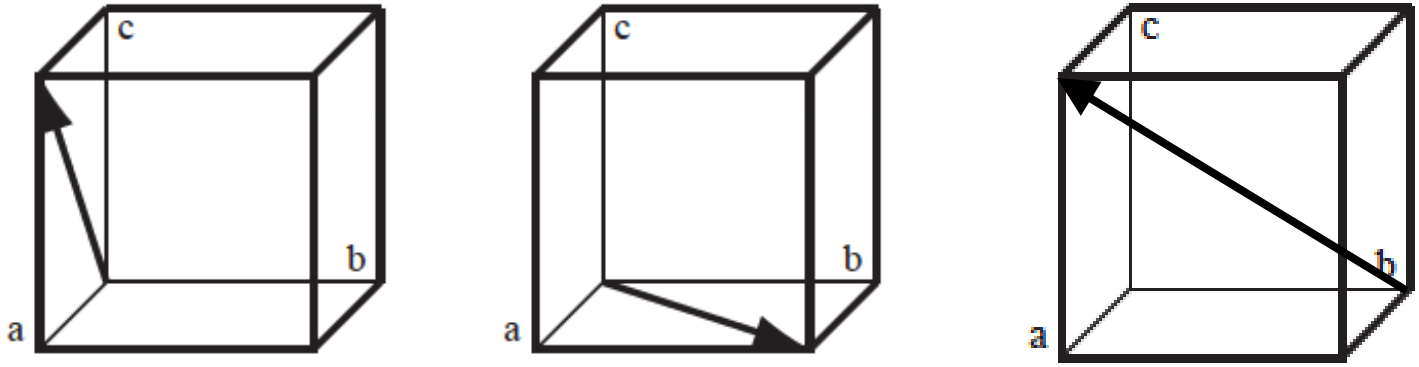
$$\vec{b}' = \frac{1}{2}(a - \vec{b} + \vec{c})$$

