Solid State Physics

فيزياء الحالة الصلبة

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The Fourth Division

Basic Education/Science

Solid State Physics

Crystal Structure

Introduction

There is a substance (elements and compounds) in three states as we knew previously or is the solid, liquid and gaseous state and the material differs in that it has one of these states according to the different distances between them and the amount of bonding force between their atoms. It should be noted here that pressure and temperature are the main causes of the change in the state of matter There is a fourth state of matter is the state of plasma, in which the substance is an ionized gas, and a fifth state in which the material appears in the form of nuclear particles with high energy and from the above we can review To come to the conclusion that "the kinetic energy of a charged molecule or microelement is responsible for determining the state in which the substance appears .".

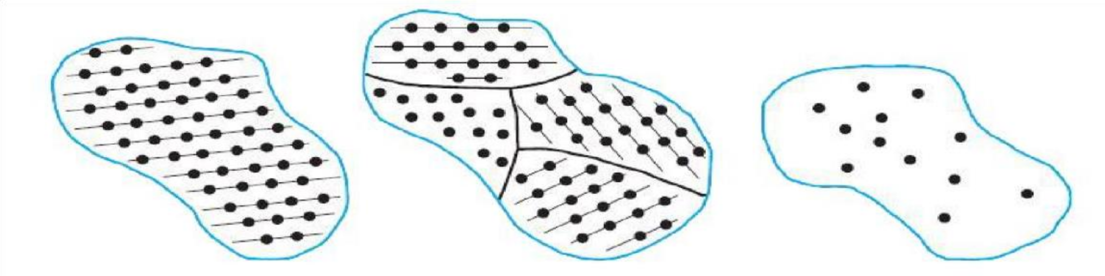
Crystallized and amorphous solids :

Crystalline materials: They are solid materials whose atoms are geometrically arranged so that their positions are boundary in this shape and this periodicity is in a long-term arrangement either in two dimensions for two-dimensional networks or three dimensions for three-dimensional networks .

The crystallized materials contain rows of atoms gathered and arranged periodically and have a kind of symmetry and can be considered a repetition of any unit cell and these materials are iron, gold, sodium **chloride** and others .

Amorphous non-crystalline materials: also called random materials (Amorphous): They are materials whose atoms gather randomly and without arrangement, and these materials include glass.

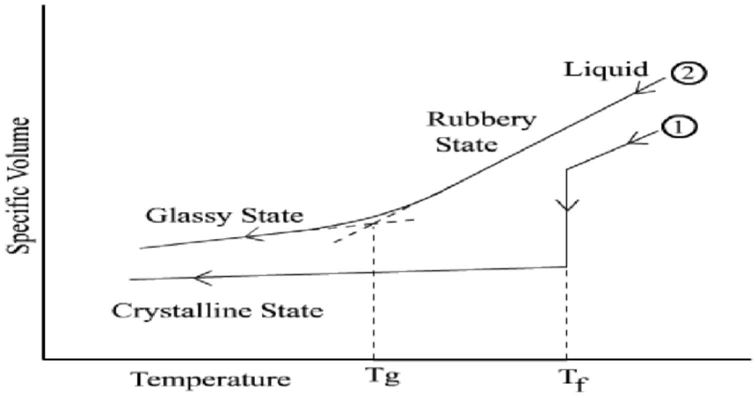
There are crystallized and amorphous materials at the same time, such as silicon and **germanium**, and the reason is due to the way they are prepared or how they are formed.

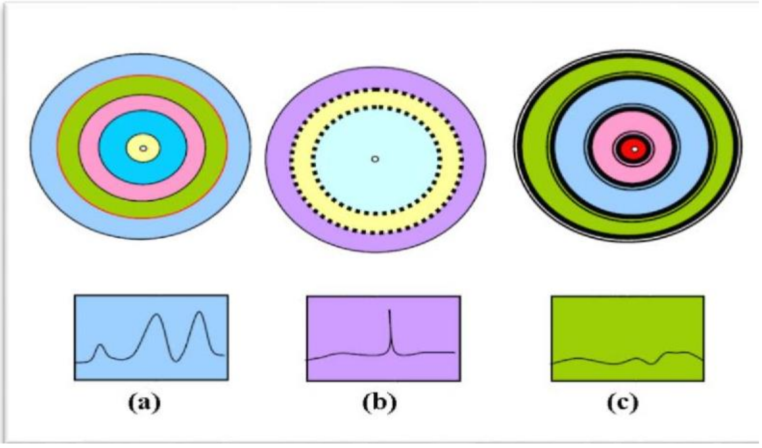


Crystalline and amorphous substances can be distinguished practically by three independent criteria:

Amorphous materials melt suddenly and at a certain temperature always constant, while amorphous materials melt over a certain temperature range.

1- **Amorphous** materials are scattered and scattered at the diffraction of X-rays in the form of concentric rings, while this formation of crystallized materials is distinct spots separated from each other and of a certain symmetry.





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

3-All crystallized materials are anisotropic and to varying degrees, while amorphous materials are all isotropic, i.e. no effect of direction on their properties.

Key terms :

Crystallography: It is the science that is concerned with the study of solids in all their forms and phenomena and is divided into :

1- **Engineering crystallography: It is concerned with the study of the symmetry of crystals and their external shapes .**
2- **Chemical crystallography: It is concerned with studying the origin of crystals and how they grow.**

Crystal: It is a solid body that contains a number of atoms lined up in a certain geometric shape and consists of very small units that are repeated regularly in three dimensions, called cell units.

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The basis of crystal construction is repetition and there are crystals of all kinds:

1- **Real crystals** represent most of the crystals found in nature and contain some defects and deformations.

2- Perfect crystals, which are assumed crystals, as we assume the existence of a perfect crystal free

Of the defects and deformations for the purpose of study and there is no perfect crystal in nature, which is similar to the idea of ideal gas and is characterized by the ideal crystal:

A- Of the defects and deformations for the purpose of study and there is no perfect crystal in nature, which is similar to the idea of ideal gas and is characterized by the ideal crystal:

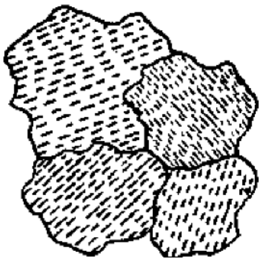
B- Periodicity regular three-dimensional where the identical groups of atoms repeat themselves at intervals or spaces exactly equal.

C-It can possess enormous configurations of periodic organizations or arrangements.

Types of real crystals:

A - Single crystal: where the periodicity of the formation or three-dimensional crystal model extends through the entire crystal.

B - Polycrystalline crystalline where the periodicity of the model does not extend through the entire crystal but ends at the boundaries inside the crystal called grain boundaries



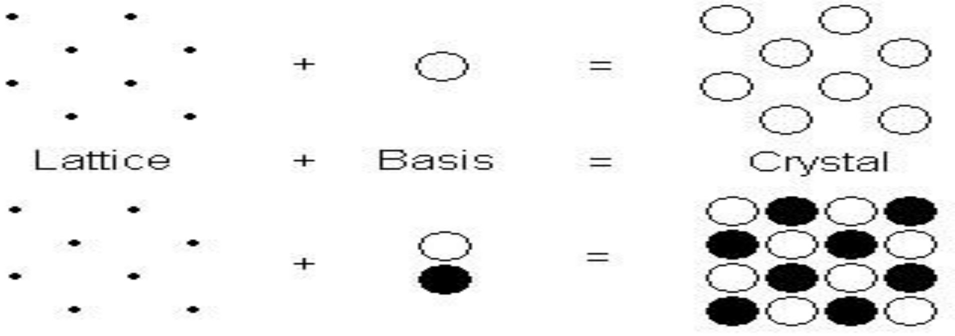
* A crystal is defined as the collection of an infinite number of identical units repeated periodically and regularly (if perfect) in all directions of space

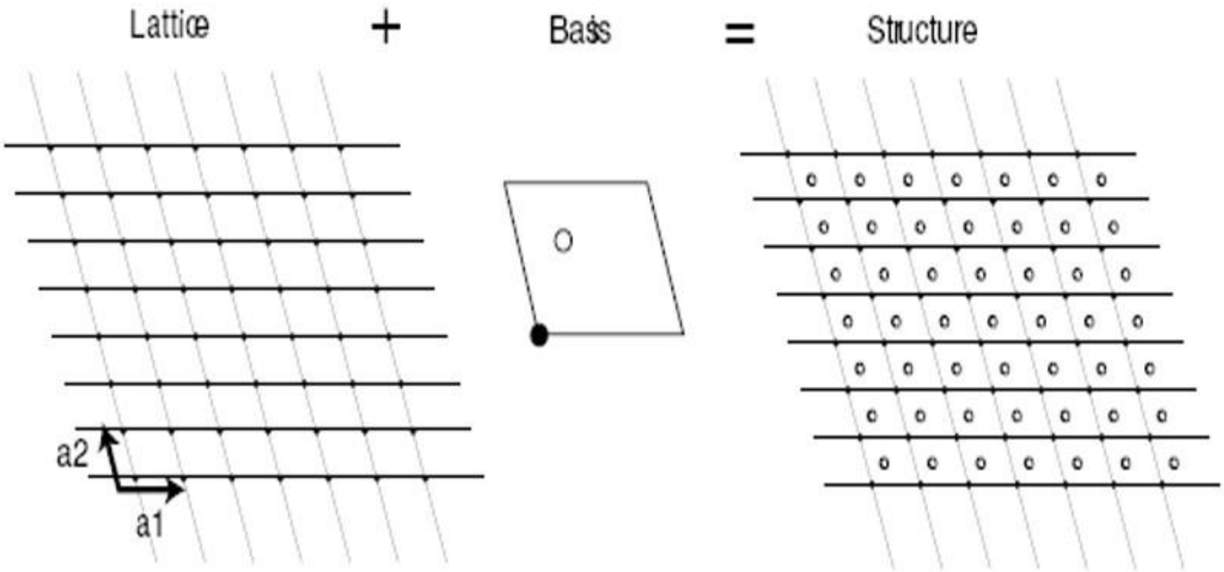
- Units are called crystal building units or bases (base).
- Each base is represented by a geometric point (in the mathematical sense) that we call a node and the group of nodes distributed regularly and periodically forming what we call a crystal lattice: a mathematical concept that expresses the geometry of a crystal.
- That is, the crystal represents a regular sequence of the base positioned in the crystal lattice nodes distributed periodically in space (space). In short:

Crystal Structure = Lattice + Basis

All bases in each crystal lattice must be identical in structure and number, and the number can be an atom, several hundred or thousands of atoms, provided that they are subject to the conditions of periodicity.

Crystal structure : It can be defined from the relationship between the basis and the lattice





Basis: The phrase of an atom, ion, molecule or group of atoms called a point and each point is linked with other points to form a specific body and the basis accompanying each point must be :

1- Symmetrical parts in terms of composition, arrangement and orientation.

2- The number of atoms in the primary unit cell is equal to the number of base atoms.

Lattice: A set of points arranged in a specific system, not a group of atoms, and to describe the crystal structure, an atom or group of atoms must be accompanied to each point of the lattice, which is called the basis

What is the difference between atomic structure and crystal structure?

Atomic structure relates to the number of neutrons and protons in the nucleus of an atom and the number of electrons in electron orbitals.

Crystal structure is concerned with the structure of atoms within crystalline solids in certain formations.

Bravais lattice and transition vectors in crystal:

Space lattice: It is a set of points arranged in a system and repeat themselves periodically in three-dimensional space and is usually called Bravais Lattice after its creator Bravais in 1848.

The one-dimensional lattice is determined by the one-dimensional vector $\vec{a}$ and the two-dimensional lattice with the two vectors $\vec{a}$ $\vec{b}$, while the three-dimensional lattice is determined in terms of the three vectors and is called the transition vector, while the vector that connects these three vectors is called the transitional effect ($\vec{T}$) Translation vector and is expressed for a dimensioned lattice

$\vec{\mathbf{T}} = \mathbf{n}\,\vec{\boldsymbol{a}}$ where n is an integer

$\vec{\boldsymbol{T}}_2 = \mathbf{n_1}\,\vec{\boldsymbol{a}} + \mathbf{n}\,\overline{\mathbf{b}}$ As for the two-dimensional network

$\vec{\mathbf{T}}_3 = \mathbf{n_1}\,\vec{\boldsymbol{a}} + \mathbf{n_2}\vec{\boldsymbol{b}} + \mathbf{n}\,\vec{\boldsymbol{c}}$ **....(1)** As for the three-dimensional network

where n_1, n_2, n_3 are integers .

The transition effect $\vec{T}$ connects any two sites within the crystal so that the atoms surrounding these two sites look the same, and this is why it is called the transition or creeping effect.

Since $\vec{r}$ and $\overrightarrow{r^1}$ are two sites inside the crystal

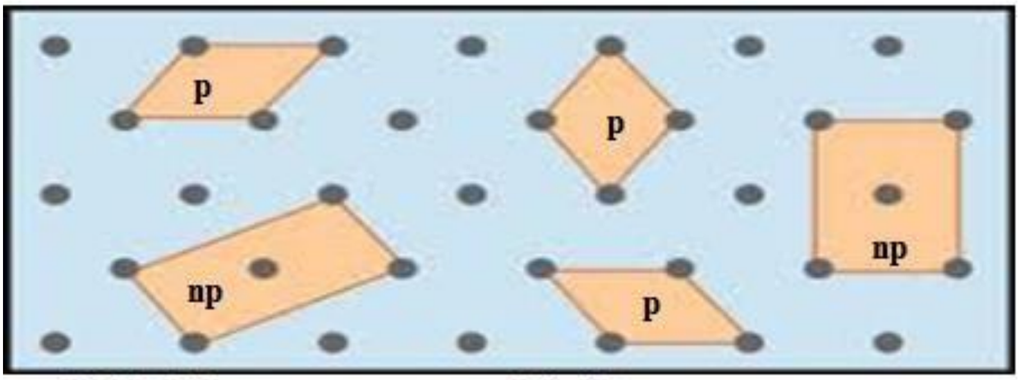
$\overrightarrow{\mathbf{r^1}} = \vec{\boldsymbol{r}} + \vec{\boldsymbol{T}}$ **.......(2)**

By substituting (1) in (2) producing

$\overrightarrow{\boldsymbol{r^1}} = \vec{\boldsymbol{r}}_3 + \mathbf{n_1}\,\vec{\boldsymbol{a}} + \mathbf{n_2}\,\vec{\boldsymbol{b}} + \mathbf{n}\,\vec{\boldsymbol{c}}$ **...(3)**

Primitive cell: It is the cell that contains only the points in its corners and its axes are of the shortest possible length. This cell can fill the entire space by means of appropriate withdrawals and rotations that return the cell to a position similar to the first position and correspond to an angle of Φ where) n=1,2,3,4,6, (the shape in which n=5,7) lacks symmetry and rotates around an axis passing through a lattice node **.**

Non-Primitive Cell: It is the cell that contains other lattice points in addition to the corners and the lengths of its axes are not as short as possible and equation (3) does not apply to it.



