Chapter 1
Generalities

I.1. Introduction

The history of human civilization has evolved through the following ages:

1) The Stone Age, approximately two million years ago, when tools were made from natural materials such as stone, clay, and wood.

2) The Bronze Age, approximately 5,000 years ago. Bronze is an alloy of copper, tin (less than 25%), and other elements.

3) The Iron Age, approximately 3,000 years ago and continuing to the present day. The Iron Age brought tools and utensils.

4) The age of advanced materials brought structural materials, such as composite materials that are both strong and lightweight, and semiconductors such as Si and Ge.

I.2 Classification of materials

One of the first methods of classifying materials is based on their obvious property, namely that there are three states of matter: solid, liquid, or gaseous. This classification is as simple as it seems fairly obvious. 1- Solids retain their shape under normal pressure and temperature conditions.

2- Liquids take the shape of the containers in which they are held. In both cases, we can talk about a defined volume of matter.

3- In gases, on the other hand, the volume of a gas depends on pressure, and the volume and pressure of a gas depend on temperature. Gas properties such as internal energy, specific heat, etc. are parameters that must be measured at constant pressure or constant volume!

Many of the physical, chemical, and functional properties of materials are closely related to the nature of the chemical bonds between their constituent atoms. This is the basis for the distinction between the main classes of materials.

I.2.1 Metals and alloys

Materials in this group are composed of one or more metallic elements (such as iron, aluminum, copper, gold, steel (iron + carbon), brass (copper + zinc), bronze (copper + tin)), and often also non-metallic elements (e.g., carbon, nitrogen, and oxygen) in relatively small quantities. The main properties of metals are:

- Good thermal conductivity
- Good electrical conductivity
- Good resistance to thermal shock
- Opaque (not transparent to visible light) and shiny when polished
- Good formability
- The atoms of metals and their alloys are arranged in a very orderly manner (crystalline

material).

 Consist mainly of metallic bonds

 Compared to ceramics and polymers, they are relatively dense.

 Mechanical properties: relatively rigid and strong, ductile and resistant to fracture.

I.2.2 Ceramics

Ceramics are compounds between metallic and non-metallic elements; they are most often oxides, nitrides, and carbides. There are no free electrons in ceramics and the bond is ionic and/or covalent, making these bonds extremely strong. Ceramics are inorganic crystalline materials.

 Traditional ceramics — clay minerals (e.g., porcelain), bricks, tiles, and cement.

 Advanced ceramics — (aluminum oxide or alumina, Al_2O_3 for spark plugs and microelectronics substrates), (ferrite Fe_3O_4 for magnetic memories used in computers), silicon dioxide (or silica, SiO_2 for electrical insulation), (silicon carbide SiC as an abrasive)

The main properties of ceramics are:

 Relatively rigid and strong—rigidity and strength are comparable to those of metals, very hard, extremely brittle (lack ductility), very sensitive to fracture (i.e., difficult to form).

 Poor thermal and electrical conductivity. Insulates against heat and electricity, low electrical conductivity, and more resistant to high temperatures (i.e., good resistance to high temperatures)

 Optical characteristics - Ceramics can be transparent, translucent, or opaque.

 Good corrosion resistance.

I.2.3 Polymers

A polymer is a large molecule composed of repeating structural units called monomers, often chain-like in nature, whose backbone consists of carbon, hydrogen, and other non-metallic elements (namely O, N, and Si).

These are materials of animal, plant, or synthetic origin: wood, cotton, wool, paper, cardboard, plastic, rubber, leather. The main properties of polymers are as follows:

 Low density, less solid than ceramics and metals.

 Extremely ductile and flexible (i.e., plastic).

 Relatively chemically inert and non-reactive in many environments.

 Easy to shape into complex forms.

 Inexpensive.

 Generally bonded by covalent forces and also by weak van der Waals forces.

 Low electrical conductivity and non-magnetic.

 Low thermal conductivity.

I.2.4 Composite

A composite is made up of two (or more) individual materials from the categories described above, namely metals, ceramics, and polymers, which are immiscible. Objective: to obtain a combination of properties that is not present in a single material. Example:

- Ceramic + metal (brake pad (steel matrix, silicon carbide reinforcement)) (concrete (ceramic matrix, steel reinforcement)),
- Polymer + ceramic (sandpaper (polymer matrix, ceramic reinforcement),
- Metal + polymer (tires (polymer matrix, steel reinforcement)).