$$c' = \frac{1}{2}(a + \vec{b} - \vec{c})$$



Crystal directions

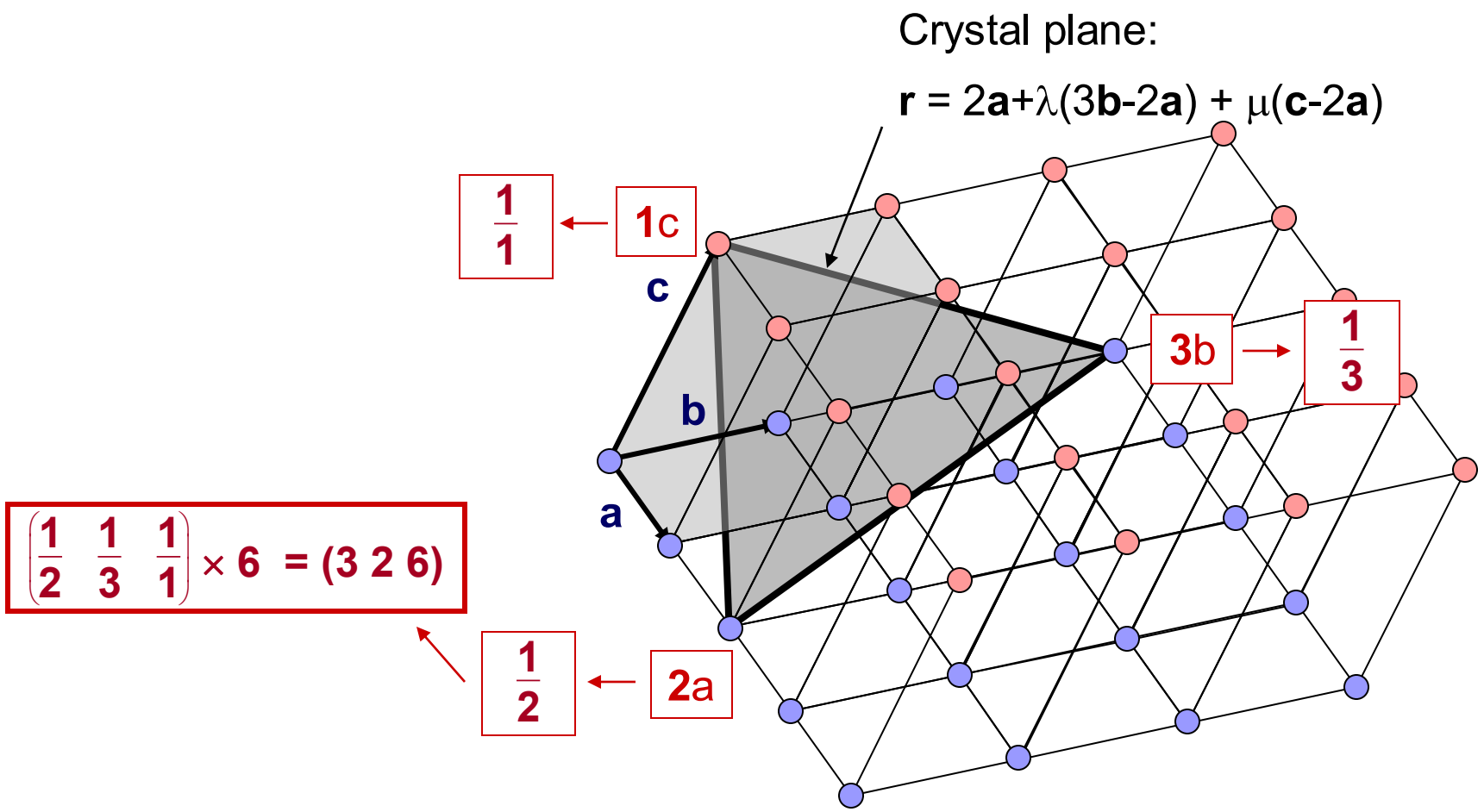
- Exemples:



- Negative indices are represented with a barre above the number.
- If the origin is translated, the lines obtained remain parallel.
- If the axis are rotated by 90° , so is the direction. However, the atomic arrangement and physical properties along the direction remains the same from symmetry !

Crystal planes

- Crystal planes are planes that pass through at least 2 lattice points.
- They can be defined by the intercept of the plan with the basis axis:

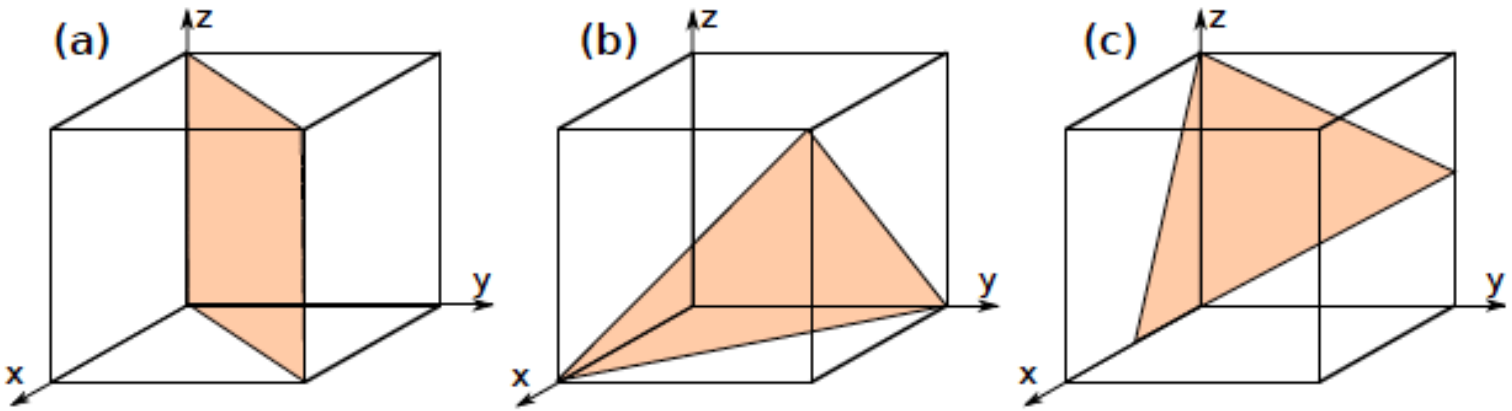


Crystal planes: Miller indices

- If the plane passes through the origin, one can translate the plane, or translate the origin, by one cell parameter along a basis vector.
- Find the coefficients (α, β, γ) such that the plan intercepts the axes (x,y,z) at $(\alpha a, \beta a, \gamma a)$ (a being the conventional lattice parameter, or the cube edge);
- If the plan is parallel to an axis, the intersection is considered to happen at infinity… (so the inverse will be zero).
- Take the inverse of these coefficients and multiply them by their lowest common multiplier (lcm)

if one of (α, β, γ) is smaller than 1, take the lcm of the coefficients greater than 1.

- The coefficients $h = \frac{lcm(\alpha,\beta,\gamma)}{\alpha}$, $\mathrm{k} = \frac{lcm(\alpha,\beta,\gamma)}{\beta}$, $l = \frac{lcm(\alpha,\beta,\gamma)}{\gamma}$ are the Miller indices of the plane
- These coefficients are co-prime !



$\mathbb{N}$ and $\mathbb{Z}$ - Divisibility

- Divisibility, congruent and prime numbers are essential parts of number theory.

- Euclidean division:

Given two integers $(a,b) \in \mathbb{Z}^2$, with $b \neq 0$, there exist unique integers q and r such that:

$a = bq + r$ and $0 \leq r < |b|$,

- Demonstration (hints):

Existence: consider $(a,b) \in \mathbb{Z} \times \mathbb{N}^*$, and the set $E = \{p \in \mathbb{Z},\ a \geq bp\}$

- E is not empty and is bounded.
- E therefore has a maximum q such that $q \in E$ and $\forall p \in E, p \leq q$.
- We define the relative integer r as $r = a - bq$:
  - $r \geq 0$ since $q \in E$ and hence $a \geq bq$;
  - $r < b$ since otherwise $q+1 \in E$ which is impossible.

Unicity: let's (q,r) and (q',r') verify the relation above, we have: $b(q'-q) = r-r'$

Since $r < |b|$ and $r' < |b|$, $|r-r'| < |b|$, which implies that $|q-q'| < 1$, so $q = q'$ and also $r = r'$

- Given two integers $(a,b) \in \mathbb{Z}^2$, a divides b if there exists an integer q such that $a = bq$.

- An equivalent definition is a divides b if and only if the rest r of the Euclidean division is zero.

$\mathbb{N}$ and $\mathbb{Z}$ - gcd and lcm

- We consider $\{x_k, k \in \mathbb{N}, and\ x_k \in \mathbb{Z}^*\}$.

- The set of the dividers of the x_k admits a maximum, called the greatest common divider and defined as gcd(x_k).

It exists because the ensemble is not empty (1 divides all x_k) and it is bounded (by any of the x_k).

Reminder: every set of finite number of integers admits an upper and lower bound.

- The set of the multiples of the x_k admits a minimum, called the lowest common multiple and is defined as lcm(x_k)

It exists since the product of the x_k is a common multiple, and it is bounded since it is greater than one.

Note that if the x_k are of different signs, we usually consider the gcd and lcm of their absolute values.

- Modular arithmetic:
  - Given an integer n > 1, called a modulus, two integers a and b are said to be congruent modulo n, noted $a \equiv b[n]$ if n is a divisor of their difference.