P=Primitive np=non-Primitive

Unit cell: It is the smallest unit in the space lattice, a unit that, repeating it in all three directions, produces a large crystal of solid matter that has the same symmetry as the unit cell.

The volume of the three-dimensional unit cell is given by

$$V = |\vec{a} \times \vec{b} \cdot \vec{c}| \quad \text{او} \quad V = |\vec{a} \cdot \vec{b} \times \vec{c}|$$

The important thing here is to perform the process of cross product first and then dot multiplication, and this law is used to calculate the size of the initial and non-prime cells.

Crystal Symmetry :

There are four processes by which symmetry processes within a crystal can be determined:

– Translation	الانتقال
– Rotation	الدوران
– Reflection	الانعكاس
– Inversion	الانقلاب

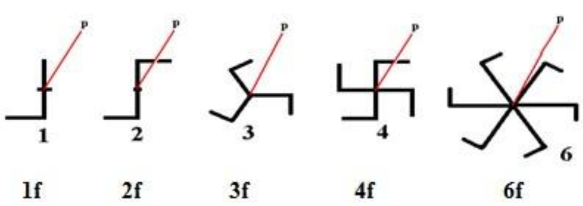
Symmetry is the repetition or congruence of parts of a shape around a plane or line or point, the circle is symmetrical about any diameter of it, and if it is possible to describe a certain position of an object in more than one direction so that it is not possible to distinguish between these surfaces, it is said that this body is symmetrical. And the sphere is symmetrical about its largest circular plane. A cube has many symmetry and is symmetrical diagonally, longitudinally, transversely, and around its center .

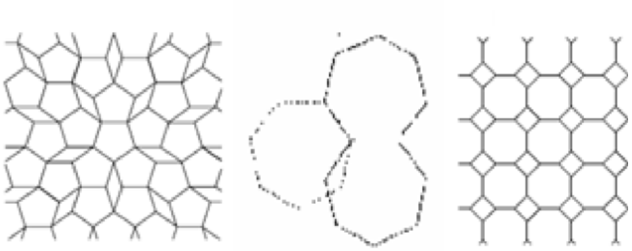
Asymmetry: It is the form that does not have the characteristic of repetition and does not have congruence in its parts, such as the right hand or the left hand of a person

Symmetry in a crystal is an imaginable process or effect that can occur on the crystal and after its completion the crystal appears to be the origin of any repetition or return its parts to the positions it occupied before these processes occurred.

The effects of symmetry or the basic elements of symmetry are :

1- Suitable axis rotation: It is an imaginary line passing through the center of the crystal so that if a full cycle (360^0) rotates without any displacement, the crystal positions will be repeated during that cycle a number of times, and the angle of rotation Ø must be one of the equal parts obtained from dividing the full cycle by integer numbers n called fold. where these numbers correspond to the permissible degrees of symmetry n = 1,2,3,4, 6 and $\emptyset = \frac{360}{n}$ Whereas, 5, 7 ,8....... is not allowed because it either leaves a vacuum or overlaps the cells of the unit with four and the simplest example of a suitable rotational axis is the rotation of a fan with three blades (3 folds) Ø = 120^o and with four blades. Ø = 90^0 (4 folds)



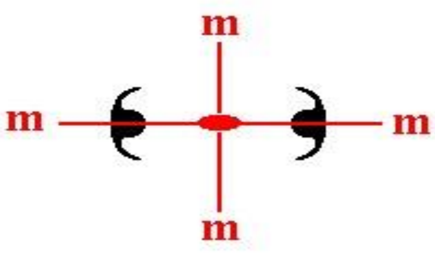


5f 7f 8f

غير مسموحة

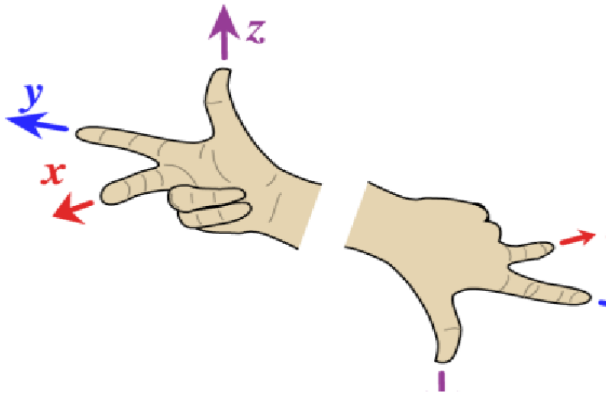
2-Inappropriate axis of rotation: It is the occurrence of a rotation process followed or followed by a reflection process in order for the body to repeat itself, that is, it is a hybrid process (rotation + reflection) and there are five reflexive rotation axes symbolized by˜4,˜3,˜2,˜1).

1- Level of symmetry: It is an imaginary level that divides the body or crystal into two similar halves so that one of the halves can be an image of the other, such as the human body if it is divided into two equal halves longitudinally. This process is symbolized by m) (mirror) and if it is possible to divide the body into several symmetral sections, for example, into two symmetrical sections up and down and two symmetry sections to the right and left, such as a rectangle, it is a double mirror (mm) (double).



2 m m

Symmetry Center: The center of symmetry is the center of inversion because this center has the property of turning all space through one point of intersection and the simplest example of our placement is the thumb of the left hand touching the thumb of the right hand and one of the hands its fingers down and its interior towards us, while the other hand has its fingers up and the back of the hand towards us, we have obtained a center of symmetry and is symbolized by $\bar{6}$, $\bar{5}$, $\bar{4}$, $\bar{3}$, $\bar{2}$, $\bar{1}$ one bar $\bar{1}$.



The most common type of unit cells are:

- **Face centered cubic (Fcc)**
- **Body centered cubic (Bcc)**
- **Hexagonal closed packed (Hcp)**

For each crystal structure mentioned above , we well determined

1- Postion of atoms

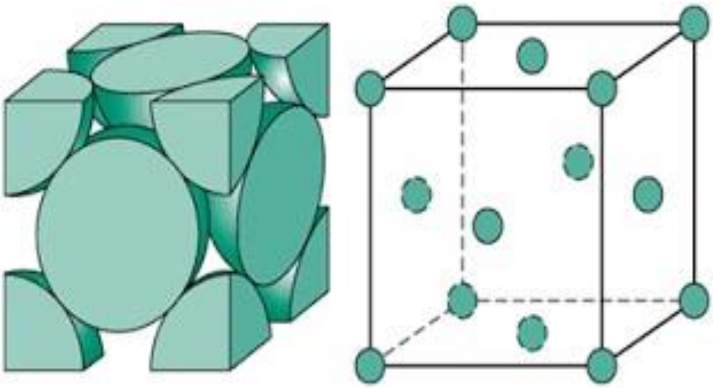
2- Examples

3- The relation between the length of the cell and the radius of atom R

4- The coordination number CN

5- Number of atom unit cell

6- Atomic packing factor APF



1- Face centered cubic structure (FCC)

1- Atom are located of the corners of all faces of cubic unit cell

2- Cu, Al, Au have this crystal structure

3- The relation between the length and the radius of the atom R (a= $2(2R)^{1/2}$.

4- The coordination number CN = the number of closed neighbors to which an atom is bonded CN (FCC) = 12

5- Number of atom per unit cell= 8*1/8 +6*1/2 =4 atoms/unit cell

6- Atomic packing factor or packing efficiency indicates how closely atoms are packed in unit cell and is given by the ratio of volume of atoms in the unit cell and the volume of the unit cell

APF = 0.74(maximum possible)

2- Body centered cubic structure (BCC)

1- **Atom are located of the corners and at center of cubic unit cell**

2- **Cr, Na, Fe have this crystal structure**

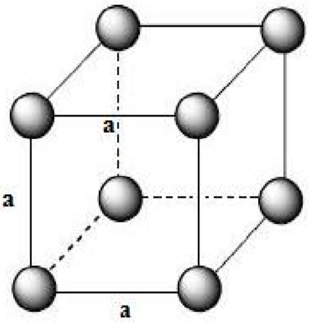
3- **The relation between the length and the radius of the atom R ($a= 4R(3)^{1/2}$.**

4- **The coordination number CN = the number of closed neighbors to which an atom is bonded CN (FCC) =8**

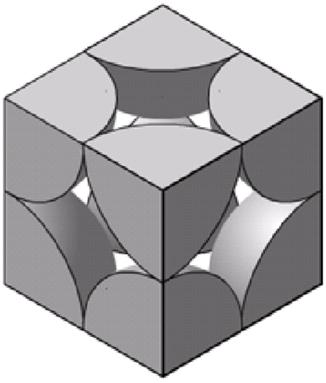
5- **Number of atom per unit cell= 8*1/8 +1 =2 atoms/unit cell**

6- **Atomic packing factor or packing efficiency indicates how closely atoms are packed in unit cell and is given by the ratio of volume of atoms in the unit cell and the volume of the unit cell**

APF = 0.68(maximum possible)



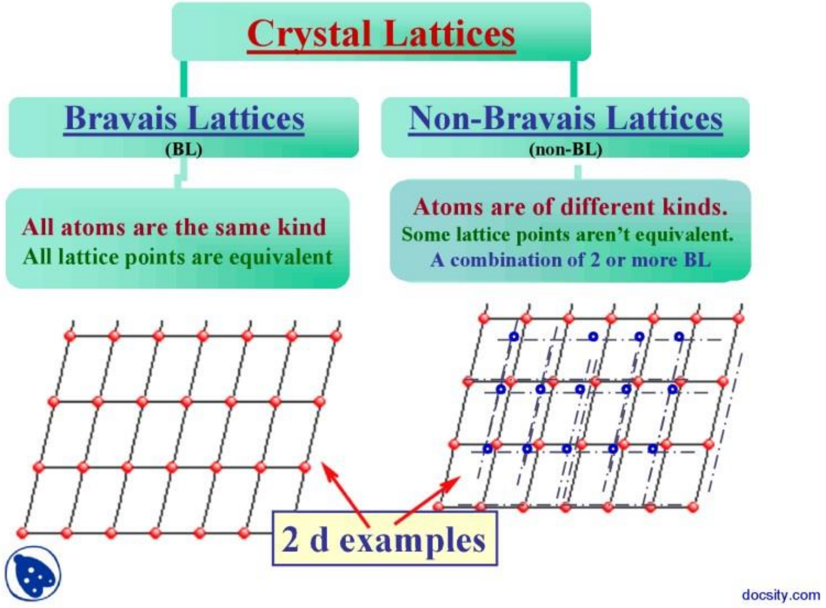
Simple Cubic



Bravais Lattice:

There are two types of nets: Bravais and Non-Bravais.

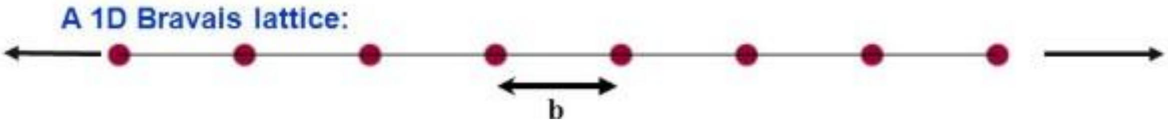
In the Pravis lattice, all lattice points are equivalent, and therefore it is necessary that all atoms in the crystal are of the same type. In non-paravis lattice, some lattice points are not equivalent.



Planar lattices and their symmetry:

The importance of these lattices is to understand the physical properties of solid objects and to understand the study of X-ray diffraction on those surfaces so that we can estimate the distance between points.

The reticence as previously passed is a set of points arranged in a certain system and repeats itself periodically and the process of repetition is in one direction and is called a linear or two-dimensional lattice and is called a plane lattice or three-dimensional and is called a space lattice and the linear reticle consists of similar points of equal dimensions and on a vertical or horizontal straight line, and for this there is one basic type of linear lattice because there is only one way to arrange the points and the only difference is the distance between the points.



As for the flat lattice, it is possible to obtain a large number of nets that can be grouped into five types:

1- Oblique lattice: It is a general lattice and there is no special relationship between the lengths of its basic vectors and the angle between these vectors is of unlimited value, that is:

$$\vec{a} \neq \vec{b}\text{،}\emptyset \neq 90^{\circ}$$

Each corner represents 1/4 point and each cell has 1 point (1/4*4=1).

2- **Initial rectangular lattice**: In this type there is a limited value of the angle $\emptyset \neq 90^{\circ}$and there is no limitation of the lengths of its axes $\vec{a} \neq \vec{b}$, each corner represents 1/4 point and each cell has 1 point (1/4 * 4 = 1).

3- **Centered rectangular lattice**: It is a non-primary lattice that represents a special case of an inclined lattice with a finite value of the angle Ø between its unequal axes when it is $\emptyset = \left(cos^{-1}\frac{a}{2b}\right)$ We get primary cells of a parallelogram shape and non-primary cells can be formed in the form of rectangles and axes are formed $\emptyset \neq 90^{\circ}$ و $\vec{a} \neq \vec{b}$. Each corner represents 1/4 point and each cell has 2 points .(2=1+4*4/1)

4- **Square lattice**: the initial axes are equal$\overrightarrow{a} = \overrightarrow{b}$ and the angle between them is right $\emptyset \neq 90^{\circ}$. Each corner represents 1/4 point and each cell has 1 point (1/4*4=1).

