Atomic Structure:

The nucleus consisting of protons and neutrons and the electrons surrounding the nucleus in order to lay a foundation for understanding how atomic structure affects the properties, behavior, and resulting applications of engineering materials. We will see that the structure of atoms affects the types of bonds that hold materials together. These different types of bonds directly affect the suitability of materials for real-world engineering applications. The diameter of atoms typically is measured using the angstrom unit (A^o or 10^{-10} m).

The Structure of the Atom

An atom is composed of a nucleus surrounded by electrons. The nucleus contains neutrons and positively charged protons and carries a net positive charge. The negatively charged electrons are held to the nucleus by an electrostatic attraction. The electrical charge q carried by each electron and proton is 1.6×10^{-19} coulomb (C).

The atomic number of an element: is equal to the number of protons in each atom. Thus, an iron atom, which contains 26 protons, has an atomic number of 26. The atom as a whole is electrically neutral because the number of protons and electrons are equal.

Most of the mass of the atom is contained within the nucleus. The mass of each proton and neutron is 1.67×10^{-24} g. But the mass of each electron is only 9.11×10^{-28} g.

The atomic number (Z) is the number of protons, which is equal to the number of electrons surrounding the nucleus in a neutral atom with electrical charges.

The atomic mass (M), which is equal to the total mass of the average number of protons and neutrons in the atom in atomic mass units, is also the mass in grams.

The Four Quantum Numbers

The quantum numbers are parameters that describe the distribution of electrons in the atom, and therefore its fundamental nature. They are:

1. PRINCIPAL QUANTUM NUMBER (*n*) - Represents the **main energy level, or *shell*, occupied by an electron**. It is always a positive integer, that is $n = 1, 2, 3 ...$

2. SECONDARY QUANTUM NUMBER (*l*) - Represents the energy sublevel, or type of orbital, occupied by the electron. The value of *l* depends on the value of *n* such that $l = 0, 1, ... n-1$.

3. MAGNETIC QUANTUM NUMBER (*ml*) - Represents the number of possible orientations in 3-D space for each type of orbital. Since the type of orbital is determined by *l*, the value of *ml* ranges between $-l$ and $+l$ such that $ml = -l, ...0, ...+l$.

4. SPIN QUANTUM NUMBER (*mS*) - Represents the **two possible orientations** that an electron can have in the presence of a magnetic field, or in relation to another electron occupying the same orbital. Only two electrons can occupy the same orbital, and they must have opposite spins. When this happens, **the electrons are said to be paired**. The allowed values for the spin quantum number *ms* are +1/2 and -1/2.

The maximum possible number of electrons in the primary and secondary shells

أقصى عدد ممكن من الالكترونات في الغلاف الرئيسي	أقصى عدد ممكن من الالكترونات في الغلاف الثانوي	الغلاف الثانوي	الغلاف الرئيسي n
2	2	s	1 = K
8	2	s	2 = L
	6	p	
18	2	s	3 = M
	6	p	
	10	d	
32	2	s	4 = N
	6	p	
	10	d	
	14	f	

Hund's rule states that electrons are distributed as individually in orbitals of equal energy as possible.

Pauli exclusion principle states that within each atom, no two electrons may have the same four quantum numbers, and thus, each electron is designated by a unique set of four quantum numbers. The number of possible energy levels is determined by the first three quantum numbers. only electrons with opposite spins can occupy the same orbital. In other words, ***if two electrons must go into the same orbital, they must be paired***. In the example shown above we have

$\frac{\uparrow\downarrow}{2p_x}$ rather than $\frac{\uparrow\uparrow}{2p_x}$

Solid Materials

Solids materials exist in two distinct types:

1- Crystalline solids

2- Amorphous solids (Non crystalline materials)

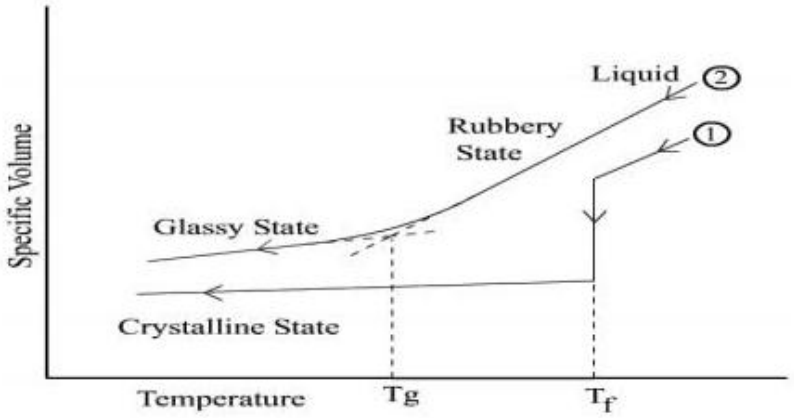
Crystalline solids: contain rows of atoms that are grouped and arranged periodically to form a formation symmetry, Therefore, it has a kind of symmetry, (three-dimension) and its repetition is described as long range order, and its structure can be considered the result of the repetition of a model or unit cell.