I.3. Areas of application

Here are some applications of the main categories of materials:

I.3.1. Areas of use for metallic materials

Construction: Building structures, beams, bridges, railroad tracks (**steel),** windows, doors, roofs, cladding (**aluminum),** pipes, electrical wiring, roofs **(copper).**

Transportation: Airplanes, car bodies, wheel rims (**aluminum),** vehicle engines, train rails, truck bodies **(steel),** aircraft parts, engine components **(titanium).**

Industry: Machine tools, cutting tools, construction equipment **(steel),** industrial machinery, robots, aircraft parts **(aluminum),** gears, bearings, machine components **(bronze).**

Consumer goods: Tools, kitchen utensils, household appliances **(steel),** food cans, beverage cans, kitchen utensils **(aluminum),** jewelry, musical instruments, faucets **(brass).**

Medical applications: Surgical implants, medical instruments, prostheses **(stainless steel),** dental implants, bone plates, joint prostheses **(titanium),** joint prostheses, dental implants, surgical instruments **(cobalt-chrome).**

Figure I.1. Some areas of use for metallic materials

I.3.2. Areas of use for ceramics

Pottery: Ceramics have been used for centuries to make pots, bowls, and other utilitarian and decorative objects.

Sculpture: Ceramics can be used to create both figurative and abstract sculptures.

Tiling: Ceramic tiles are used to decorate floors, walls, and roofs.

Bricks: Ceramic bricks are used to build walls and other structures.

Tiles: Ceramic tiles are used to cover roofs

Sanitary ware: Sinks, toilets, and washbasins are often made of ceramic.

Cutting tools: Ceramic tools are used to cut hard materials such as metal and glass.

Medical implants: Ceramic implants are used to replace damaged joints and other tissues.

Filters: Ceramics are used to make filters for gases and liquids.

Figure I.2. Some areas of use for ceramics

I.3.3. Areas of use for polymers

Bottles and containers: Plastic bottles for beverages and containers for household products are made from polyethylene terephthalate (PET), high-density polyethylene (HDPE), and polypropylene (PP).

Food films: Plastic films are used to wrap food to protect it from air, moisture, and contaminants. They are made from PE, PP, and polyvinyl chloride (PVC).

Pipes and tubes: Plastic pipes and tubes are used for water supply, sewage disposal, and the transport of gas and chemicals. They are made from PVC, HDPE, and polyvinylidene chloride (PVDC).

Windows and doors: Plastic windows and doors are lighter and more energy efficient than wood or aluminum windows and doors. They are made from PVC and composite polymers.

Flooring: Plastic flooring, such as vinyl flooring and carpet tiles, is durable, easy to clean, and affordable. It is made from PVC, PP, and PET.

Automotive: Dashboards, seats, and door trim are made from PP, PS, and ABS. Bumpers, fenders, mirrors, and taillights are made from PP, ABS, and polycarbonate (PC). Fuel tanks, air intake pipes, and hose clamps are made from nylon, PE, and PP.

Textiles: Polymer materials are used in the textile industry to manufacture fibers, fabrics, and clothing. Polyester, nylon, and acrylic are used to make clothing, upholstery fabrics, and technical textiles.

Technical clothing, such as sportswear and diving suits, is made from waterproof, breathable, and durable fabrics.

Biomedical: Surgical instruments, such as scalpels and forceps, are made from stainless steel and polymers that are resistant to heat and chemicals. Artificial organs, such as heart valves and pacemakers, are made from biocompatible polymers that are resistant to bodily fluids.

Implants, such as hip and knee replacements, are made from biocompatible polymers such as titanium and PEEK (PolyEtherEtherKetone).

Figure I.3. Some areas of polymer use

I.3.4. Areas of use for composites

Aeronautics: Carbon-based composites are used for their lightness and strength, improving the energy efficiency of aircraft and satellites.

Automotive: Carbon-based composites are used to reduce vehicle weight and improve fuel economy. They are used to manufacture lighter and stronger seats, dashboards, and door trim.

Bridges, buildings, and other structures: Glass and carbon composites are used for their strength and durability, enabling the construction of lighter, more energy-efficient structures.

Sports equipment: Composites are used to make lighter, higher-performance tennis rackets, golf clubs, skis, and bicycles.

Prosthetics and implants: Composites are used to make lighter and stronger prosthetics and implants.

Others: sandpaper, glass wool,

Figure I.4. Some areas of application for composites

Example: What are the different materials used in the manufacture of a car?