5- **Hexagonal lattice**: A hexagonal lattice can be formed from an inclined lattice with special specifications, so that the axes of the lattice $\overrightarrow{a} = \overrightarrow{b}$, and the angle between them $\emptyset \neq 120^{\circ}$is a special case of a rectangular lattice centered when I left it , primary rhombic with specifications $\overrightarrow{a} = \overrightarrow{b}$ and $\emptyset \neq 60^{\circ} or\ 120^{\circ}$

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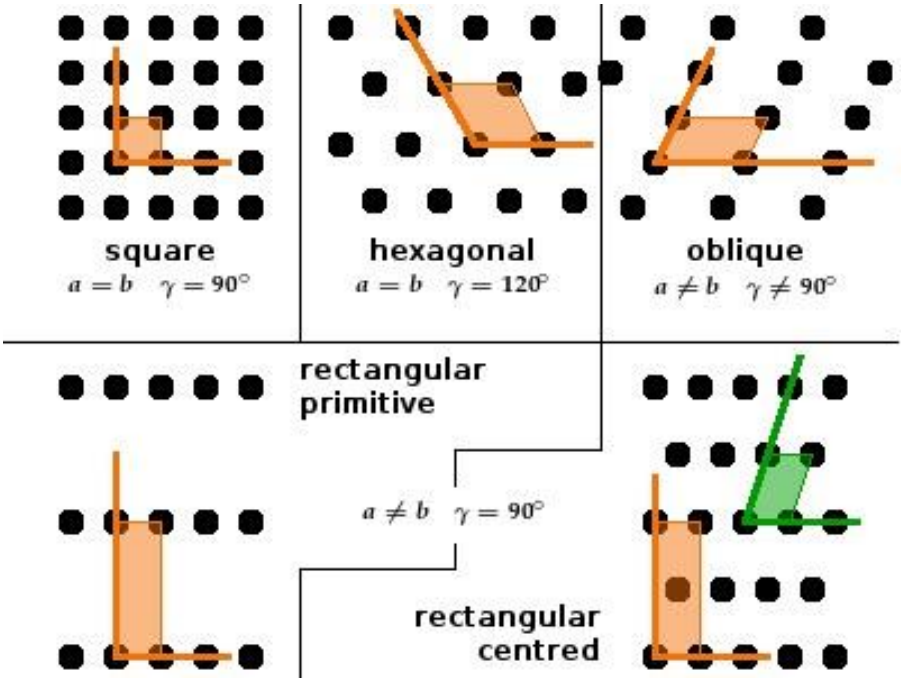


Space lattice (3D) and crystal systems:

There are five basic types of Pravise networks (in three dimensions).

1- Primitive Lattice

It is denoted by the symbol (P), where each unit cell contains a point in each of its eight corners, so that each primary unit cell contains one lattice point (point). $8 * \frac{1}{8} = 1$

2- Face Centered Lattice

It is marked with the symbol (F) and it contains a lattice $\frac{1}{8}$ point in its eight corners in addition 1/2 to a lattice point in the six faces, that is, the sum of what these nets contain is 4 points. $(8 * \frac{1}{8} + 6 * \frac{1}{2} = 4 \text{ نقاط})\ 4 \text{ نقاط}$

3- Body Centered Lattice

It is denoted by the symbol (I) and contains a lattice point in its eight corners in addition to one lattice point in the center of the body, meaning that the sum of what these nets contain is two points. $(8 * \frac{1}{8} + 1 = 2 \text{ نقطة})$

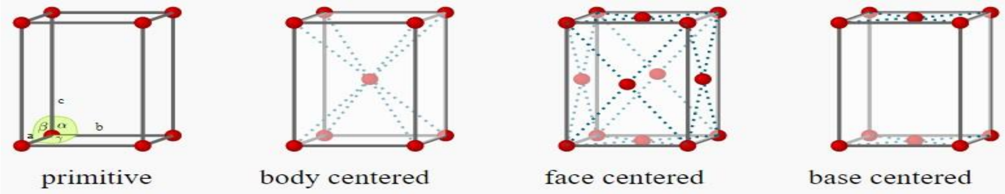
4- Base or Side Centered Lattice

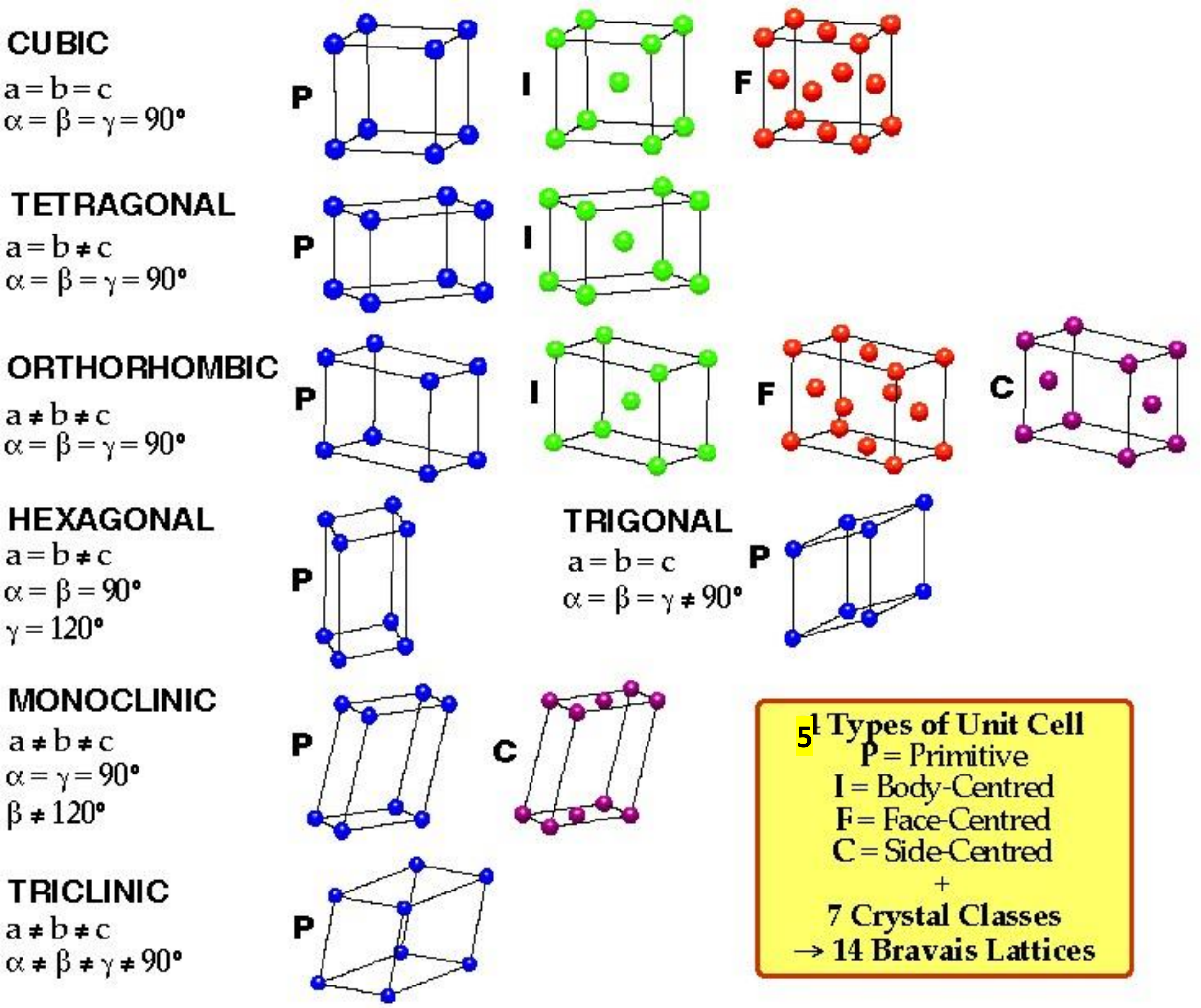
This type is characterized by containing $\frac{1}{8}$ a lattice point in its eight corners in addition to a lattice point in two opposite faces of its six faces, and therefore the total of the points it contains is two points $(8 * \frac{1}{8} + 2 * \frac{1}{2} =$

These lattices are denoted by the symbol A, B or C depending on the location of the two points on the faces of the cell

5- Rhombohedral Lattice

It is a special case of primary lattices and is denoted by R. The shape of the cell is rhombic but the three axes are not perpendicular, that is,
$(\propto = \beta = \gamma) \neq 90^{\circ}$ و $\vec{a} = \vec{b} = \vec{c}$





The seven crystalline systems can be arranged from the highest symmetrically (cube) to the lowest symmetrical (triclinical).

The five types of basic lattices are distributed among seven crystal systems with fourteen praffesian lattices .

The seven crystal systems and fourteen paraphysite lattices are as follows:

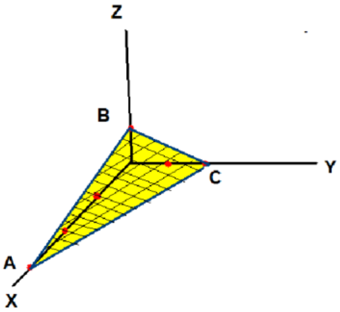
Miller indices (أدلة ميلر) معاملات الاوجه

• To describe the physical state of the crystals, the positions and direction of the crystal planes that are determined for any crystal plane must be determined by three nodes that are not on one line through which the coordinates of the crystal plane are determined, provided that the nodes are located on the crystal axes.

• We can determine the above by choosing a set of coordinate axes that apply and agree in direction with the sides of the primitive cell so that the principle of these axes lies on one of the nodes of the crystal lattice where the sides of the primitive cell intersect.

• If points A, B, S have coordinates A(3,0,0),B(0,2,0),C(0,0,1) representing the three nodes, they will determine a crystalline plane what this plane can be determined by the three numbers (123).

- From the point of view of crystal structure, the position and direction of the crystal plane can be determined by a convention used to describe crystal planes and trends in a crystal called Miller's coefficients, which are very useful in the inverted lattice convention As we will see later, Miller's coefficients are determined as follows:



To find them, we follow the following steps:

1) We select the origin point (0) and three reference axes (x, y, z)

2) We determine the intersection of the surface with each of the three axes with values (p, q, r).

3) We flip the values of the intersections p, q, r, if they are all integers representing hkl and if some or all of them mixed numbers that we multiply by the least common multiple to convert them to integers to get (hkl).

4) When placing Miller's coefficients in parentheses (hkl) it means one set of parallel or equal surfaces in surface and not Miller's coefficients for one given surface

5) Miller's coefficients may all be positive, negative, or mixed numbers, but they are always integers.

6) When there is a surface parallel to one of the crystal axes such as the axis, the coefficients of this surface are written as kl(0) because this surface crosses the axis at infinity (∞) and the reciprocal of ∞ is 0

Example (1): Find the Miller coefficients of a surface whose intersection with the axes is as follows:

p = 3 , q = 6 , r = 2

الحل: نجد المقلوب $\frac{1}{2}$ $\frac{1}{6}$ $\frac{1}{3}$

نضرب بالمضاعف المشترك الاصغر $\frac{1}{2} * 6$ $\frac{1}{6} * 6$ $\frac{1}{3} * 6$

∴ معاملات ميلر لهذا السطح هي (312)

Example (2): Find the Miller coefficients of a surface whose intersections are

$\mathbf{p = 4}$ و $\mathbf{q = \infty}$ و $\mathbf{r = \frac{1}{2}}$

P q r

$4 \quad \infty \quad \frac{1}{2}$

$\frac{1}{4} \quad \frac{1}{\infty} \quad 2 \quad \big\} *4$ م.م .أ

8)0 1 معاملات ميلر لهذا السطح هي (8 0 1

Example (3):

المقلوبات $\mathbf{p = 4}$, $\mathbf{q = \infty}$, $-\frac{\mathbf{1}}{\mathbf{6}}$ **:**

$\frac{1}{4}$ 0 -6

$\}$ * 4

1 0 -24 : م .م أ.

$\mathbf{p} = -\frac{\mathbf{1}}{\mathbf{2}}$, $\mathbf{q} = \frac{\mathbf{1}}{\mathbf{3}}$, $\mathbf{r} = \infty$ **:**(h k l) (1

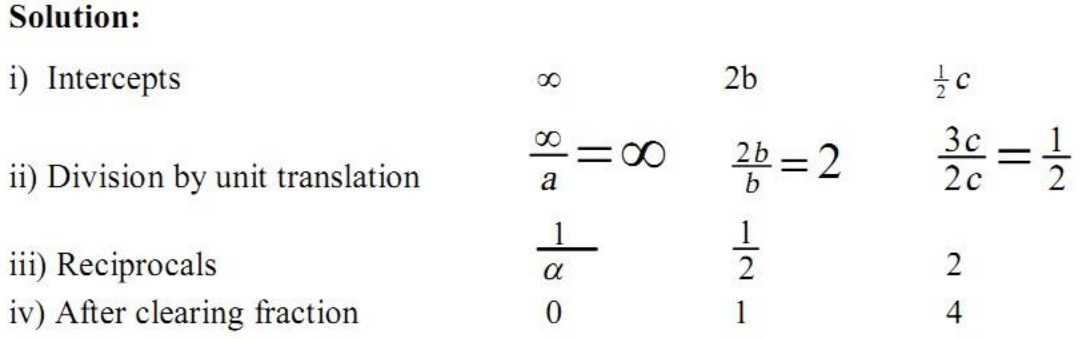
Example 4)

P q r

$-\frac{1}{2}$ $\frac{1}{3}$ ∞

المقلوبات0 3 2 −0)3̄2 ((h k l

Ex5: Determine the Miller Indices of a plane which is parallel to x-axis and cuts intercepts of 2 and 1/2, respectively along y and z axes.