Amorphous solids are those whose atoms are collected randomly and without an order, forming a range. So complex that their structure cannot be considered a repetition of any unit cell, they are called amorphous solids, such as carbon, glass (silicon oxide), which are described as short range order.

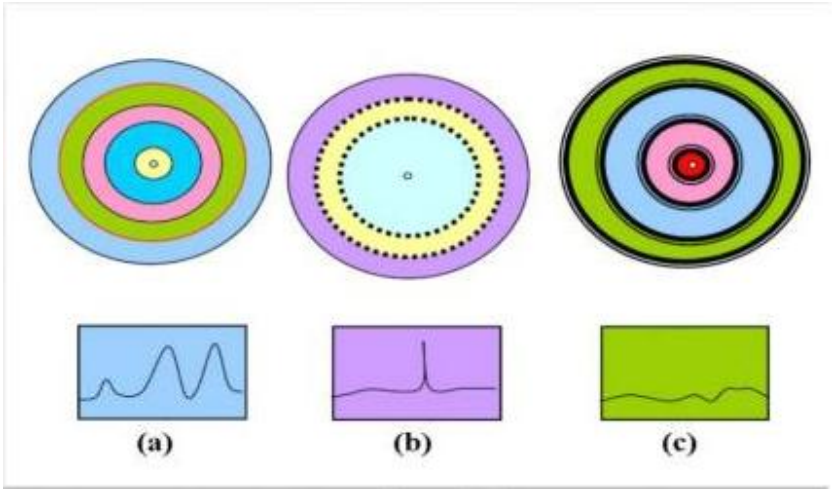
- **How can we distinguish between crystalline solids and amorphous solids?**

It is possible to distinguish between crystalline and amorphous solids through three criteria:

1- Amorphous materials melt within a certain temperature range, while crystalline materials suddenly melt at a specific temperature that can be measured experimentally, no more than. (±0.01).



2- Amorphous materials are dispersed and dispersed when X-rays are diffracted, while crystalline materials form a pattern that consists of distinct and separate spots.



(XRD) of (a) Polycrystalline (b) single crystal (c) Amorphous crystal

3- Crystalline materials have directional anisotropy, meaning that their distinctive properties depend on the direction in which that property is measured, while amorphous materials are all directionally isotropic.

Materials in general cannot be completely pure and usually contain impurities and defects, and these impurities and defects sometimes have the same effect on the materials. Discovery of X-rays and then the technique of X-ray diffraction had a major impact on modern physics. Also, the successive developments and discoveries

contributed significantly to the development of solid state physics. For example, the discovery of pure and impure semiconductors, and then the selection of impurities that can be added to very pure materials in a precise manner, has contributed to obtaining new qualities and properties of solid materials. It must be noted that there is no possibility of obtaining very pure materials, as materials remain impure even if they have a high purity rate of 99.999%, as in physics we always need materials with high purity that reach the limits of (1×10^6) or even ($1x10^8$), and thanks to the great development in modern technologies, physicists have been able to obtain pure materials through purification processes that differ from common chemical methods in purification processes.

Substances can exist in the form of the three known states: gaseous, liquid, and solid, in addition to the state of plasma. The number of atoms per unit length is concentrated at (10^{28}-10^{29}) atoms/m^3. Each atom is located between many neighboring atoms, and this effect and interaction between atoms can be attributed to the huge number of atoms, knowing that these atoms are not static, but rather mobile and have a movement known as vibrational movement. At absolute zero temperature, there is a vibratory movement called absolute zero temperature movement.

- **Why do we study solid state physics?**

The study of solid state physics is very important for understanding many of the properties of solid materials and how to use those properties in the industrial, medical, military, and other fields. On the other hand, the study of solid state physics is because materials in this state are represented by the least kinetic energy and therefore it is possible to study them in detail and accurately. The solid has a constant shape and size when the temperature is constant.

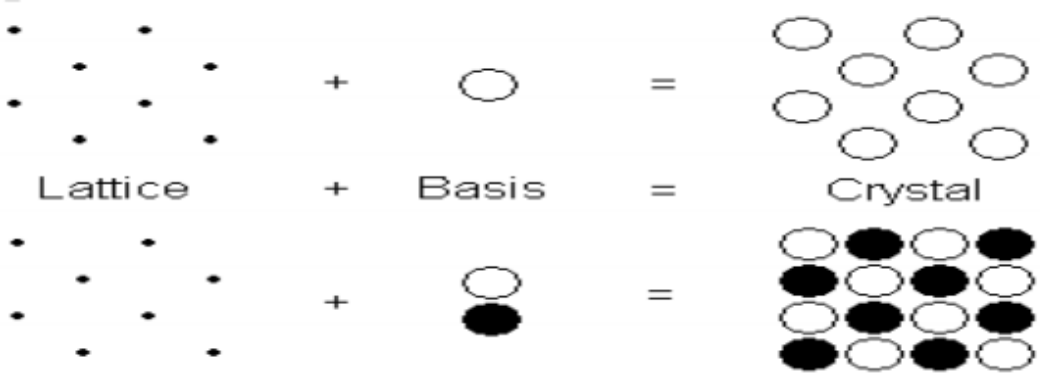
Crystal: is defined as a solid body that contains a number of atoms, has a specific geometric shape, and consists of very small units that are repeated regularly in three dimensions.