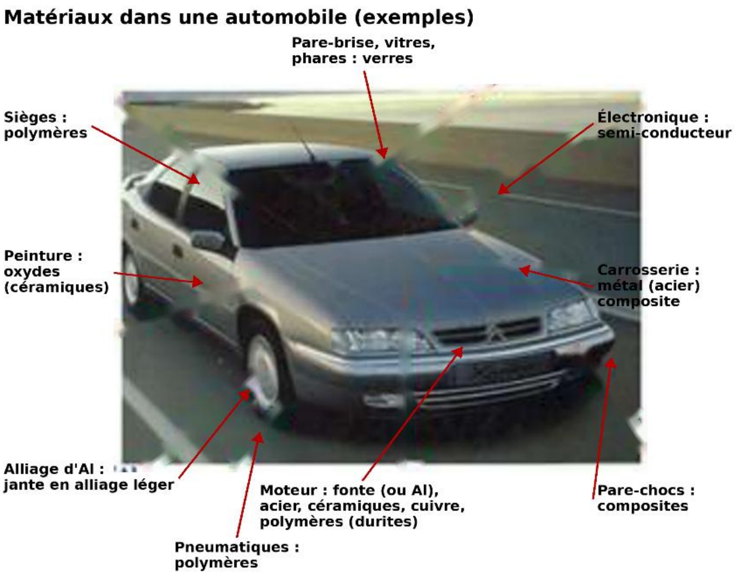


Figure I.5. Different materials used in a car

I.4. Structure of materials

I.4.1. Amorphous materials

An amorphous compound is a compound in which the atoms do not follow any order at medium and long distances, which distinguishes it from crystallized compounds. Glasses, elastomers, and liquids are amorphous compounds.

I.4.2. Crystalline materials

This is a network that reproduces the arrangement of atoms in a crystal; it is defined as a solid body that consists of the periodic repetition in the three dimensions of space of an atomic or molecular pattern, contained in a periodic repeating unit called a lattice, in the same way that wallpaper consists of the repetition of the same pattern.

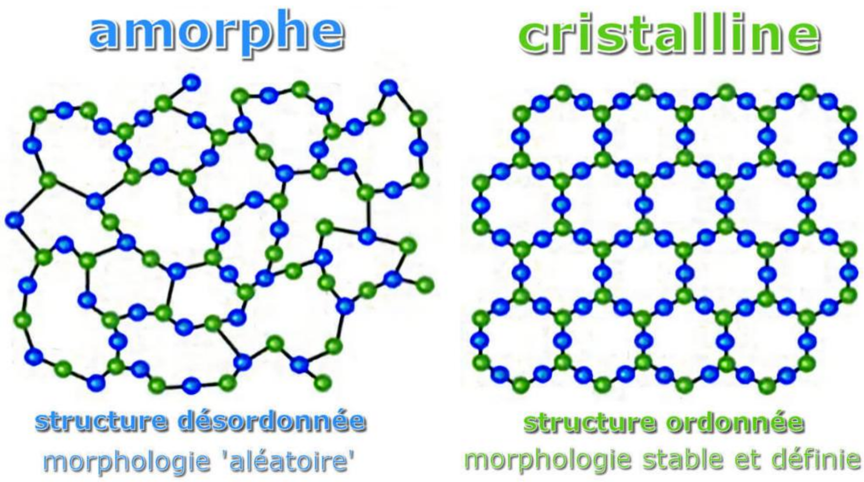


Figure I.6. Types of structures

I.4.3. The difference between amorphous and crystalline structures

The properties of amorphous bodies differ greatly from those of crystalline bodies. Amorphous bodies are characterized by the chaotic arrangement of their atoms, which gives them a disordered internal structure (like a liquid). An amorphous body has no natural geometric shape; they are like frozen liquids.

Today, amorphous solids are of great interest in the field of technology. Amorphous semiconductors can replace electronic components. Computer memories have been developed using amorphous materials.

Criterion	Crystalline structure	Amorphous structure
Arrangement of atoms	Orderly and repetitive	Disordered and random
Shape	Well-defined geometric	Amorphous
Physical properties	Anisotropic	Isotropic
Melting point	Single melting point	No defined melting point
Examples	Table salt, quartz, diamond	Glass, plastic, wax

Table I.1. The difference between amorphous and crystalline structures

I.5. Concepts of crystallography

Crystallography is a science that studies crystals, i.e., the formation, growth, external shape, internal structure, and physical properties of crystallized matter. Crystallography is gradually moving away from mineralogy and closer to physics and chemistry, becoming an independent science.