Solution:

i) Intercepts	∞	2b	$\frac{1}{2}c$
ii) Division by unit translation	$\frac{\infty}{a} = \infty$	$\frac{2b}{b} = 2$	$\frac{3c}{2c} = \frac{1}{2}$
iii) Reciprocals	$\frac{1}{\alpha}$	$\frac{1}{2}$	2
iv) After clearing fraction	0	1	4

The six faces of the cube can be expressed as follows

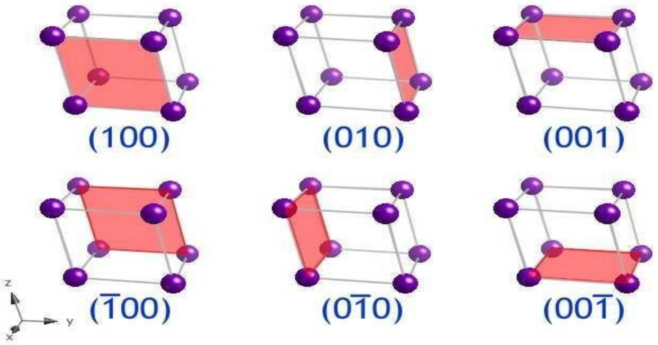
((100)) or {100} They represent the surfaces : (001),(0̄01),(00̄1),(001),(010),(100̄)

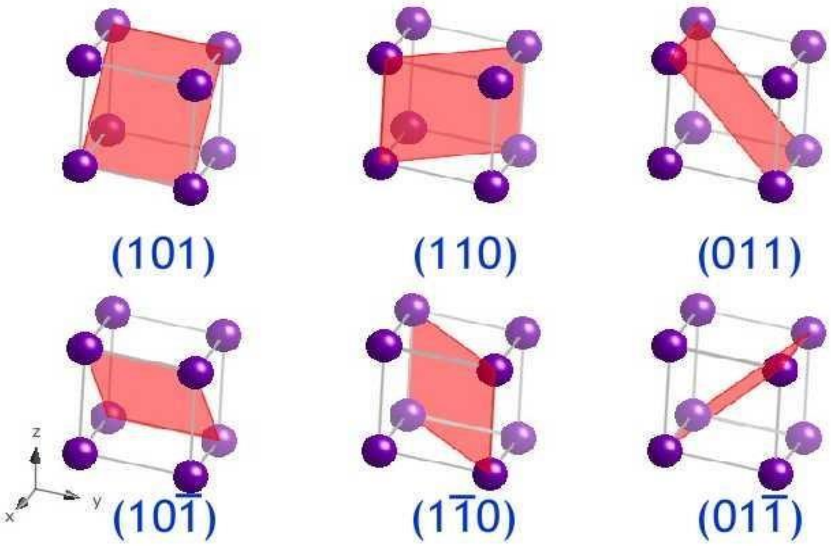
The relationship { } or)) ((means all the surfaces equivalent to that surface, for example{333} means: (333),(3̄33), (33̄3),(333̄),(3̄3̄3), (3̄33̄),(33̄3̄),(3̄3̄3̄)

If all the surface values are different for {h k l} we get 48 different equivalent surfaces such as , {352}, {324}{431} and others}. If two values are similar from the values of {h k l), it is possible to obtain 24 equivalent surfaces, such as:

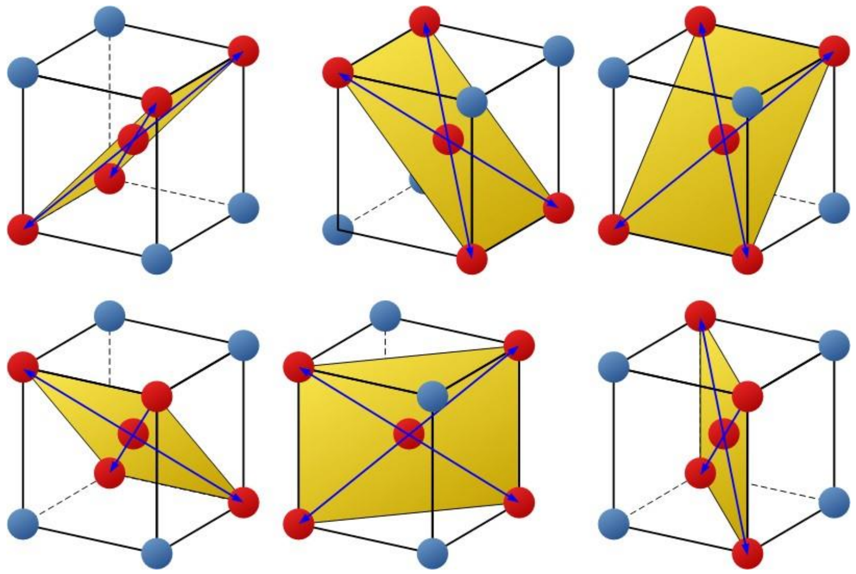
{331}, {422}, {511} Try to find the 24 equivalent surfaces.

`Q / Draw the following crystal surfaces of the cube system:
(200),(004),(023),(120),(0$\bar{1}$0),(001),(010),(222),(011),(331),(420),(2$\bar{1}$1),($\bar{1}$31),(110),($\bar{1}$10),(111),(020)





Q: Determine the Miller coefficients for the following crystal surfaces:



Miller's coefficients for hexagonal shape :

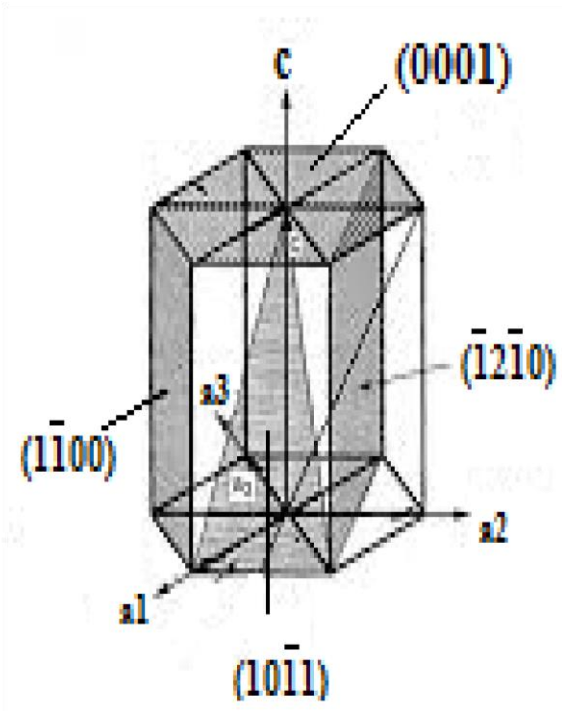
The crystal surfaces of the hexagram are represented by four coefficients instead of three and are written (h k i l)

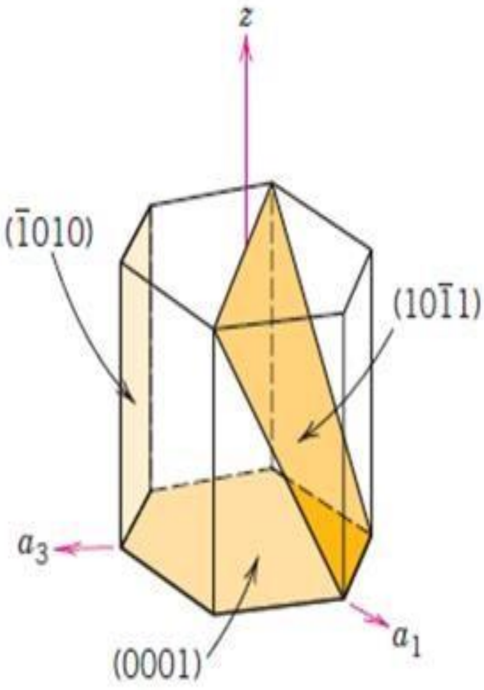
Example: Calculate the Miller coefficients of a surface in the hexagon whose intersections

$a_1 = 1$ $a_2 = -1$ $a_3 = \infty$ $c = \infty$

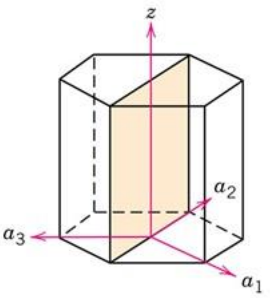
التقاطعات	1	-1	∞	∞
المقلوبات	1	-1	0	0
معلومات ميلر	$(1\ \bar{1}\ 0\ 0)$			

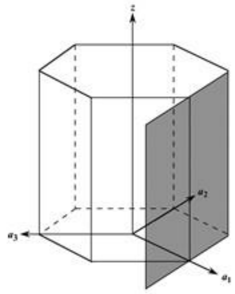
The upper base has Miller's coefficients (1000) and the lower rule is that the axes of this lattice are called Praviz axes and are subject to the directional relationship :

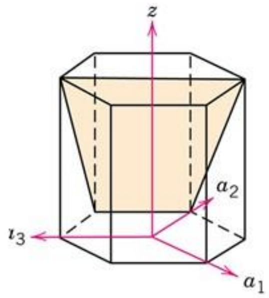


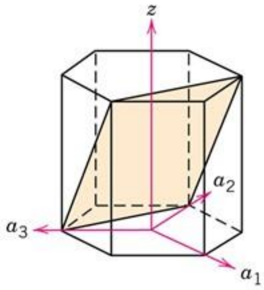


Q: Determine the Miller coefficients for the following crystal surfaces of the hexagon:









Definition of amorphous

Amorphous solids are solids in which the particles that make up a substance are organized in a random pattern, and they are amorphous solids where atoms are not arranged in a regular pattern in the solid lattice.

Amorphous solids are materials that lack a specific structure arranged from atoms and molecules, and the majority of solids are amorphous and used in a variety of industries, and glass, commonly used in the automotive industry, is one of the most famous examples of amorphous solids.

The most common examples of amorphous solids are: mineral glass, rubber, plastic, glass, polymers, gel.

Properties of amorphous solids

These materials have some properties, including:

- Amorphous solids gradually soften over a temperature range and can be formed into different shapes when heated.
- Amorphous solids are pseudo-solids or supercooled liquids, which means they have a slow flow rate, if you look at the glass panels connected to the windows of old houses you will notice that they are thicker at the bottom than at the top.
- Amorphous solids have an irregular shape because their constituent molecules are not arranged in a specific geometry.
- When amorphous solids are cut with a sharp-edged tool, irregular surfaces are produced.
- The reason for the irregular arrangement of particles is that amorphous solids do not have a specific melting temperature.

Due to the irregular arrangement of particles, amorphous solids are anisotropic, which means that the value of any physical property will be the same in any direction.

Uses of Amorphous Solids

Amorphous solids have a wide range of uses including the following:

- Rubber is mainly used in the production of tires, shoes, chains and camp fabrics, in addition to being used in many raw materials in a variety of industries.

- Glass is commonly used in packaging such as food cans, cosmetic boxes, soft drink bottles and cutlery, and for building construction such as windows, lighting and shelves.

- A common use is the use of amorphous silicon in converting sunlight into electricity.

- The polymer is used in the manufacture of pipes, medicines and as raw materials in many factories.

Definition of crystalline solids

Crystalline solids are solids in which the molecules that make up the material are organized in a certain way, and the composition of these solids contains crystals, each of which has a distinctive geometric shape, also crystalline solids are the most stable types of solids due to their low potential energy.

Almost all solids are known as crystalline solids including metal elements such as iron, silver, and copper as well as non-metallic elements such as phosphorus, sulfur, and iodine.

Crystalline solids are often formed by many compounds such as sodium chloride, zinc sulfide and naphthalene, but the statement that glass is a crystalline solids is not true

Properties of crystalline solids

- Crystalline solids have a characteristic melting point and begin to melt at a certain temperature.

- The shape of crystallized solids is described in typical particle arrangements

- It has split properties, which means that when sliced using the edge of a sharp tool, it splits in two leaving smooth and simple surfaces.
- Contrasting crystalline solids, which means that when physical properties such as electrical resistance or refractive index are calculated in different directions in the same crystal, they display different values.

Since crystalline solids do not flow like pseudosolids, they are also known as true solids.

Uses of crystalline solids

Crystalline solids have a huge range of uses, including the following:

- Diamonds are frequently used in the development of fine jewelry.
- Quartz is widely used in the production of watches and watches, and in many industries crystalline solids are used as raw materials.

Types of crystalline solids

Crystallized solids are divided into four groups based on the presence of intermolecular forces or chemical bonding:

For molecular solids

The particles that make up molecular solids are molecules, and in general molecular solids are insulators, soft in nature, and have a very low density.

Molecular solids are classified into three types based on the nature of the molecules: (non-polar molecular solids, polar molecular solids, hydrogen-bonded molecular solids)

• Ionic solids

Ions are the particles formed in ionic solids, these are formed by powerful Colombian forces that arrange cations and anions, which are fragile and difficult in nature.

In the solid state, they are insulators, while in the molten and aqueous state, they are conductors, and they have a very high melting point, e.g. sodium chloride, MgO, ZnS, CaF2 etc.

• Metal solids

Electron-positive metal ions are uniformly distributed throughout the crystal, and they are responsible for high electrical and thermal conductivity due to the presence of free and moving electrons.

In both the solid and liquid state they are conductors, and these solids have a solid physical nature but they are flexible and spreadable, and they have the greatest melting points such as: Fe, Cu, Ag, Mg.

•Covalent solids

A variety of non-metallic crystalline solids form a giant molecule or macromolecules by forming covalent bonds between neighboring atoms in a crystal.

These solids are carbon isotopes, hard like diamonds and soft like graphite, they are insulators like diamonds, but because of free electrons they conduct electricity and act as a conductor like graphite.

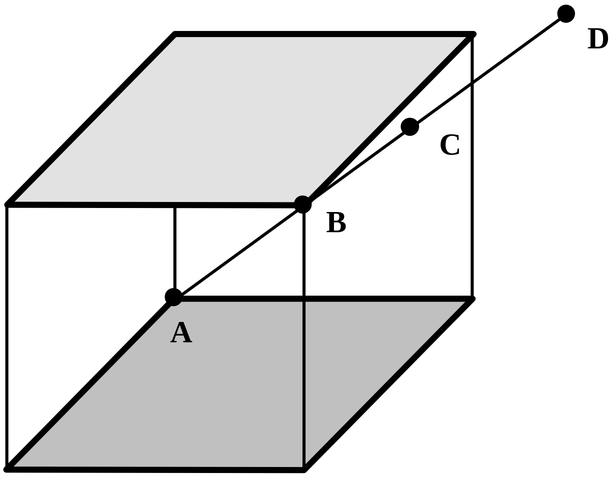
CRYSTAL DIRECTIONS الاتجاهات البلورية

Since the physical properties of crystals are heterogeneous in different crystal directions, it is necessary to find a way to designate and name directions in the crystal.

The direction in the crystal can be determined as follows. Suppose that a straight line passes through lattice points A, B, and C, as shown in Figure 3-1. To identify these points, we select one of the lattice points and consider it the origin of the point A. Then we select the lattice vector connecting point

A to any point on the line, be point B, and so on. This vector can be expressed by base vectors of the form

$$R = n_1 a + n_2 b + n_3 C \qquad 1\text{-}3$$



.Figure 3-1 Crystal vector

The trend is now determined by a set of numbers [n_1,n_2,n_3]. The common factor between these numbers should be omitted, if any, i.e. this group should be the smallest of the numbers with the same ratio.

Thus, the direction shown in Figure 3-1 and denoted in terms of Miller's evidence is as [111].

Note that the direction guides for a given direction are the same as the Miller guides for the plane perpendicular to that direction, for example, the guides are the guides of the direction perpendicular to the plane[321]

When a unit cell has some rotating symmetry, there may be many non-uniform directions that are equivalent from the point of view of symmetry, so the directions [100], [010], and [001] in the cubic crystal are equivalent. All directions equivalent to the direction [n1n2n3] are denoted by the symbol 3n1n2n with angular arcs Thus, the symbol 100 in the cube system refers to the following six directions,[001],[1 00], [010], [001], [100], [010]. The negative sign of the number s indicates the negative value of the number, and similarly the symbol 111 refers to the diagonals of the cube, which of course is not equivalent to the 100 direction.

Figure 3-2 shows Miller's guides for three faces in the cube and Miller's guides for directions perpendicular to them.

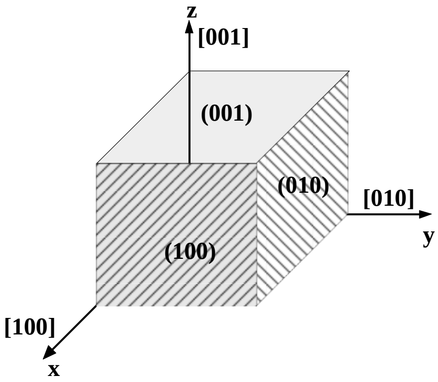


Figure 3-2 Basic directions in the cube.