Crystal structure التركيب البلوري

The solid body contains a number of units that are repeated regularly for certain dimensions, which constitute the structure, as for the crystalline structure, it represents a relationship linking the basis and the lattice

Basis: It is a group of atoms, ions, molecules with the same arrangement and orientation that are added to the points of the lattice, forming the crystalline structure.

Lattice: A group of points arranged in a specific order, not a group of atoms. To describe the crystal structure, an atom or group of atoms must accompany each point of the lattice, which is called the basis.



Studying the crystal structure means knowing the shape and specifications of the unit cell of the crystal and the atoms this cell contains in terms of type, number, location, and the way they are connected to each other. The crystal structure is studied in terms of a single periodic structure or space lattice with a group of atoms

accompanying each point of the space lattice or space lattice. This basis repeats itself in space in a symmetrical manner, and this group of atoms is called the basis of space to form the crystal. This can be expressed with a simple mathematical relationship:

(space lattice + basis = crystal structure)

The idea of a space lattice is an abstract mathematical idea, and it means a group of arranged points that repeat themselves periodically in space. This means that any gathering of points around a particular lattice point is similar to the gathering around any other lattice point. The space lattice is usually called a Bravais lattice is named after Braves, the inventor of this idea in 1848 AD.

Transition vectors in lattice متجهات الانتقال في البلورة

The lattice is defined in terms of three vectors a, b, c, and they are called the basic transition vectors.

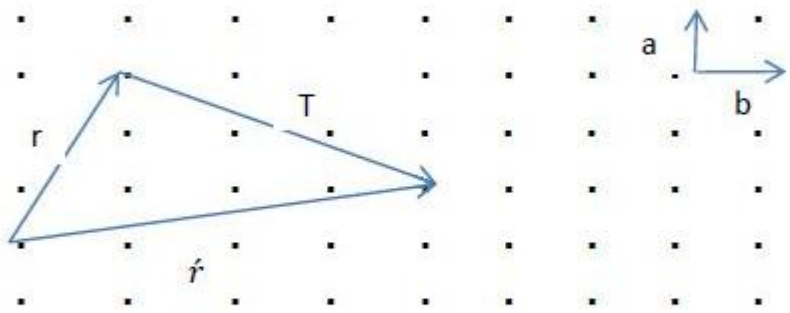
The vector that connects these three vectors is called the translational vector of the lattice or crystal (fundamental translation vector).

It is expressed mathematically as follows:

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \dots\dots\dots(1)$$

Whereas n_1, n_2, n_3 are arbitrary integers, and the translational vector of the lattice T connects any two locations inside the lattice so that the atoms surrounding these two locations appear identical. This is why it is called the creeping effect, as the result when any location inside the crystal creeps by the amount of the access vector to another location $r^{\rightarrow}$ appears The atoms around it are like those atoms surrounding the site $r^{\rightarrow}$, as shown in Figure No. (2), that is:

$$\vec{r}' = \vec{r} + \vec{T} \quad \ldots\ldots\ldots (2)$$



الشكل رقم (٢)

Translation vector: Vector that connects any two lattice points.

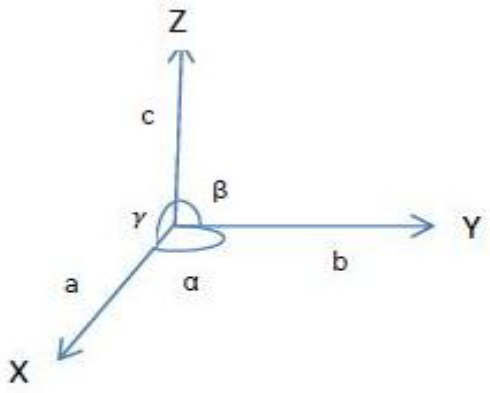
The lattice and its transitional axes are defined as primitive if any two points in the lattice are subject to the relationship.

$$\vec{r}' = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \ldots\ldots\ldots (3)$$

With appropriate choices of the integers n_1, n_2, n_3, but if the points of the lattice are not all subject to relationship number (3), then it is a non-prime lattice n_1, n_2, n_3 and the axes that are determined by it are non-prime axes. On this basis, the primary axes of the lattice are forms of parallelepipeds called a primary unit cell, while the non-primary axes are non-primary unit cells.