Crystalline bodies are characterized by flat faces, straight edges, and vertices such as: F + S = A + 2

Where: F: faces, S: vertices, A: edges.

I.5.1 Crystal lattices

A geometrically perfect single crystal is a set of ions evenly distributed in space. To describe this arrangement, **a crystal lattice** is defined as a set of nodes obtained from **an elementary cell** that determines the three-dimensional periodicity of repetition **of an elementary pattern** (see diagram opposite).

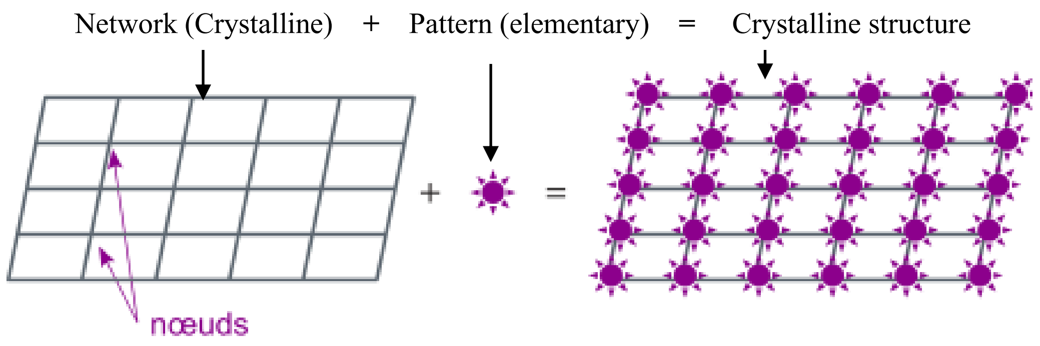


Figure I.7. Crystal structure

The unit cell is a parallelepiped defined by the three primitive vectors, also called lattice parameters. Note that the angles between vectors a, b, and c can be arbitrary. The position of a given vector in the lattice is given by the vector r= ua + vb + wc (with u, v, and w as integers), which generally represents a translation of the lattice.

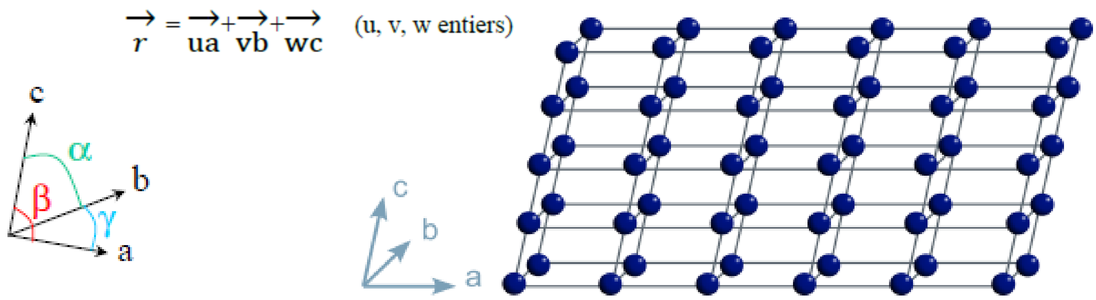


Figure I.8. Crystal lattice

To represent the type of distribution of lattice points in space, seven different coordinate systems are required. These coordinate systems are called crystal systems. We can also give names to crystal systems based on geometric shape and symmetry. The seven crystal systems are:

(1) Cubic

(2) Tetragonal

(3) Orthorhombic

(4) Monoclinic

(5) Triclinic

(6) Trigonal (or rhombohedral)

(7) Hexagonal.

In 1948, Bravais showed that 14 lattices are sufficient to describe all crystals. These 14 lattices are known as Bravais lattices. They are classified into seven crystal systems based on the parameters of the cells or lattice points present per unit cell.

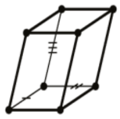
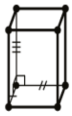
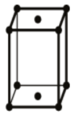
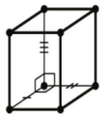
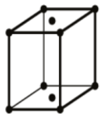
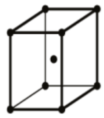
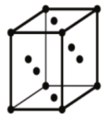
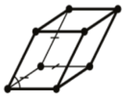
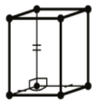
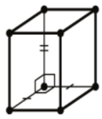
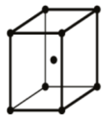
Système cristallin	Relations entre les axes	Relations entre les angles	Réseaux de Bravais			
			simple	à bases centrées	centré	à faces centrées
triclinique	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$				
monoclinique	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$				
orthorhombique	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$				
rhomboédrique	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$				
hexagonal	$a = b \neq c$	$\alpha = \beta = 90°$ $\gamma = 120°$				
quadratique	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$				
cubique	$a = b = c$	$\alpha = \beta = \gamma = 90°$				

Table I.2. Fourteen crystal structures (or Bravais lattices)

However, although their shapes are similar from one mineral to another, they vary in **size**. The length, width, and height of a lattice are specific to each crystalline chemical form.