<u>Example 3-1</u>

Draw plane [110] and vector [110] in a simple cube

Solution

From Figure (3-3)a the level BFHD is the level [110] where the intersections of this plane with the axes are , i.e. ∞,1,1. The vector EG is the vector perpendicular to the previous plane and has the evidence [110] and has its projection on the x-axis is 1, on the y-axis is 1, and its projection on the z-axis is 0.

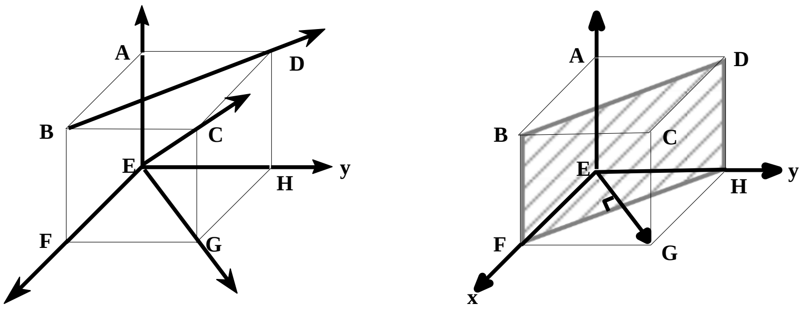


Figure 3-3

Identify Miller's guides for the vectors defined in Figure (3-3)b.

Solution

The Miller indices for the vectors shown in Figure 3-3(b) are as shown in Figure 3-4.

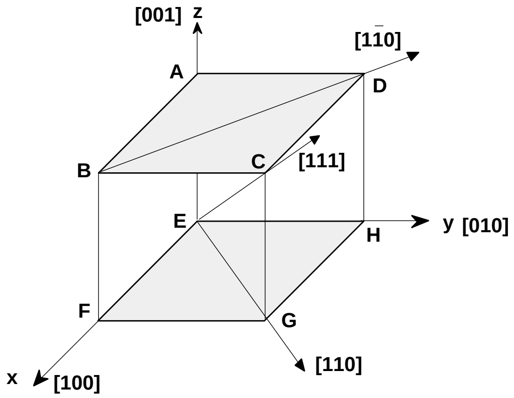


Figure 3-4

Distance between parallel planes

In X-ray scattering by crystal, one needs to know the distance between parallel planes (which have the same Miller indices, [hkl]). The real equation for this distance depends on the crystal structure, where we will consider only the case in which the axes are perpendicular, in order to simplify (and we will study the case of the cube in detail in a later chapter). We can calculate this distance by referring to Figure 3-5.

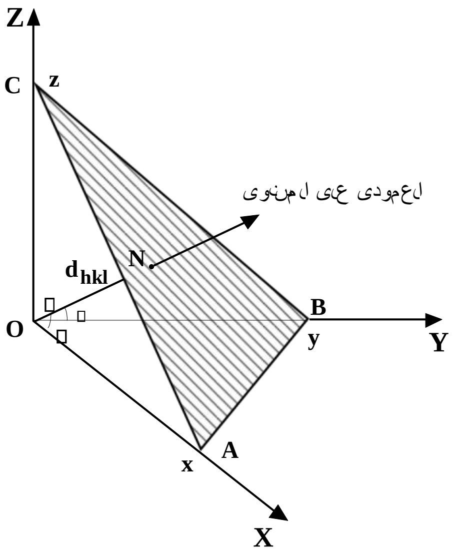


Figure 3-5 Finding the distance between the planes

The shaded plane belongs to the set of levels hkl . We imagine another plane parallel to the shaded plane passing through the origin. Thus, the length of the column ON drawn from the origin on this plane represents the dhkl distance separating this set of parallel planes. We assume that this perpendicular makes g, ya α, β, and γ with the x, y, and z axes and that the plane crosses these axes at points x, y, and z, respectively. Figure 3-5 shows that:

$$d_{hkl} = x\cos\alpha = y\cos\beta = z\cos\gamma. \qquad 2\text{-}3$$

Whereas, according to the law of the right of the angle,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1. \qquad 3\text{-}3$$

From the previous equations 3-2 and 3-3, after substituting the cosines of the angles, we obtain an expression for the distance dhkl separating the parallel planes hkl as follows ,

$$d_{hkl} = \frac{1}{\sqrt{\frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2}}} \qquad 4\text{-}3$$

ATOMIC DENSITY OF CRYSTAL PLANES الكثافة الذرية لمستويات البلو رة

In order to determine the mechanical properties (especially the plastic behavior) of metal crystals, the density of the arts located at the different crystal levels must be known in order to determine whether or not the planes slide on each other. The atomic density of a crystal plane J is defined as the number of arts per unit area in a given crystal plane. How to calculate the atomic density of a plane can be illustrated by the following examples :

Example 3-11

In a lead crystal, I calculate the atomic density of levels a-[100], b-[111] and c-[110], given that lead crystallizes in the form of a centered cuboid and has a = 4.93 A.

Solution

(A) In the level [100] the distribution of arts is as shown in Figure (3-11 a) . This level contains two atoms 1/4 * 4 + 1 = 2 and therefore the atomic density of this level, ρ $_{100}$, is equal to the number of arts divided by the area, i.e .

$$\rho_{100} = \frac{2\ atom}{(a\ mm)^2} = \frac{2\ atom}{\left(4.93 * \ x10^{-7}\right)^2} = 8.23\ \ x10^{12}\ \ atom/mm^2$$

(b) At the level [111] the distribution of art's is as shown in Figure 3-11 (b). This plane contains two atoms (2 = 3 * 1/6 + 3 * 1/2) for each PRQ triangle, its height is h =$\sqrt{2}$ acos30 and the length of its base is equal to a ' 2 √and therefore its area is equal to

$$\frac{1}{2} * \ \sqrt{2}a * \ \sqrt{2}a * \cos 30 = \frac{\sqrt{3}}{2} = a^2$$

And the atomic density of this plane is equal to

$$\rho_{100} = \frac{4\ atom}{\sqrt{3}(2)^2} = \frac{4\ atom}{\sqrt{3}\left(4.93 * x10^{-7}\right)^2} = 9.5\ x10^{12}\ \ atom/mm^2$$

Q: What are the three relatively simple crystal structures that contain the most common minerals?

الجواب: *FCC* و*BCC* و *HCP*

Features of cubic lattice

The cube system includes three types of lattice

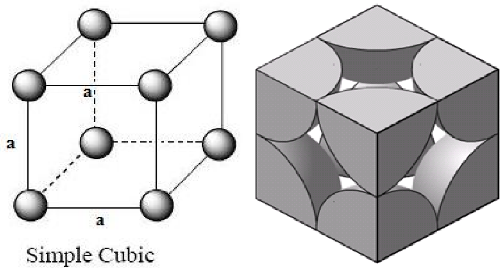
1- Simple Cubic (SC أو sc)

It has one lattice point $\frac{1}{8}$ A point in each of the eight corners and its vectors

$$\vec{a} = a\hat{i}\ ,\quad \vec{b} = b\hat{j}\ ,\quad \vec{c} = c\hat{k}$$

They are prime vectors of length L or . a

$$\frac{1}{8} * 8 = 1$$ نقطة واحدة

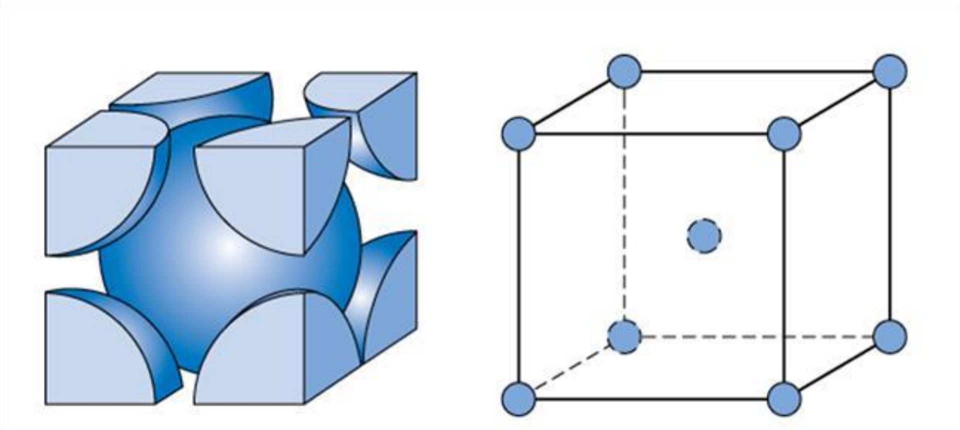


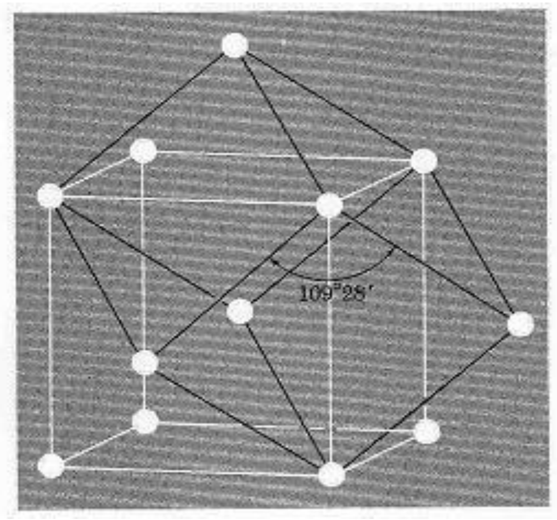
Simple Cubic

2- Body Centered Cubic (BCC أو bcc)

It contains two points, one in the corners and one in the center of the cell, which is one of the non-primary networks because it is a unit cell for it is non-primary, and the initial vectors can be calculated and then the primary unit cell has as follows:

We draw three vectors from a lattice point in the center of the cube and consider it the origin, ending in three points located at the corners of the cube as in the diagram and complete the diagnosis of rhombic to obtain the initial unit cell with Elementary Vectors $\vec{\mathbf{a}}'$ $\vec{\mathbf{b}}', \vec{\mathbf{c}}'$,




109°28′

For the initial lattice $$\begin{cases} \vec{a}=\overrightarrow{a_1}=\frac{a}{2}\left(\hat{i}+\hat{j}-\widehat{k}\right) \\ \vec{b}=\overrightarrow{a_2}=\frac{a}{2}\left(-\hat{i}+\hat{j}+\widehat{k}\right) \\ \vec{a}=\overrightarrow{a_3}=\frac{a}{2}\left(\hat{i}-\hat{j}+\widehat{k}\right) \end{cases}$$

The cell of the primary unit is a rhombic with side length $\left(\frac{\sqrt{3}}{2}L\right)$ and axes and occurs with each other $\vec{\mathbf{c}}`$, $\vec{\mathbf{b}}`$,$\vec{\mathbf{a}}`$, An angle of approximately (109^{o}) and the positions of the two points: $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$, 000

Q1 / Prove that the angles between the tetrahedral bonds of diamonds are the same as the angles between the diameters of the BCC, as in the adjacent figure. Use prime vector factorization to evaluate the angle. :

Angles between: $\vec{a_1}$ and $\vec{a_2}$,$\vec{a_2}$ and $\vec{a_3}$, or $\vec{a_3}$ and $\vec{a_1}$.

$$cos\theta = \frac{a_1 \times a_2}{\|a_1\|\|a_2\|} = \frac{\frac{1}{4}a^2(-1-1+1)}{\frac{1}{4}a^2(1^2+1^2+1^2)} = -\frac{1}{3}$$

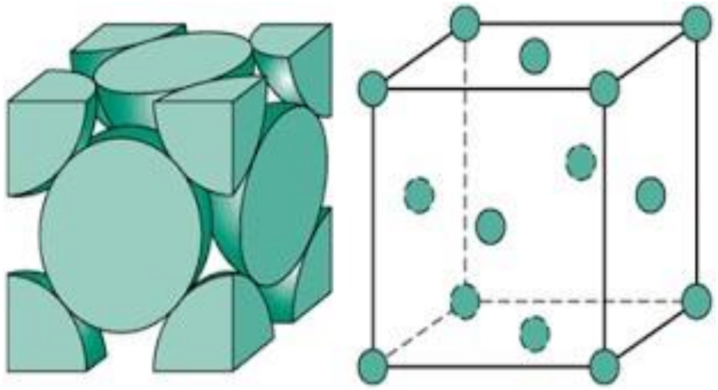
$$\theta = cos^{-}1(-\frac{1}{3}) \approx 109.47^0$$

Q2 / Prove that the volume of the primary unit cell of the bcc cube is equal to the volume of the normal unit cell of the same lattice.

$$V = \left|\vec{a} \times \vec{b} \,.\, \vec{c}\right| \qquad = \qquad \left|\vec{a} \,.\, \vec{b} \times \vec{c}\right|$$

3- Face Centered Cubic (FCC أو fcc)

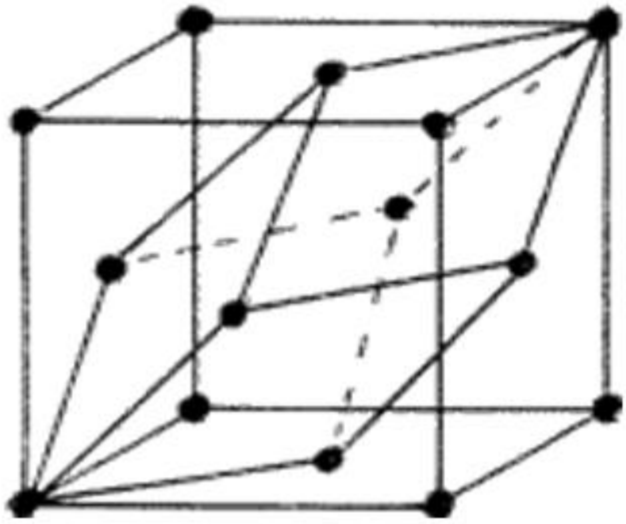
It has four lattice points, one of the corners and half a point in each of the six faces. It is not a primary network because his unit cell is not primary.