Unit cell وحدة الخلية

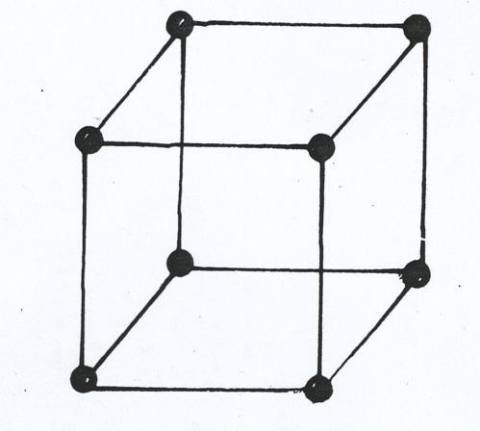
Every solid has a crystalline form, and this crystalline form is arranged in units. A unit cell is a place where ions or atoms are grouped in three directions within a crystal structure. It occupies the least possible space, and these three directions form parallelogram surfaces. The unit cell usually specified by the vector $\vec{a}$, $\vec{b}$, $\vec{c}$ and angles between them usually denoted α, β, γ.



الشكل رقم (٣)

The unit cell has two types: it is either primitive or non-primitive:

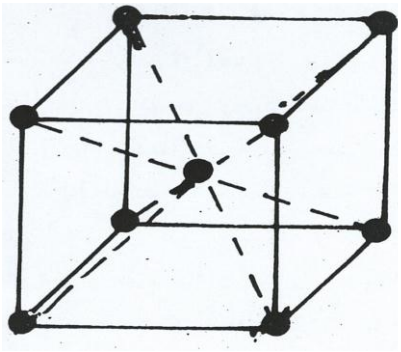
1-primitve cell: if the translation vector $\vec{a}$, $\vec{b}$, $\vec{c}$ are chosen to make the unit cell as small as possible, both translation vectors and unit cell are said to be primitive. It is symbolized by the symbol and is in the form of a rectangular prism, and each primitive ornament contains one lattice point or one atom.



2-non primitive cell: It is a cell resulting from the intersection of two or more lattices. Each cuboid and each primitive cell contains one lattice point or one atom and contain two or more lattice points.

There are three types of non-primitive cells

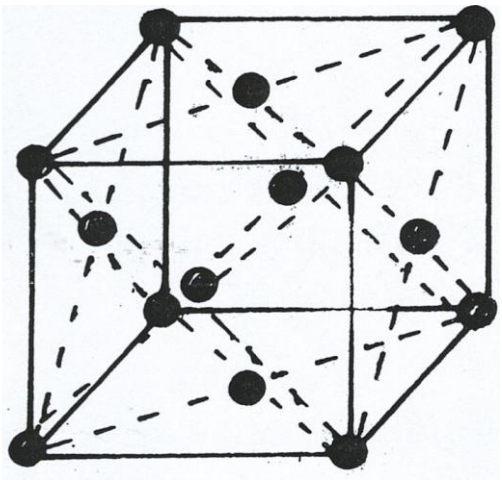
1- **Body-centered cell**: symbolized by the symbol (I). This type of cell contains one grid point in the center of the body, in addition to a grid point at each corner point shared with eight neighboring primitive cells. This means that each body-centered cell contains two retinal points.



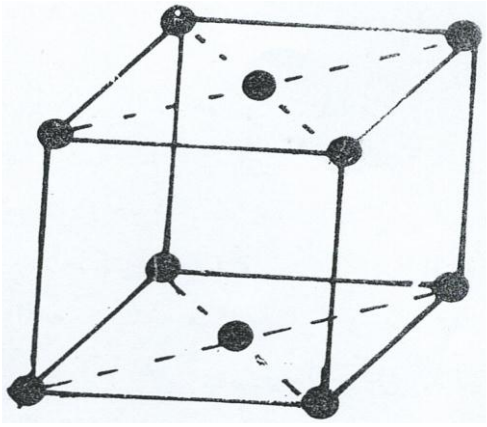
2- **A facet-centered cell**: symbolized by the symbol (F). This type of cell contains, in addition to a grid point at each corner point shared with eight primitive cells adjacent to a grid point at the center of each facet. Since each face is shared by two

adjacent cells, 1/2 of the point belongs to one cell. This means that each body-centered cell contains two retinal points. Therefore, it is (3=6*\1 2) .

Each faceted ornament contains four lattice points.



3- Base or End- cell centered: is symbolized by the symbol (C). This type of cell contains, in addition to a grid point at each corner point shared with eight primitive cells adjacent to a grid point in the center of each two opposite faces. Since each face is shared between two adjacent cells, and therefore 1/2*2=1. Each ornament centered on two opposite sides contains two lattice points.