Examples:

Hexagonal: many metals, including cobalt and zinc Titanium, zirconium, cadmium, hafnium , have a variant of the hexagonal crystal structure called "compact hexagonal."

Simple cubic: the only element that is simple cubic is polonium

Face-centered cubic: many metals, including lithium, sodium, potassium, and chromium, iron α, tantalum, vanadium, molybdenum

Face-centered cubic: many metals, including copper, silver, gold, and platinum, aluminum, nickel

Trigonal: quartz, calcite

I.5.2. Crystal directions and planes

Now that we know how atoms organize themselves to form crystals, we need a way to identify the directions and planes of the atoms.

Deformation under load occurs on certain crystal planes and in certain crystallographic directions.

Other properties of materials (electrical conductivity, thermal conductivity, modulus of elasticity) can vary within a crystal with orientation.

Many properties and processes of materials vary with direction in crystallographic directions and planes are described using three integers—Miller indices.

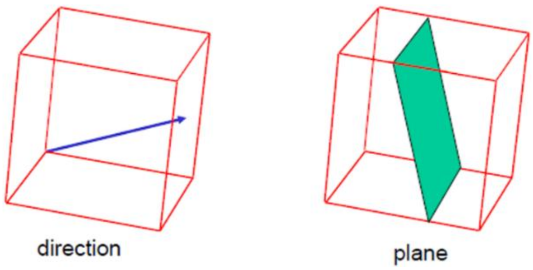


Figure I.9. Crystallographic directions and planes

I.5.3. Miller indices of the direction

1) Draw a vector in the elementary mesh that is parallel to the direction and passes through the origin;

2) Project the vector onto the axes and express its coordinates in the basis (a, b, c);

3) Remove the units [ua vb wc]---[uvw], for example [2a 3b 5c]--[2 3 5].

4) The uvw are multiplied and divided by a common factor to reduce them to the smallest integer values

5) Designate the direction by [uvw]

6) All parallel directions have the same Miller indices; direction family <uvw>

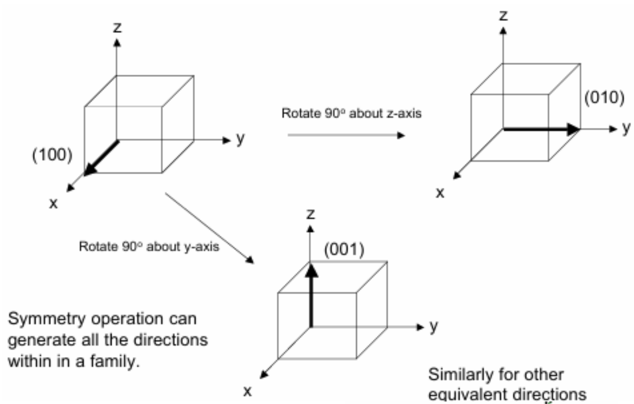
7) Material properties along any direction in a family are the same, e.g., [100], [010], [001] in a simple cubic system are the same.

8) For uniform crystalline materials, all parallel directions have the same properties

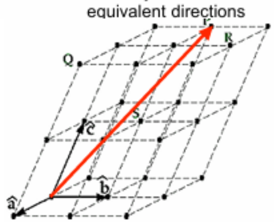
9) Negative index: a bar over the index

Families and symmetry: cubic symmetry

<100> = [100], [010], [001]



Examples



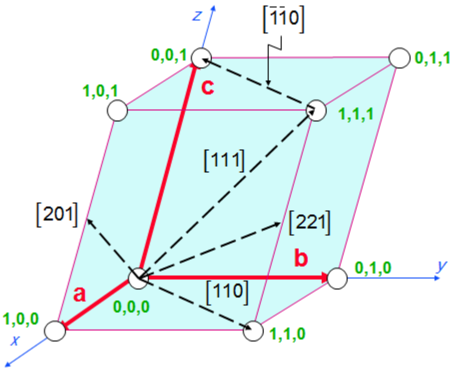
a) What is the lattice point given by point P? -112