To obtain the prime vectors, we draw three vectors emitted by a lattice point in one of the corners of the heel and consider it the origin point so that it ends with the lattice points located in the centers of the faces near the origin as in the adjacent figure. We complete the rhombic faces to obtain the prime unit cell with prime vectors:

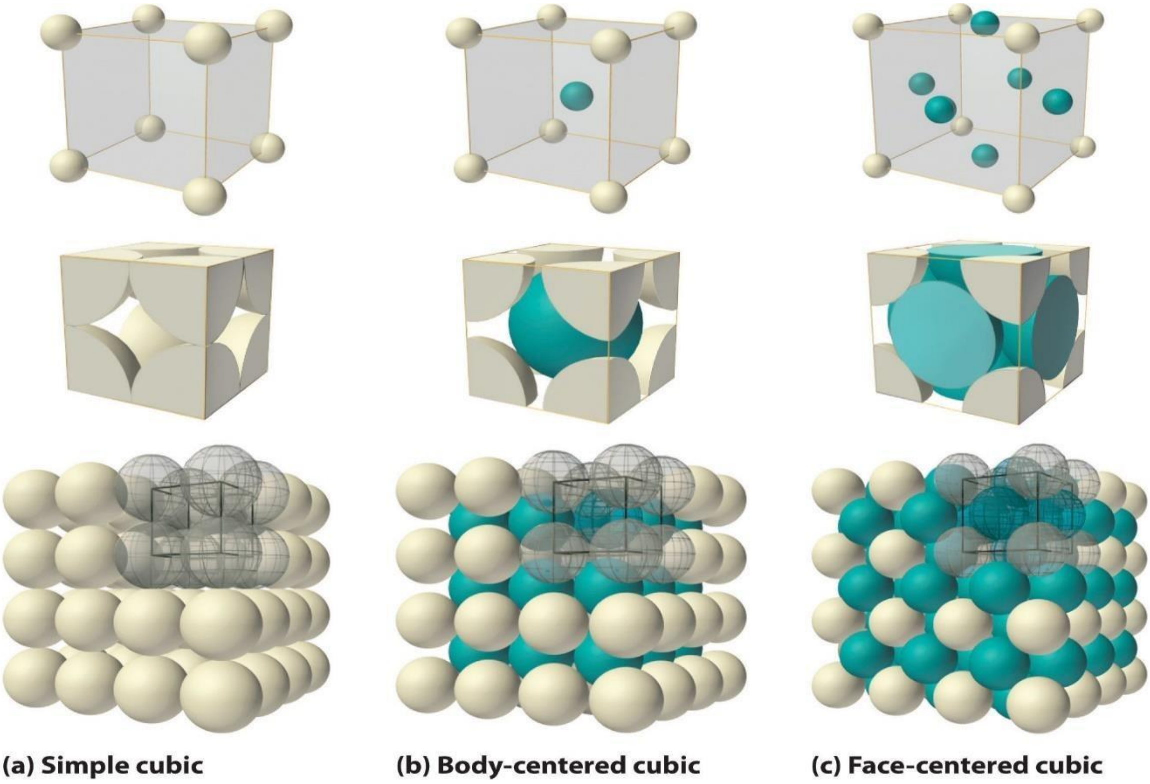
For the initial lattice

$$\begin{cases} \vec{\grave{a}} = \overrightarrow{a_1} = \dfrac{a}{2}\,(\hat{\imath} + \hat{\jmath}) \\ \vec{\grave{b}} = \overrightarrow{a_1} = \dfrac{a}{2}\,\left(\hat{\jmath} + \hat{k}\right) \\ \vec{\grave{c}} = \overrightarrow{a_1} = \dfrac{a}{2}\,\left(\hat{\imath} + \hat{k}\right) \end{cases}$$



Point Locations $000\ ,\ 0\frac{1}{2}\frac{1}{2}\ ,\ \frac{1}{2}0\frac{1}{2}\ ,\ \frac{1}{2}\frac{1}{2}0$

Q: Prove that the primary cell size of the FCC lattice is the normal cell size of that lattice.



:Packing Fraction or Filling fraction

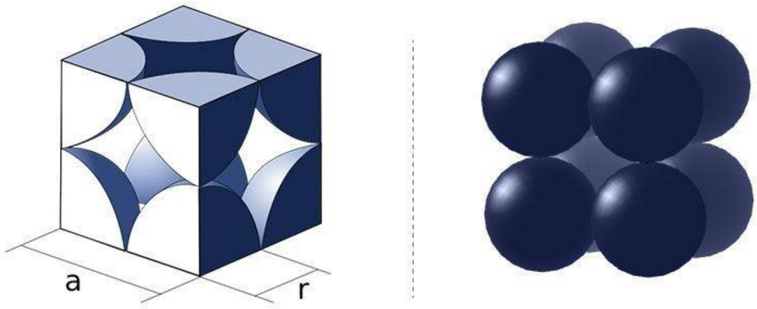
For the purpose of calculating the filling ratio, we assume that very adjacent atoms are in contact, that is, the shortest distance between two lattice points represents the diameter of the atom (the distance of the nearest neighbor = 2r) and the stacking ratio is calculated as follows:

$$\text{Stacking ratio}= \frac{\text{The volume of one atom} * \text{the number of atoms in a unit cell}}{unite\ cell\ size} * 100\%$$

$$PF= \frac{\frac{4}{3}\pi r^3 N}{V} * 100\% = \frac{4}{3}\pi r^3 \frac{N}{V} * 100\%$$

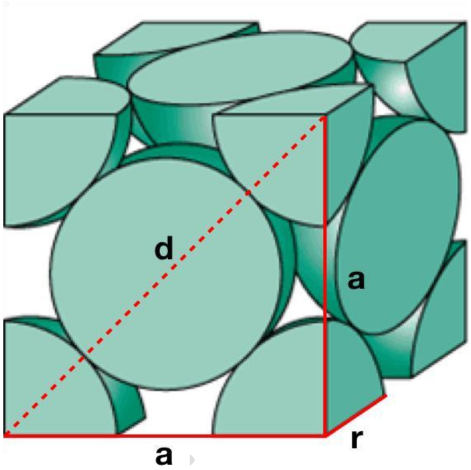
r : radius of the atom , 2r : diameter of the atom and represents the distance of the nearest neighborhood

SIMPLE CUBIC UNIT CELL



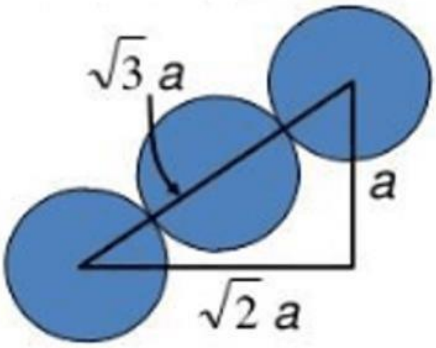
SC

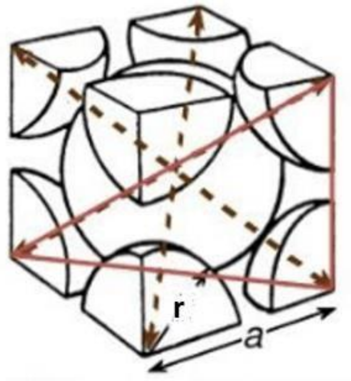
2r=a



FCC

4r=$\sqrt{2}$ a





BCC

4r=$\sqrt{3}$ a

Q / What is the magnitude of the stacking ratio of FCC, BCC, SC and diamonds The table represents some of the advantages of the networks of the cube system, namely FCC, BCC, SC where (a=L)

	sc	bcc	fcc
حجم الخلية الاعتيادية	L^3	L^3	L^3
عدد نقاط الشبيكة لكل خلية اعتيادية	1	2	4
حجم الخلية الوحدة الاولية	L^3	$\frac{1}{2}L^3$	$\frac{1}{4}L^3$
عدد نقاط الشبيكة لكل وحدة حجم $\left(\frac{N}{V}\right)$	$\frac{1}{L^3}$	$\frac{2}{L^3}$	$\frac{4}{L^3}$
عدد الجوار الأول (العدد التناسقي)	6	8	12
مسافة الجوار الاول	L	$\frac{\sqrt{3}}{2}L$	$\frac{1}{\sqrt{2}}L$
عدد الجوار الثاني	12	6	6
مسافة الجوار الثاني	$\sqrt{2}L$	L	L
نسبة الملء	0.52	0.68	0.74
نسبة الجزء الفارغ	0.48	0.32	0.26

How to calculate theoretical density

$$\boldsymbol{\rho = \frac{N\, A_w}{V\, N_A}}$$

where ρ represents the theoretical density $\left(\frac{g}{cm^3}\right)$ N represents the number of atoms in a unit cell V represents unit cell size (cm^3) and NA represents the number of avogadro $=10^{23}*3.023$ (atom/mol

Example / Copper has an FCC crystal structure and an atomic radius of 0.128 .nm, and an atomic weight of gmol 33.6. Calculate its theoretical density

Solution / Number of Atoms 4

$V=a^3$ ، $4r=\sqrt{2}\,a$, $V=\left(\frac{4}{\sqrt{2}}r\right)^3$ −

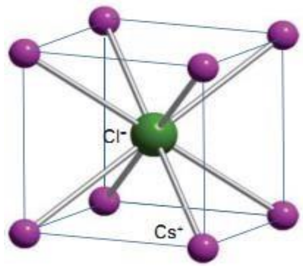
$$\rho = \frac{4 * 63.5\ \text{g\textbackslash mol}}{\left(\frac{4}{\sqrt{2}} * 0.128 * 10^{-7} cm\right)^3 * 6.023 * 10^{23}\text{atom/mol}}$$

$=8.89\ g\backslash cm^3$

1- Simple Crystal Structure

Cesium chloride has a simple cubic praviz lattice SC with a side length of 4.IIA and the base is composed of two ions, Cl+, Cs. If it is assumed that the cesium ion occupies one of the corners of the lattice and the origin of the cube is (000) + Cs, then The chlorine ion occupies the center of the cube, i.e. the site Cl $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$

31

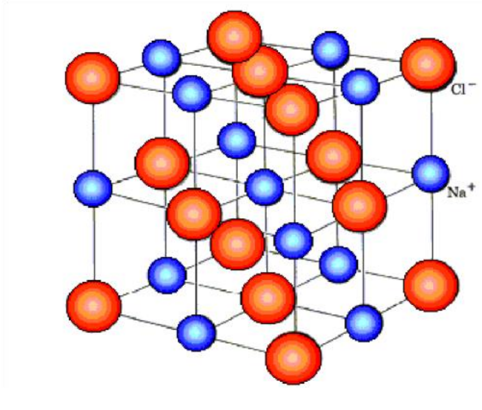


Cs^+ : 000

Cl^-: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

2- Sodium Chloride NaCl

The Praviz lattice has a cubic type centered on the fcc with a side length of Å5.63 The normal single cell contains four lattice points, each of which is accompanied by a base consisting of two ions, one of them +Na and the other -Cl, separated by a distance of the radius of the cubic unit cell, so the normal unit cell includes four sodium ions and four chlorine ions, i.e. four molecules of sodium chloride, and chlorine and sodium ions are distributed on the following sites:



تحفظ مهمة جدا

$$Na^+ :\ 000\ ,\ \frac{1}{2}\frac{1}{2}0\ ,\ \frac{1}{2}0\frac{1}{2}\ ,\ 0\frac{1}{2}\frac{1}{2}$$

$$Cl^- : \ \frac{1}{2}\frac{1}{2}\frac{1}{2} \ , \quad 00\frac{1}{2} \ , \quad 0\frac{1}{2}0 \ , \ \frac{1}{2}00$$

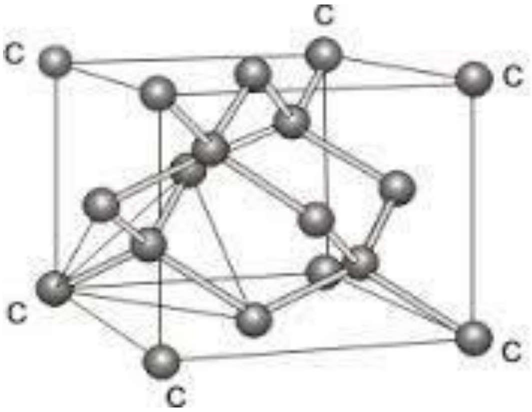
There are structures similar to that of sodium chloride such a Potassium chloride, potassium bromide, silver bromide .... etc

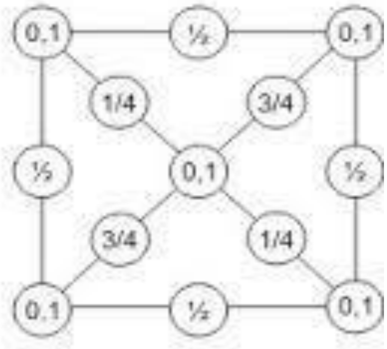
Diamond Structure -3

The composition has a Praviz lattice of the type of cubic centered faces fcc side length Å3.56 and the basis is of two similar carbon atoms C and the distance between them is estimated at a quarter of the diameter of the cubic unit cell and that the normal cubic unit cell contains 8 carbon atoms distributed on the following sites : One atom in one corner of the cell 000 and three in the centers of the cell faces $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}0\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$

And four atoms inside the cell, two close to its lower base at the sites $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, $\frac{3}{4}\frac{3}{4}\frac{1}{4}$

And four atoms inside the cell, two close to its lower base at sites and two close to its upper base, i.e. at sites $\frac{1}{4}\frac{3}{4}\frac{3}{4}$, $\frac{3}{4}\frac{1}{4}\frac{3}{4}$ At the sites as in the figure:





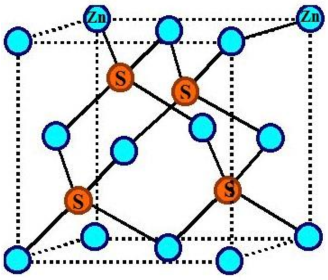
Each carbon atom is covalently linked to four adjacent atoms (first neighborhood) and is surrounded by twelve atoms as a second neighborhood, and despite the high hardness of diamonds, the filling rate does not exceed 34%.

4-Cubic Zinc Structure ZnS

The cubic structure of zinc sulfide and similar compounds is called zinc volcano, which is a similar structure to the composition of diamonds, and the only difference is that the basis in the case of ZnS is made up of two atoms, Zn and S, instead of the two carbon atoms that are similar in diamonds, and the Zn and S atoms are arranged so that they occupy the following atomic sites:

$Zn : 000\ ,\ 0\frac{1}{2}\frac{1}{2}\ ,\ \frac{1}{2}0\frac{1}{2}\ ,\ \frac{1}{2}\frac{1}{2}0$

$S\ :\ \frac{1}{4}\frac{1}{4}\frac{1}{4}\ ,\ \frac{1}{4}\frac{3}{4}\frac{3}{4}\ ,\ \frac{3}{4}\frac{1}{4}\frac{3}{4}\ ,\ \frac{3}{4}\frac{3}{4}\frac{1}{4}$



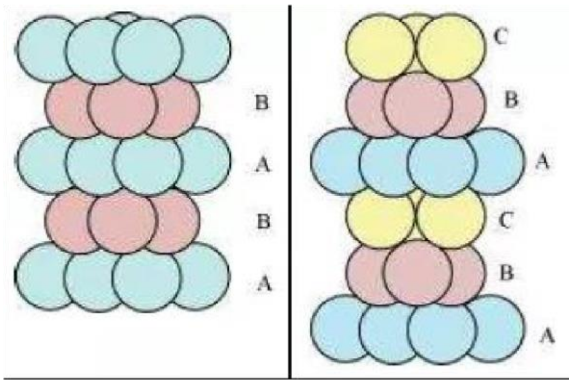
The size of the unit cell of zinc sulfide is about three and a half times the size of the diamond cell as the side length of the unit cell of zinc sulfide is Å5.41 which makes the filling ratio small .