Crystal Symmetry التماثل البلوري

means the repetition or conformity of the parts of a shape around a plane or point of symmetry. For example, a circle is symmetrical (repeats or repeats itself) around any of its diameter, and a ball is symmetrical around its largest circular plane. As for a shape that does not have the characteristic of repetition and does not have identity in its parts, it may be the shape of asymmetry. Crystal symmetry depends on two important factors: the symmetry element and the symmetry process. Examples of asymmetric and opposite objects are a pair of shoes, the right hand, and the left hand. The element of symmetry can be considered the location or plane around which the symmetry process takes place.

Elements of crystal symmetry عناصر التماثل البلوري

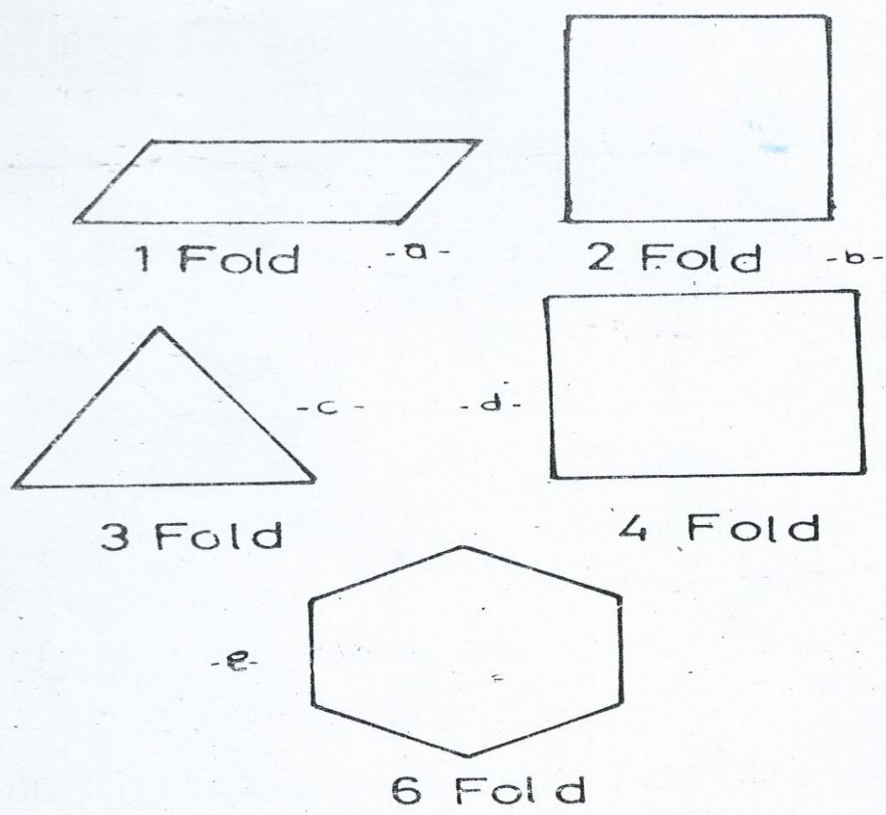
The basic elements of symmetry can be listed as follows:

1- A**xis of symmetry** محور التماثل

It is known as a straight line. If the shape rotates around itself at a certain angle, the shape replaces itself. In order to ensure that repetition occurs or the formation is completed after a specific number of rotations n, the rotation angle Ø must be one of the equal parts resulting from dividing the complete rotation by integers, that is,

$$\emptyset = \frac{2\pi}{n} = \frac{360^o}{n}, \qquad n = 1,2,3,4,6 \dots \dots \dots \quad (5)$$

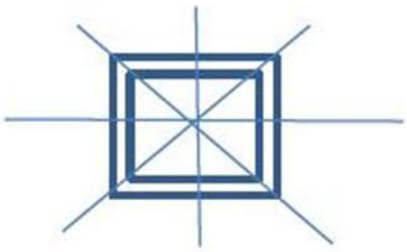
Where no. 1,2,3,4,6 is degree of rotational symmetry of a crystal.



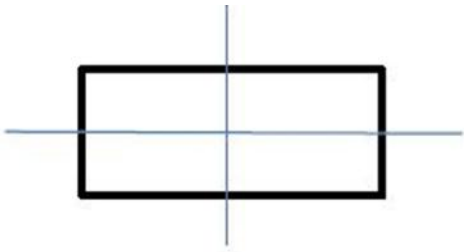
2- Plan of Symmetry مستوي التماثل

An imaginary plane that divides a body or crystal into two similar halves, such that one half is a mirror image of the other half. Everybody that has this characteristic is reflectively symmetrical. An example of this is our bodies when imagining the presence of a vertical mirror that divides the body into two similar halves and symbolizes Some crystals have several levels of symmetry, as in... m for the level of symmetry or level of reflection in the letter Cubic-cell crystals contain nine levels of symmetry, each of which divides the cubic cell into two halves, they are similar, one of them is a mirror reflection of the other half. The body or crystal may not have any plane of symmetry, and sometimes the body has two planes of symmetry intersecting

at a right angle, and they are called a double mirror it is symbolized by mm, as in the case of a rectangular, square, or hexagonal table. Figure 5 represents the level of symmetry.