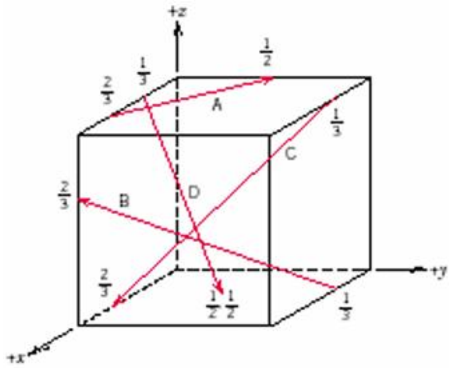
(b) What is the crystallographic direction of the origin of P? [$\bar{1}$12]

To which lattice direction does lattice point 264 correspond?

The lattice direction [132] from the origin.

Determine the indices of the line directions





Draw the following directions: [110], $[\bar{1}\bar{2}1]$, $[\bar{1}02]$

I.5.4. Miller indices of the plane

Draw a plane in the elementary mesh that does not pass through the origin

1. Determine the points of intersection.

2. Take the reciprocals.

3. Reduce the 3 fractions to the lowest common denominator

4. Take the numerators.

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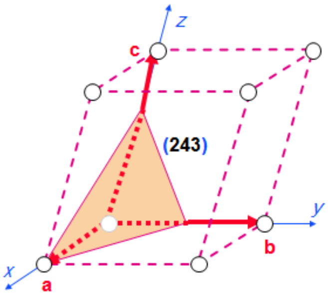
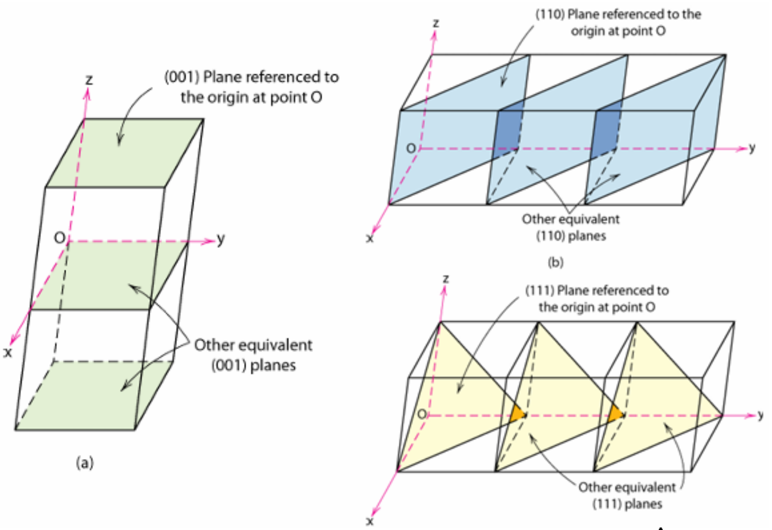
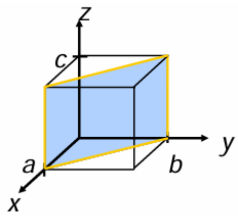


	axes		
step	Ox	Oy	Oz
1	(1) a	(1/2) b	(2/3) c
2	1/1	2/1	3/2
3	2/2	4/2	3/2
4	h = 2	k = 4	l = 3