$\mathbb{N}$ and $\mathbb{Z}$ - prime numbers

- A prime number is a number greater than one that is only divided by 1 and itself.
- *p* is a prime number if and only if *a* divides *p* implies that *a =1* or *a* = *p*.
- Fundamental theorem of arithmetic (unique factorization, or prime factorization theorem):
  - Every integer greater than 1 can be represented uniquely as a product of prime numbers, up to the order of the factors.
    In other words, for all integers *n* there exists prime numbers p_i and integers n_i $(1 \leq i \leq k)$, such that

$$n = \prod_{i=1}^{k} p_i^{n_i}$$

- Demonstration:
  - Existence: using strong induction: 2 is a prime. If it is true for all integers < n, either n is prime, or there is two integers *a* and *b* such that *n*=*ab*. Since *a* < *n* and b < n, *a* and *b* have a representation in prime numbers, and so also does *n*.
  - Uniqueness: Let's *n* be the smallest integer to have two sets of primes p_i and q_i such that $n = p_1 \ldots p_k = q_1 \ldots q_l$. p_1 divides $q_1 \ldots q_l$, so according to the Euclid lemma, p_1 divides one of the q_i, which by re-ordering could be q_1. Since they are both primes, $p_1 = q_1$. As a result, $p_2 \ldots p_k = q_2 \ldots q_l < n$, which contradicts the hypothesis on *n*.
  - Euclid's lemma: If a prime *p* divides the product *ab* of two integers *a* and *b*, then *p* must divide at least one of those integers *a* or *b*. We will see it soon using the relation of Bezout.
- Prime numbers are the building blocks, the fundamental particles, of numbers.
- A parallel can be made between prime numbers and bonds in materials !

$\mathbb{N}$ and $\mathbb{Z}$ - mutually prime numbers

- Two integers *a* and *b* are mutually prime (or co-prime, relatively prime), if *gcd(a,b) = 1*.
  In other words, they don't have a common prime number in their factorization.

  Example: 6 and 25 are not prime numbers but are mutually prime: 6 =2x3 and 25 = 5^2

- This definition can be extended to *n* integers x_i , which are called mutually prime if *gcd(x_1,…,x_n) = 1*.

- Theorem of Bézout:
  For *n* non zero integers x_i, $gcd(x_1, \dots, x_n) = d$. Then, $\exists\ (d_1, \dots, d_n) \in \mathbb{Z}^n$ such that

$$\sum_{i=1}^{n} d_i x_i = d$$

- Proof:
  Let's consider the set $S = \{\sum_{i=1}^{n} u_i x_i, : (u_1, \dots, u_n) \in \mathbb{Z}^n \ and \sum_{i=1}^{n} u_i x_i \ > 0\}$
  S is not empty ($x_1 or -x_1 \in$ S) and it is then bounded and has a minimum $\mathrm{d} = \sum_{i=1}^{n} d_i x_i$.
  d divides all x_k : if $x_k = dq_k + r_k$, and $0 < r_k < d$, then $r_k = (1 - d_k q_k)x_k + \sum_{k \neq i} d_i x_i \ \in S$ which contradicts that d is the minimum of S, so necessarily $r_k = 0$ and *d* divides x_k.
  d is the gcd: if $\exists\ c, \forall k, c/x_k$, then c/d, and hence necessarily $c \leq d$.
  So *d* is the greatest divider of all x_k, or *d* = *gcd(x_1,…,x_n)* and the *(d_1, …, d_n)* verify the proposition.

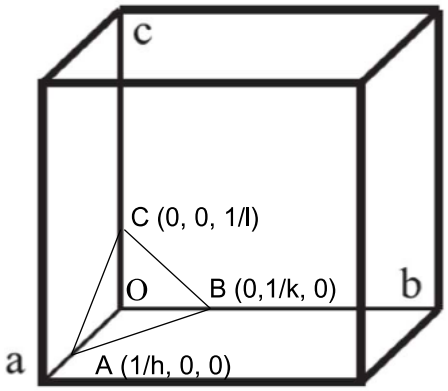
- No need to know the proofs of theorems, but rather the idea of the proof, and how to apply a theorem to practical problems as we see in exercises.