4m



2m

(two mirror image)

3- **Inversion axis of symmetry**

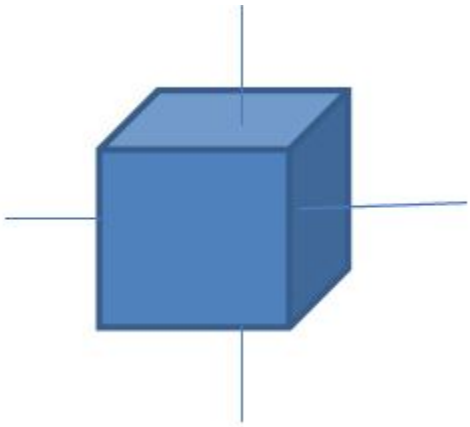
An inappropriate axis of rotational symmetry repeats the left side of the body from its right side Vice versa. The symmetry effect that can be such as these groups or pairs of opposite bodies is called the reflection effect. If the rotation process is followed by a reflection process in order for the body to repeat itself, then these two processes are considered one hybrid process and it is called the rotational-reflective process.

4- **Centre of symmetry** **مركز التماثل**

A crystal has a center of symmetry if the line passing through the center from any point on the surface of the crystal meets a point, it is completely similar on the opposite part and at an equal distance. The center of symmetry is a center of inversion because this center has the property of inverting all space through a point.

It is possible to connect the center of symmetry with the appropriate axis of rotation to form a new element of symmetry called the inversion rotational axis. The

inversion rotational axis is distinguished by placing a sign (-) above the appropriate rotation axis symbol (one process with two successive stages that begins with the rotation stage and is followed by the inversion stage).