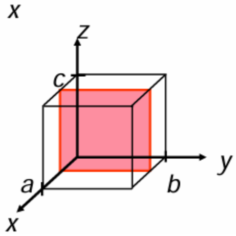
Example

		a	b	c
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		



Example

		a	b	c
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		



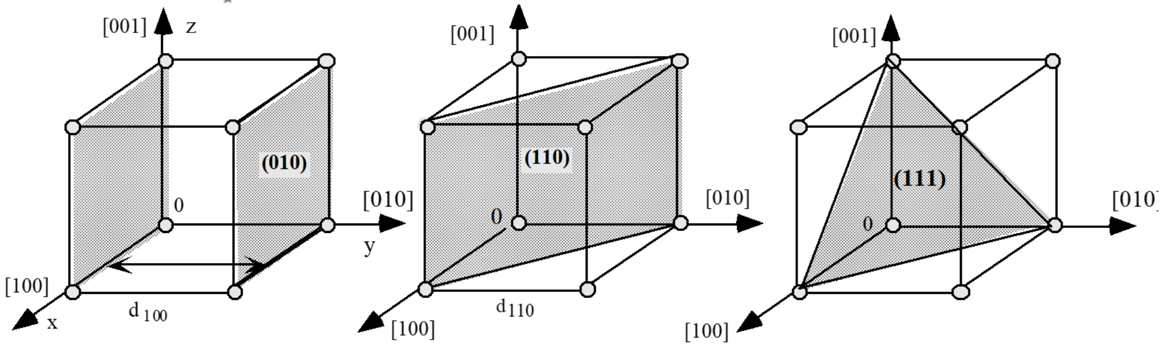


Figure I.10. Some crystallographic planes

I.5.5. Coordination number and number of atoms per unit cell

A unit cell is the smallest representation of an entire crystal. All crystal lattices are made up of repeating unit cells. In a unit cell, the coordination number of an atom is the number of atoms it touches.

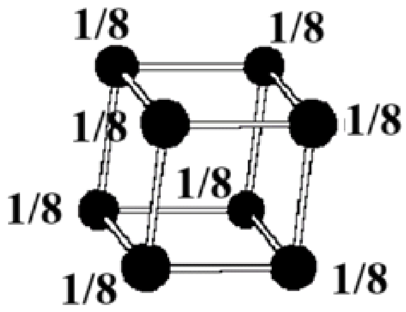
A- Simple Cubic (SC) (primitive **P**)

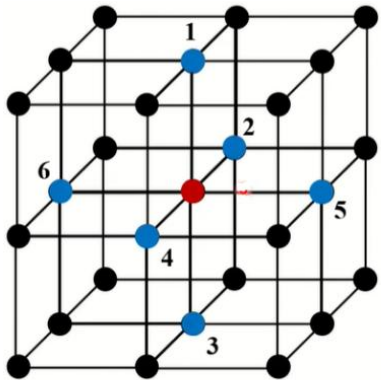
The SC structure consists of ***one atom per lattice***,

8 nodes at the 8 vertices, each shared between 8 lattices; $8 \cdot \frac{1}{8} = 1$

Coordination: number of neighboring motifs at equal distance

The coordination number of CS is **6**.



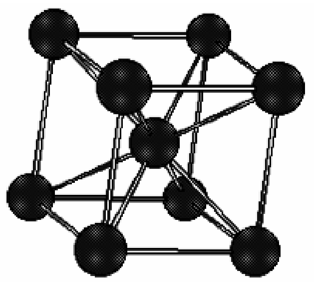


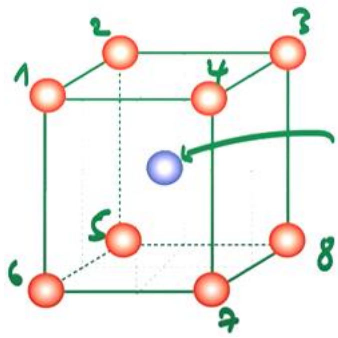
B- Body-centered cubic (BCC) (**I**, from the German Innenzentriestes)

The CC structure consists of ***two atoms per lattice***, one at the center of the cube (1x1=1) and eight nodes at the eight vertices, each shared between eight lattices$8 \cdot \frac{1}{8} = 1$.

Coordinate: number of neighboring motifs at equal distance

The coordination number of CC is **8**.





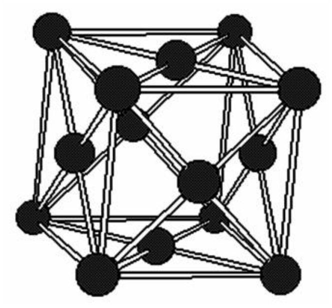
C- Face-centered cubic (FCC) (**F**, from the German Flächenzentriestes),

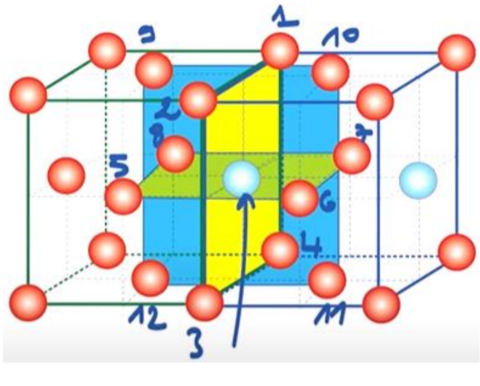
The FCC structure consists of **four *atoms per mesh***,

8 nodes at the 8 vertices, each shared between 8 meshes; $8 \cdot \frac{1}{8} = 1$

6 nodes at the centers of the 6 faces of the cube, each shared between 2 units. 6x1/2 = 3

Coordination: number of neighboring motifs at equal distance. The coordination number of CFC is **12**.