$\mathbb{N}$ and $\mathbb{Z}$ - mutually prime numbers

- Important corollary to Bézout's theorem:
  If *n* non zero integers x_i are mutually prime, or co-prime, ie if $gcd(x_1, \dots, x_n) = 1$,
  then $\exists\ (d_1, \dots, d_n) \in \mathbb{Z}^n$ such that:

$$\sum_{i=1}^{n} d_i x_i = 1$$

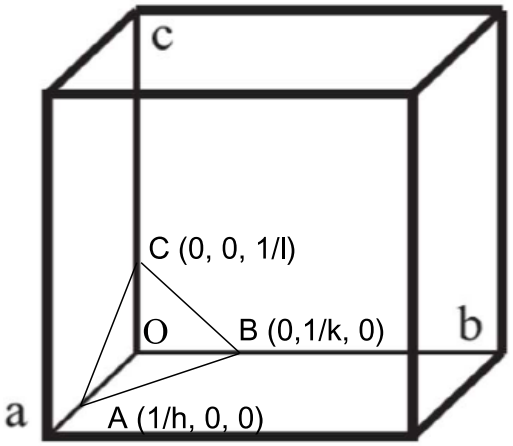
- Important results from Bézout formulation:
  - If for *n* integers x_i, there is $(d_1, \dots, d_n) \in \mathbb{Z}^n$ such that $\sum_{i=1}^{n} d_i x_i = 1$, then the x_i are mutually prime.
    Straightforward since if $\delta = \gcd(x_i)_{\ 1 \le i \le n}$ then $\delta | \sum_{i=1}^{n} d_i x_i$ and so $\delta = 1$.
  - Corollary: $\forall\ (a, b, c)(\mathbb{Z}^*)^3, \{c|b\ \&\ \gcd(a, b) = 1\} \Longrightarrow \gcd(a, c) = 1.$
  - Gauss Theorem: $\forall\ (a, b, c) \in (\mathbb{Z}^*)^3, \{a|bc\ \&\ \gcd(a, b) = 1\} \Longrightarrow a|c$



- For any three co-prime numbers (*h,k,l*), the plane shown here cutting the axis at points A, B and C is a crystal plane.

  This can be shown using Bézout relation !

Crystal (or lattice) planes



- This plan can be defined in two ways:
  - $P = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \boldsymbol{AM}.\boldsymbol{n} = 0 \right\}$ where $\boldsymbol{n}$ is the normal to the plane;
  - $P = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \boldsymbol{AM} = \lambda \boldsymbol{AB} + \mu \boldsymbol{AC}, (\lambda, \mu) \in \mathbb{R}^2 \right\}$

- The normal to the plane is given by $\boldsymbol{N_{(hkl)}} = \boldsymbol{AB} \times \boldsymbol{AC}$
- **In the cubic system, the direction [hkl] and the planes (hkl) are perpendicular !**
- In an orthonormal basis, the equation of the plane is obtained as follow:

$$\mathcal{P}_1^{(hkl)} = \{(x, y, z) \in \mathbb{R}^3 / hx + ky + lz = a\}$$

- Does it really intercept lattice points ?
- Using Bézout on the co-prime h,k and l numbers defined previously, we hence know that:

$$\exists (n_1, n_2, n_3) \in \mathbb{Z}^3, hn_1 + kn_2 + ln_3 = 1$$

- We can deduct that the point $P(n_1 a, n_2 a, n_3 a) \in \mathcal{P}_1^{(hkl)}$.

SUMMARY

- We introduced the basic notions of divisibility, prime and co-prime numbers, and discussed several important concepts like the Bézout relation, or the Euclid lemma, that can be useful in understanding discrete configurations such as Bravais lattices.

- We also reviewed basic calculation in 3D geometry involving vectors, directions and planes.

- We use all these notions to review a foundational aspect of Materials Science that is crystallography and the structure of materials. Notions discussed:
  - Bravais lattices;
  - Crystal directions and planes, Miller indices
  - The cubic structure
  - The hard sphere model

- Next week
  - We will show a few examples of using number theory to approach crystal planes, reciprocal spaces and X-ray diffraction.
  - We will review some properties of real and complex numbers;
  - We will give some examples as to how to manipulate them, and of their use in Materials Science and engineering.