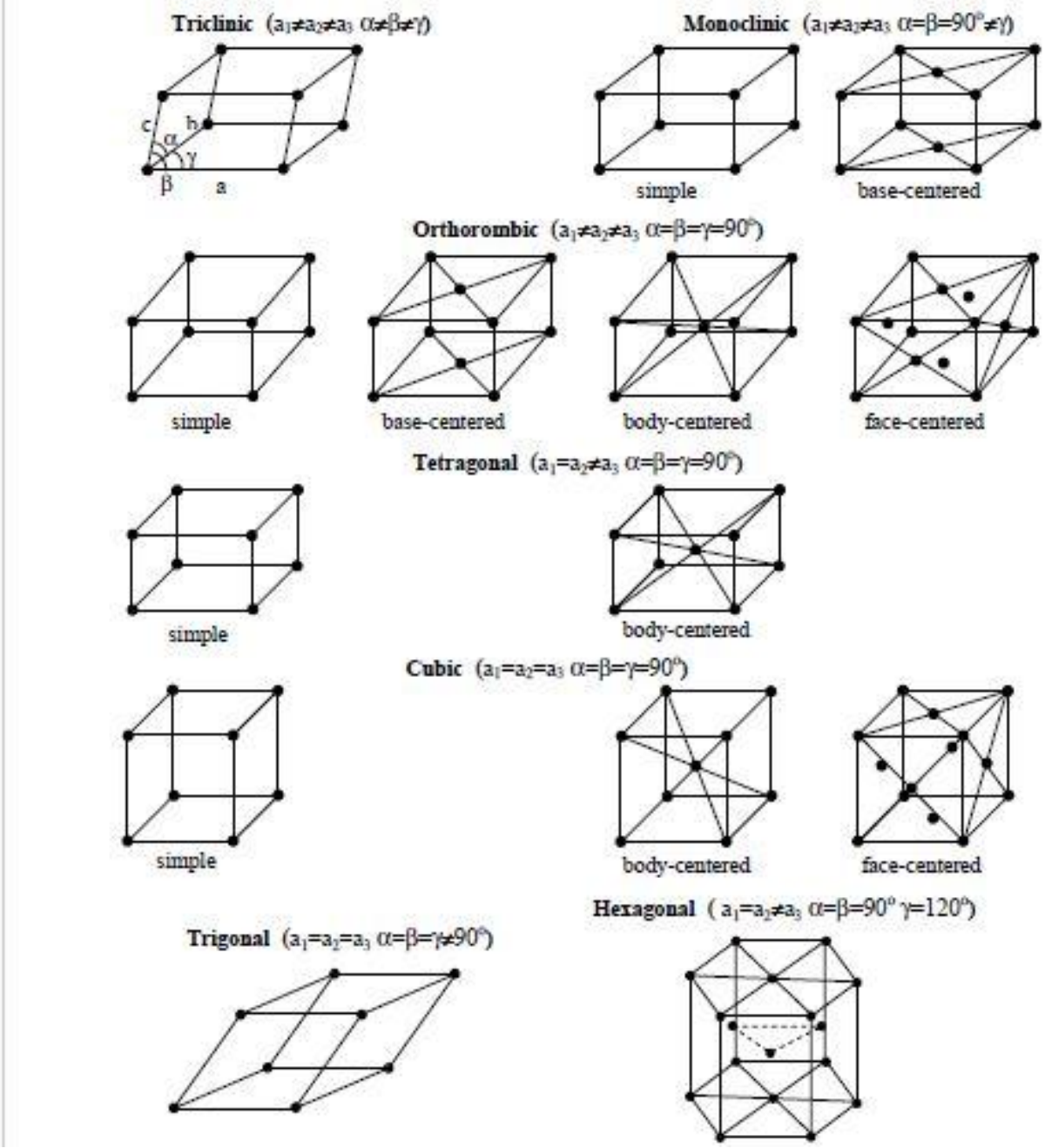
Centre of symmetry

Three – dimensional lattice and crystal systems الشبائك الثلاثية الابعاد والانظمة البلورية

The French crystallographer (Bravais) is credited with classifying crystal lattices into fourteen crystal lattices distributed into seven crystal systems shown in Table and Figure. The number of crystalline lattices and seven systems is limited to the number of possible ways to arrange the lattice points such that the environment surrounding any One point is completely identical to the environment surrounding another point. The parasitism is simple if its points are only at the corners and is symbolized by the letter P, and when it includes additional points in special locations, it is facet-centered (F), body-centered (I), or base-centered (C).

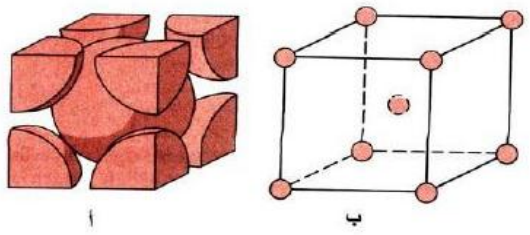
Crystal system	The Bravais lattice	Unit cell properties
Triclinic - ثلاثي الميل	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$

Monoclinic – أحادي الميل	P , C	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic - معيني قائم	P , C , I , F	$a \neq b \neq c$ $\alpha = \gamma = 90° = \beta$
Tetragonal – رباعي	P , I	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
Cubic – مكعب	P , I , F	$a = b = c$ $\alpha = \beta = \gamma = 90°$
Trigonal - ثلاثي التماثل	P	$a = b = c$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal - سداسي	P	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120o$

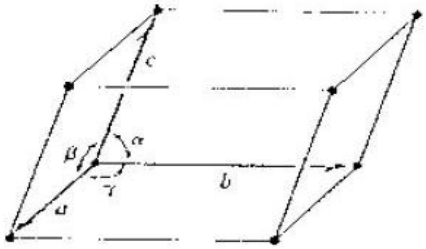


4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

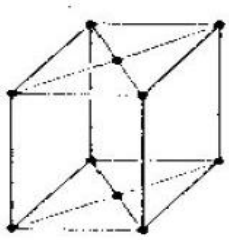
For example, some alloys are simple or elementary if their points are at the corners only and are symbolized by the letter P. When they include additional points in special locations, they are facet-centered (F), body-centered (I), or base-centered (C), as shown in the figure. (8).



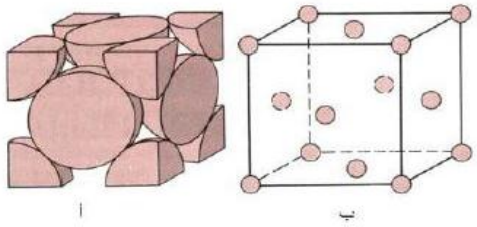
شبيكة متمركزة الجسم



شبيكة اولية



شبيكة متمركزة القاعدة



شبيكة متمركزة الاوجه

Table: important properties of lattices of the cubic crystal system

Property	Simple cube (sc)	Body-centered cube (bcc)	face centered cubic (fcc)
Unit cell size (The side length of the cell a)حجم خلية الوحدة	a^3	a^3	a^3
Number of lattice points per unit cell (عدد نقاط الشبيكة لوحدة الخلية)	1	2	4

The number of reticle points per unit volume عدد نقاط الشبيكة لكل وحدة حجم	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors (عدد اقرب الجيران)	6	8	12
Distance to nearest neighbors المسافة لأقرب الجيران	a	$\sqrt{3/2}\ a$	$\sqrt{2}\ a$
Number of second neighbors عدد الجيران الثاني	12	6	6
The distance of the second nearest neighbor مسافة اقرب الجيران الثاني	$\sqrt{2}\ a$	A	a
Filling ratio or compaction ratio نسبة الملء او نسبة الرص	0.52	0.68	0.74

Example: Iron crystallizes in a body-centered cubic atomic arrangement (bcc). Calculate the amount of the lattice constant (the side length of the unit cell a), noting that: the density of iron (ρ = 7.94 g/cm^3), its atomic weight (w=55.85), and Avogadro's number (NA = 6.02× 10^{23}).