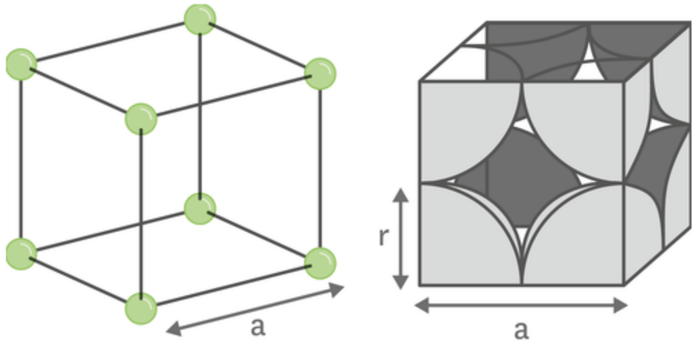


I.5.6. Relationship between the lattice parameter and the atomic radius

a- Simple Cubic (SC)

Contact at the edge:

a = 2r



b- Body-centered cubic (BCC)

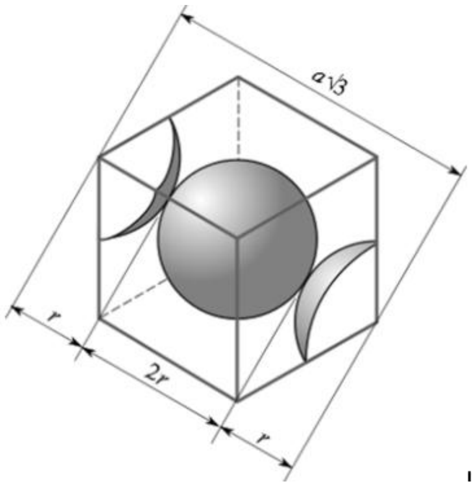
d = diagonal of the cube face d =a √2

D = diagonal of the cube $D^2 = a^2 + d^2 = a^2 + 2.a^2 = 3.a^2$

Let D = √3.a

We also have D = 4.r, hence √3.a = 4r

a = 4.r/√3

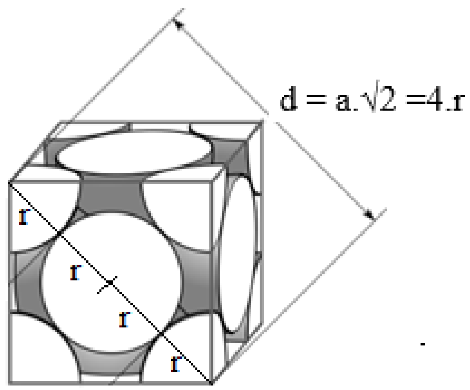


c- Centered Face Cubic (CFC)

d = diagonal of the cube face

d = a.√2 =4.r

Hence: **a= 2.√2.r**



I.5.7. Packing density or compactness

The stacking density or stacking fraction of a stack in a given space is the fraction of space occupied by the figures that make up the stack. In simple terms, it is the ratio between the volume of the bodies in a space and the volume of the space itself. In stacking problems, the goal is generally to obtain a stack with the highest possible density.

ρ = (volume occupied by atoms/volume of the lattice)

a- Simple Cubic (SC)

Volume occupied by atoms: 1 atom/lattice = $(4\pi r^3/3)$

Volume of the lattice = a^3 Let us note that: $a = 2.r$

$\rho = (4\pi r^3/3)/8.r^3 = \pi/6 = 0.52$ **ρ = 52%**

b- Body-centered cubic (BCC)

Volume occupied by atoms: 2 atoms/mesh = $2.(4\pi r^3/3)$

Volume of the lattice = a^3 Note that: $a = 4.r/\sqrt{3}$

$\rho = 2.(4\pi r^3/3)/(4.r/\sqrt{3})^3 = \pi.\sqrt{3}/8 = 0.68$ **ρ = 68%**

3- Face-centered cubic (FCC

Volume occupied by atoms: 4 atoms/lattice = $4.(4\pi r^3/3)$

Volume of the lattice = a^3 Let us note that; $a = 2.\sqrt{2}.r$

$\rho = 4.(4\pi r^3/3)/(2\sqrt{2}.r)^3 = \pi/(3.\sqrt{2}) = 0.74$ **ρ = 74%**