5- Hexagonal Closed Filling and Coherent HCP and Closed Cube Fill (CCP)

The crystal structure of a cubic – closed packed (ccp) is a face-centered cube or hexagonal closed packed (hcp) and examples of a coherent cubic structure are crystals:

Cu , Ag , Al , NH_3 , HCl , HBr , Ar While the composition is hexagonal coherent crystals] SiO_2 , N_2 , O_2 , H0.

The filling ratio of both CCP and HCP is 0.74 which is the largest filling ratio value that can be obtained for any crystal structure.



(hcp) (ccp)

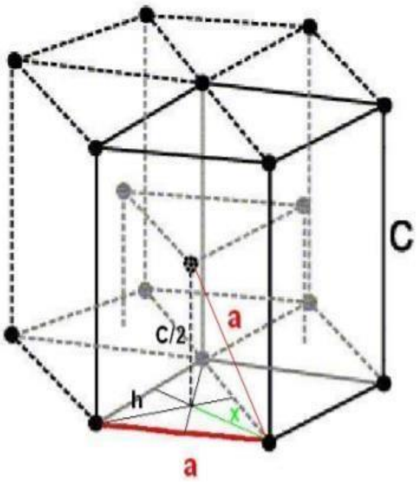
Q/show that the ratio c/a for the ideal hexagram structure is: 3 = 1.633/8 = c/a

س/ بين أن النسبة c/a للتركيب السداسي المثالي هي : 3 = 8/633.1 = c / a

h. . .height of the equilateral triangle

a. . .lattice constant

$$h = \sqrt{a^2 - (a/2)^2} = \sqrt{1 - \frac{1}{4}} * a = \sqrt{\frac{3}{4}} * a$$



Distance x from an atom to the middle of the triangle:

$$x = \frac{2}{3} * h = \frac{2}{3} * \sqrt{\frac{3}{4}} * a$$

$$x = \frac{1}{\sqrt{3}} * a$$

$$\frac{c}{2} = \sqrt{a^2 - x^2} = \sqrt{a^2 - \frac{1}{3}a^2} = \sqrt{\frac{2}{3}} * a$$

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

X-ray diffraction in crystals.

Three types of beams are used in diffraction experiments: X-rays, neutron beams and electron beams. The mathematical treatment of the three types is almost the same so we will examine in detail only the case of X-rays. After a brief discussion of the generation and properties of X-rays, we will provide a brief conclusion of Prague's law of scattering rays by crystal planes. We will also discuss the scattering of rays by atom and by crystal. In this context, we will discuss the inversion lattice and various practical methods for studying crystal structure.

5.1 Rays used to study the crystal structure

For the rays to be suitable for studying the crystal structure of a solid state, the wavelength of the rays must be approximately equal to the distance between atoms. Since the distance between the atoms of a solid is in the range of 10-8 cm, the rays by which important information about the structural structure of the material can be obtained must have a wavelength of the same order (-01 cm). When some types of radiation fall on a solid material, they are scattered by the atomic levels of the material, deviate from its course and overlap together to form a diffraction pattern that carries with it information about the structural structure of the material. This information can be extracted and the details of the structural structure of the crystallized material can be obtained by analyzing good diffraction models of the rays within this material.

Many types of photons can be used in diffraction experiments to study the structural structure of crystallized material, including X-rays, neutrons and electrons. Although these types differ in energy (and therefore wavelength), the mathematical treatment of the three types is almost the same.

The diffraction angles of photons in a material depend mainly on both the structural structure of the diffraction material and the wavelength of the photons used. The energy of an X-ray photon is determined according to its wavelength from the relation:

$$E = h\text{u} = hc/\lambda \text{ ‘} \qquad 1\text{-}5$$

where *h* is Planck's constant (n,(6.62´x 10-27 erg.sec) wave frequency and c is the speed of light (1-m.sec 108x3). From this relationship, the wavelength of the X-ray can be written on the image,

λ (A^{o})= 12.4/ E(Kev). 2-5

It is clear from this relationship that the energy of a ray photon in the range of 10-50 kV gives a wavelength in the range of 1.2-0.4 angstroms. Figure 5-1 shows the location of X-rays in the spectrum of electromagnetic waves. In this spectrum, due to the absence of precise values of the upper and lower limits of the different electromagnetic wave regions, the boundaries between the regions are optional.

Accelerated neutron rays are suitable for studying the structural structure of some types of solids due to their magnetic momentum, which makes them interact strongly with the electrons of the atoms that make up the material.

The energy of a neutron moving very quickly is related to the wavelength of the de Broglie associated with it according to the relationship,

$$E = \frac{h^2}{2M_n \lambda^2} \qquad 3\text{-}5$$

where Mn is the mass of the neutron (gm 42-10´1.675)

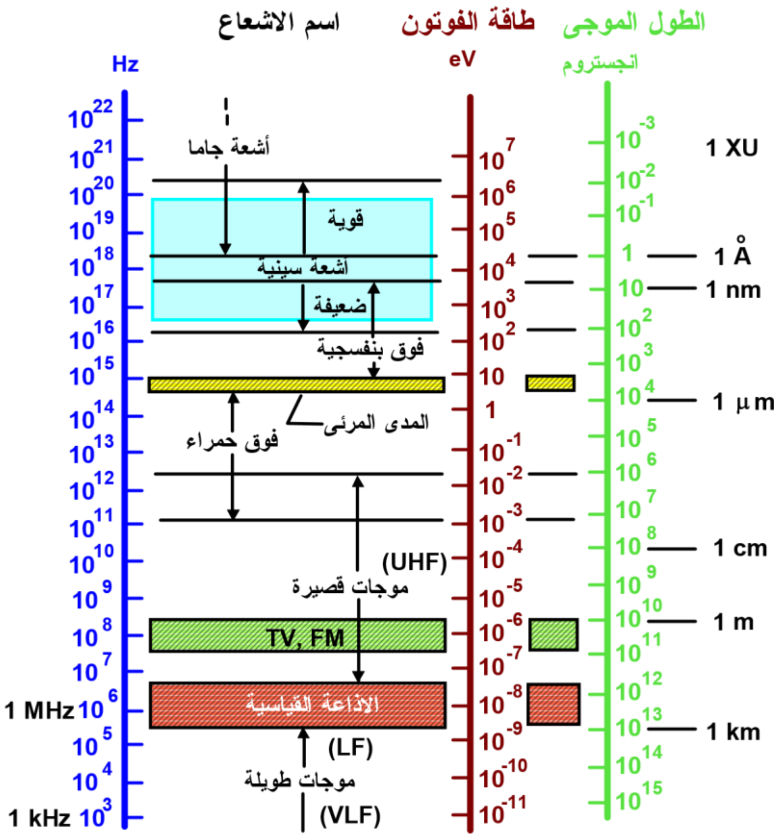


Figure 5-1 Spectrum of electromagnetic waves.

Substituting the mass of the neutron and Planck's constant into this equation, the wavelength in the form can be obtained,

$$\lambda\,(A_\circ) = \frac{0.28}{[E\,(eV)]^{\frac{1}{2}}} \qquad . \quad 4\text{-}5$$

The wavelength of a neutron with energy eV 08.0 is in the range of oA1 and such neutrons are called thermal neutrons.

Accelerated electrons are suitable for use in diffraction experiments because of their electric charge, which causes them to react strongly with atoms of matter. Also, because of their charge, the penetration distance of electrons is less than in the case of X-rays, so electronic rays are used to study the crystal structure of thin films of materials or to study the surfaces of thick crystals.

The energy of electrons moving very quickly is related to the wavelength of de Broglie associated with it according to the relationship,

$$E = \frac{h^2}{2m\,\lambda^2} \qquad 5\text{-}5$$

where m is the mass of the electron (gm 43-10´9.11). The wavelength associated with the electron can be written as

$$\lambda\,(A^\circ) = \frac{12}{[E\ \ (eV)]^{\frac{1}{2}}} \qquad 6\text{-}5$$

5.3.1 **X-ray generation**

X-rays were discovered in the summer of 1895 by the German scientist Roentgen. Roentgen was interested in generating cathode rays and accidentally noticed a flash (rays) emission from a fluorescent screen placed at a distance when an electrical discharge occurred in the cathode ray tube. From that moment on, Roentgen devoted all his energy to studying.

The characteristics of these unknown rays that cause this effect and he called them X-rays (meaning unknown rays). This discovery was met with much interest in scientific circles and was soon used in imaging in the medical field. Only the next fifteen years produced little information about the nature of these waves, when Max von Laue in 1912 was able to confirm this in practice. Knipping and Friedrich were also able after several successful attempts to conduct a successful experiment to scatter X-rays on the crystal of copper sulfate, and it was observed that there were spots scattered around the central spot where the rays fell on the plate as a result of the scattering of radiation by the atomic levels of the crystal. They have conclusively concluded that radiation consists of waves and that the crystal is composed of atoms arranged in a space lattice.

X-rays can be generated by a vacuum tube containing an anode (target) and a cathode, as shown in Figure 5-2. When the cathode is heated by a filament, it emits electrons that are accelerated towards the anode by the high voltage difference applied between the anode and the cathode. The accelerated electrons collide with the anode and generate X-rays that emit it to exit a side opening (window) that is a thin membrane of metal. Since most of the accelerated electron energy is lost upon impact with the elevator in the form of thermal energy (99% thermal energy and 1% to generate rays), the elevator must be made of metal with a high melting point and must have a large mass to extend its operating life. The elevator is cooled by a cooling (water) circuit to eliminate excess heat generated. The potential difference between the cathode and the anode is large and ranges from 1 to 50 kV (and sometimes more).

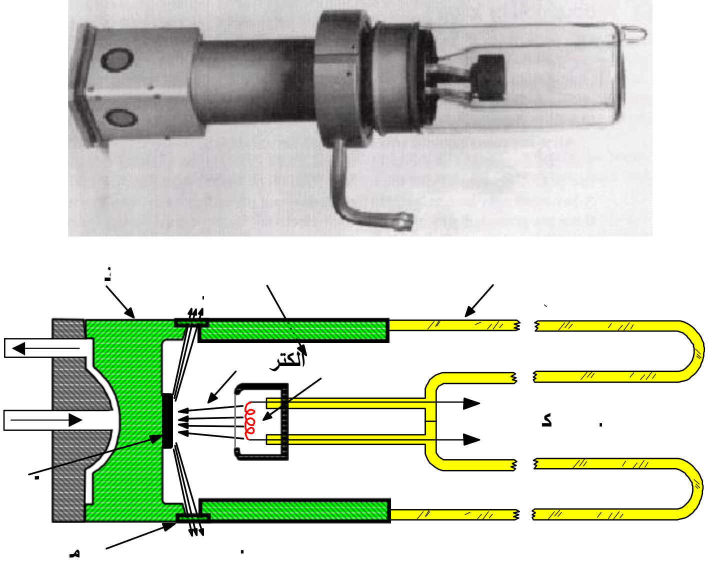


Figure 5-2 Picture and diagram of the X-ray generating tube.

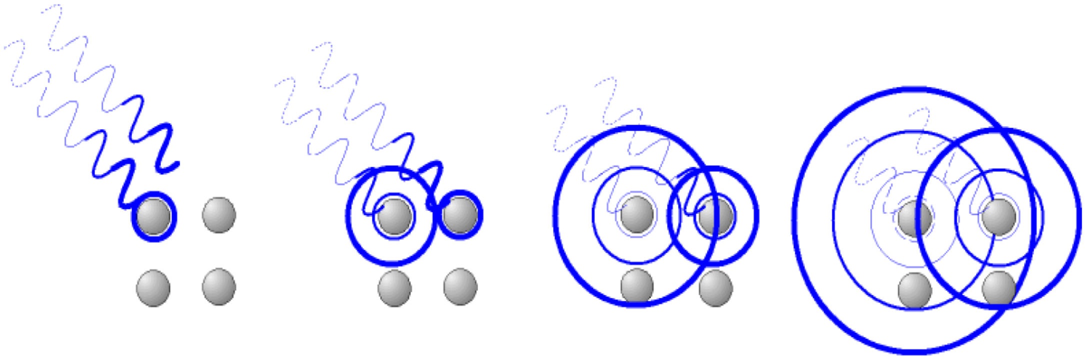
Prague's Law of Diffraction

In 1913, Prague set the geometric conditions for the diffraction of a single-length wave-ray beam and it was assumed that the beam of rays incident on the crystal is reflected just as ordinary rays are reflected from a plane mirror (the angle of incidence is equal to the angle of reflection) relative to the various atomic levels in the crystal, and that the link between the angle of incidence and the wavelength of the light used and the distance between the reflection levels is a prerequisite for good reflection (Prague).