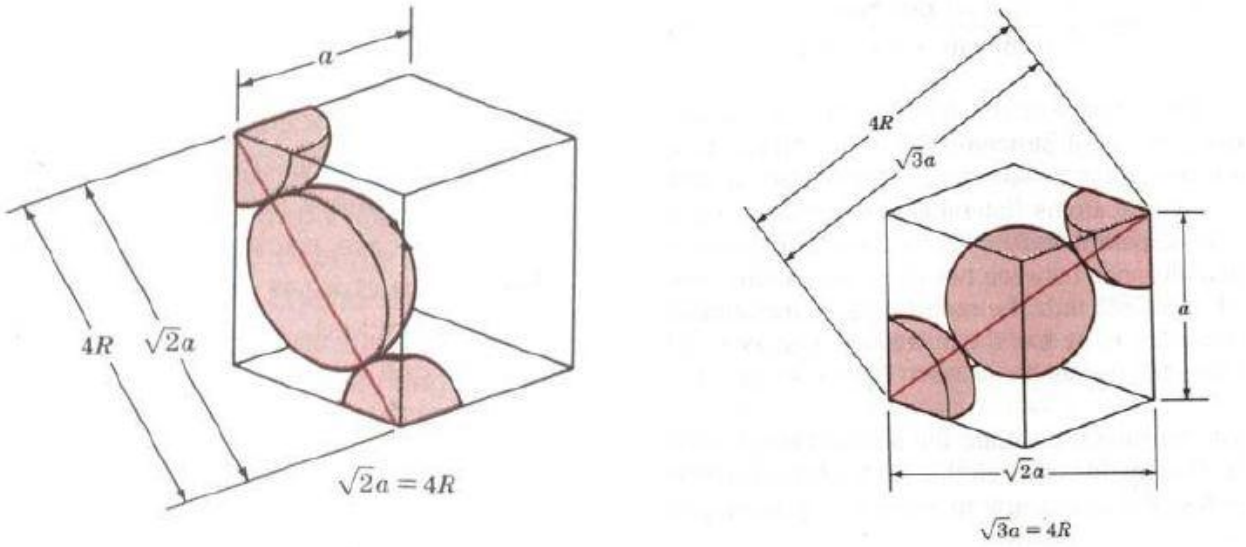
$$\text{الكثافة} = \text{كتلة وحدة الحجوم} = \frac{\text{كتلة الوحدة خلية}}{\text{حجم الوحدة خلية}}$$

وبما أن عدد الذرات الحقيقية لكل خلية وحدة في بلورة الحديد $(n)=2$

$$\rho = \frac{nw}{N_A a^3} \Rightarrow a^3 = \frac{nw}{\rho N_A} = \frac{2\times55.85}{7.94\times6.02\times10^{23}} = 2.86 \times 10^{-8} = 2.86\text{Å}$$

Filing fraction or Packing fraction نسبة الملء او نسبة الرص

The three types of cubic ingots differ in the percentage of filling or the percentage of compaction that represents or is known as It is the largest proportion of the volume of a normal cell that can be occupied by identical atoms located at the points of the lattice or Accompanying the lattice points. This means the ratio between the volume of atoms in the cell to the volume of the cell or the volume of the atom one multiplied by the density of the lattice points and the number of atoms composing the foundation. For the purpose of calculating the filling ratio (P.F.), we assume that the very adjacent atoms are in contact, meaning that the shortest distance between two lattice points represents the diameter of the atom.



(b) (a)

a- The relationship between cell dimensions and atom radius in lattices (bcc).

b- The relationship between cell dimensions and atom radius in lattices (fcc).

Calculating the filling factor of the cubic crystal system

$$P.F. = \frac{volum\ of\ the\ atom \times number\ of\ atoms\ in\ the\ unit\ cell}{volum\ of\ the\ unit\ cell}$$

$$(P.F.)_{sc} = \frac{\frac{4}{3}\pi r^3 \times 1}{a^3} = \frac{\frac{4}{3}\pi r^3}{8r^3} = 0.52$$

$$(P.F.)_{bcc} = \frac{\frac{4}{3}\pi r^3 \times 2}{a^3} \models \frac{\frac{4}{3}\pi r^3 \times 2}{(\frac{4r}{\sqrt{3}})^3} = \frac{\pi\sqrt{3}}{8} = 0.68$$

$$(P.F.)_{fcc} = \frac{\frac{4}{3}\pi r^3 \times 4}{a^3} = \frac{\frac{4}{3}\pi r^3 \times 4}{(2\sqrt{2}r)^3} = \frac{\pi\sqrt{2}}{6} = 0.74$$