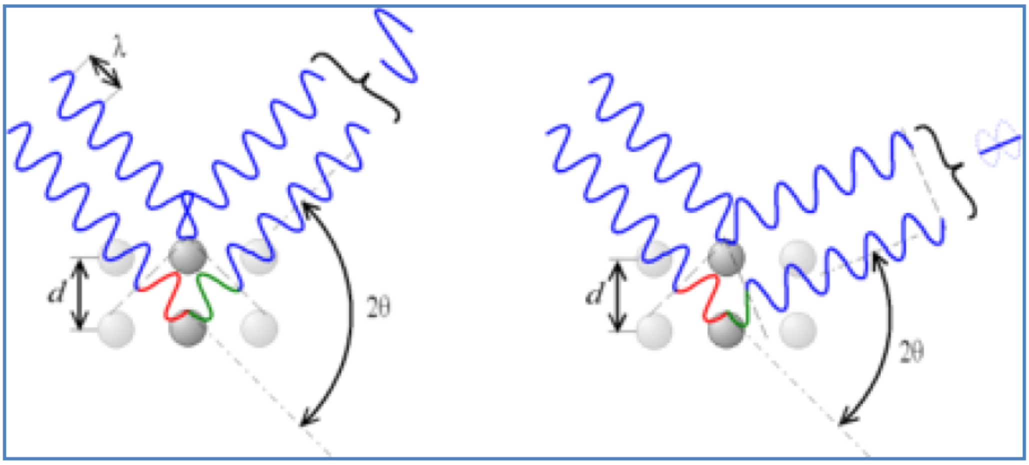
X-rays fall in the form of a parallel beam on atomic levels (follow the shapes accurately from 1-8) where they are supposed to penetrate the different layers of the crystal and exchange influence with all atomic levels, even the deep ones, and it is also assumed that the atomic levels reflect a small section of the rays and the rest penetrates to the other levels

Since the crystal consists of several atomic levels and any plane has a periodic arrangement of atoms, these levels will interact with X-rays as if they were plane diffraction networks, and this will lead to diffractions of different orders from the first plane to the second to the third...... Etc. The entry of X-rays into the depths of the crystal will lead to the emergence of a huge amount of reflected rays resulting from thousands of atomic levels (diffraction networks), but the largest part of them weakens its intensity as a result of the interference process and the other part increases in intensity and this condition is achieved when the path difference between the incident rays (incoming) and reflected is equal to an integer of the wavelength used, i.e.:

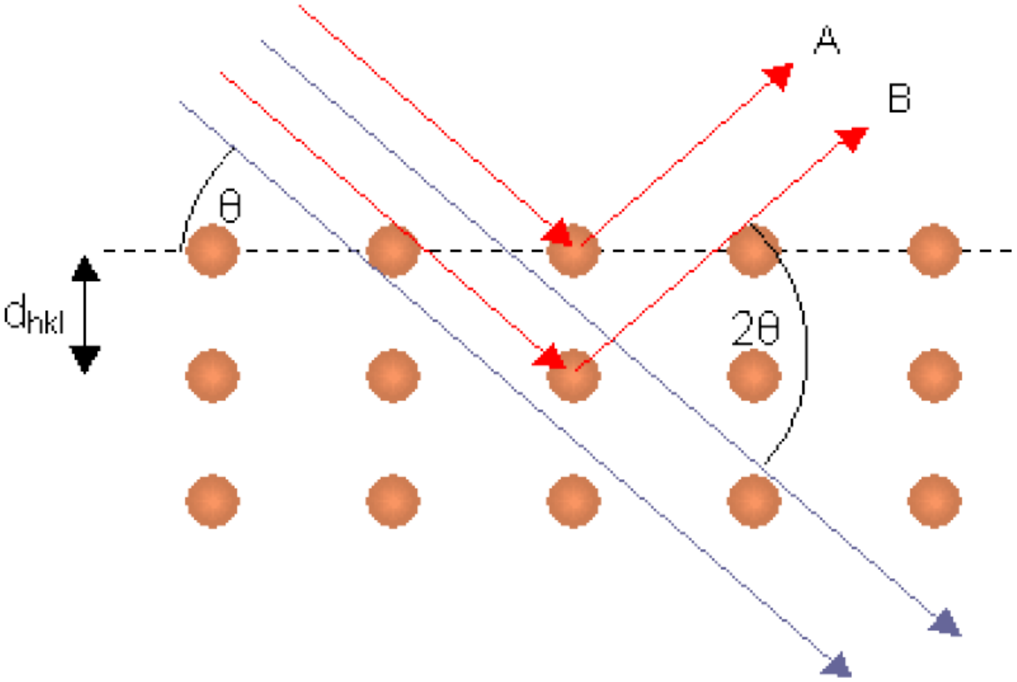
1.......... $\Delta = n\lambda$



شكل(1):تفاعل الإشعاع مع المادة



شكل(2):الحيود عن مستويين ذريين



شكل(3): الحيود واختراق الأشعة للمستويات

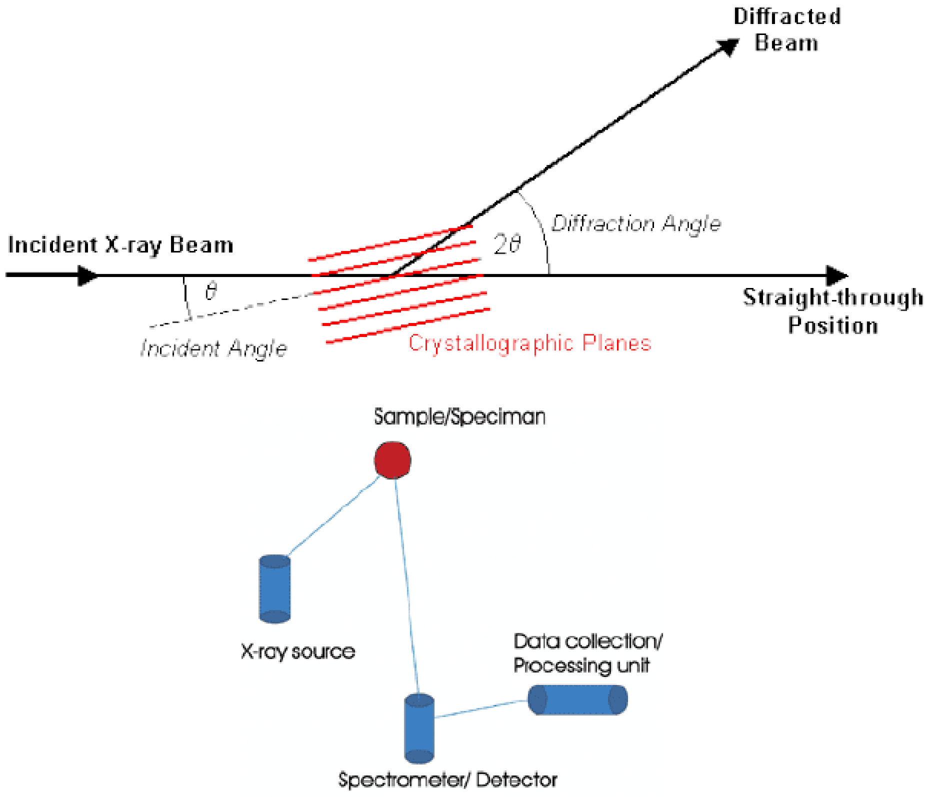
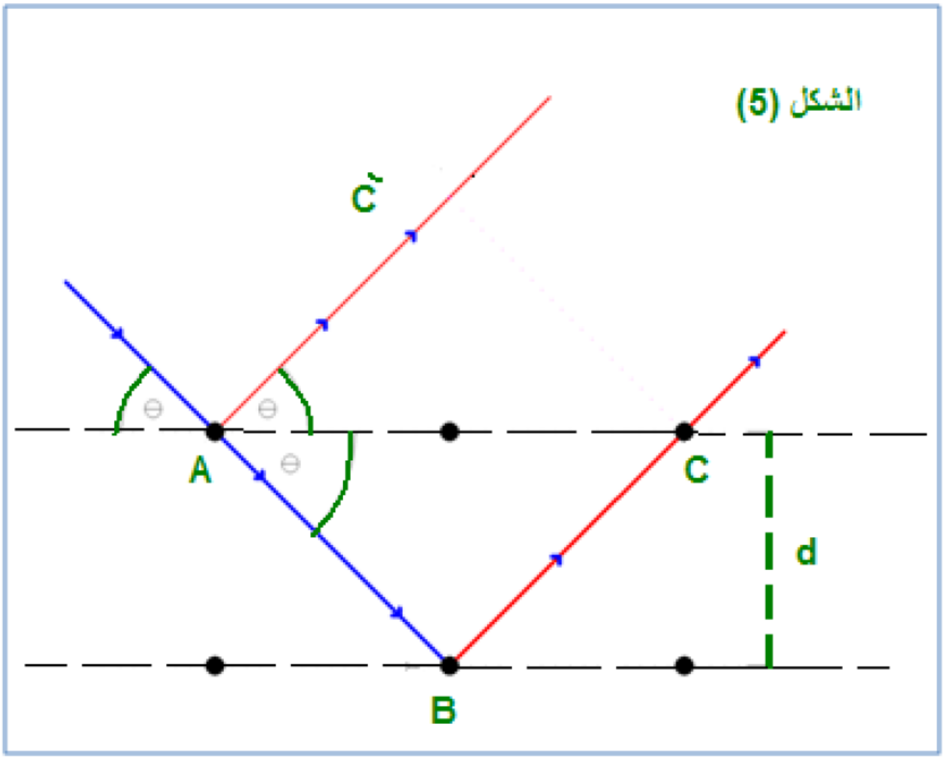


Figure 1

شكل(4) : شكل تخطيطي يمثل أشعة اكس الساقطة والشعاع المنعكس وفق نظرية الحيود لبراغ


الشكل (5)

From schematic figure (5) where a ray at point A falls on the crystal, we find the path difference between the ray reflected on the first plane at point A and the remainder of the original ray reflected on the lower plane at point B is equal to:

2………. $$(AB + BC) - (AC')$$

If this difference satisfies relation (1), we can write the following relationship:

3………… $$(AB + BC) - (AC') = n\lambda$$

We can also see from Figure (5) the following trigonometric relationships:

4………. $$AB = \frac{d}{\sin\theta} \qquad BC = \frac{d}{\sin\theta}, \qquad AC = \frac{2d}{\tan\theta}$$

We also find that:

5………… $$AC' = AC \cdot \cos\theta = \frac{2d}{\tan\theta}\cos\theta$$

We substitute in relation (3) and we find:

6………. $$n\lambda = \frac{2d}{\sin\theta} - \frac{2d}{\tan\theta}\cos\theta = \frac{2d}{\sin\theta}(1 - \cos^2\theta) = \frac{2d}{\sin\theta}\sin^2\theta$$

From it we get Prague's law of diffraction:

7………… $$n\lambda = 2d \cdot \sin\theta$$

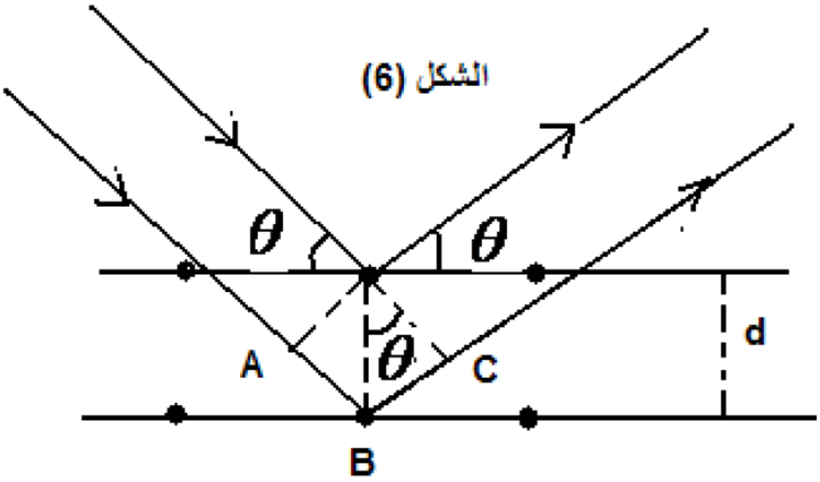
Or briefly from Figure (6) also the difference of the path between two rays, one of which falls on the first plane and the second on the second plane, we find:

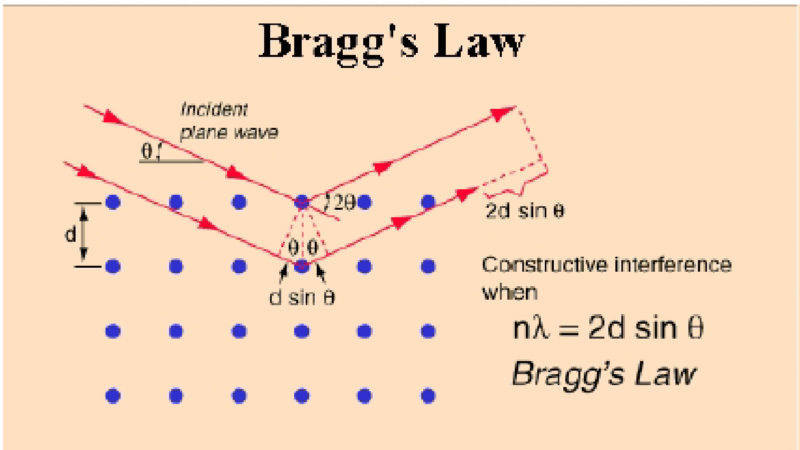
$$\Delta = ABC = 2BC = n\lambda$$

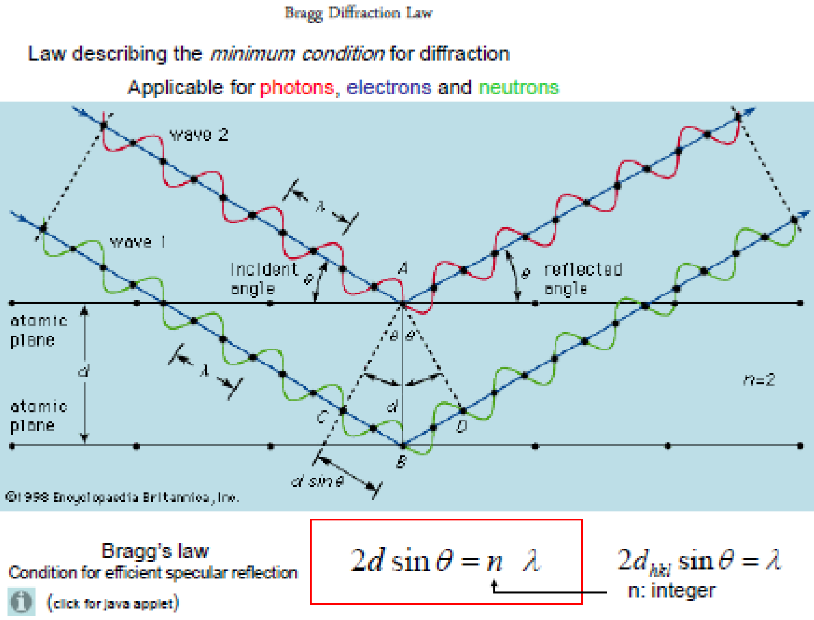
$$\sin\theta = \frac{BC}{d} \Rightarrow BC = d\,\sin\theta$$

$$\Delta = 2BC = 2d\,\sin\theta = n\lambda$$ **8..........**

It is the same relationship (7). It initially gives us the distance between atomic planes, and more than one wavelength must be used to obtain a spatial visualization of the crystal.






Bragg Diffraction Law

Law describing the *minimum condition* for diffraction

Applicable for photons, electrons and neutrons

Bragg's law

Condition for efficient specular reflection

(click for java applet)

$$\boxed{2d\sin\theta = n\ \lambda}$$

$$2d_{hkl}\sin\theta = \lambda$$

n: integer

شكل (7):قانون براغ وعملية الحيود هندسيا

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