

Aim

To study various crystals structures.

Theory

Matter exist usually in solid or fluid (liquid, gas) state. According to modern concept matter classification is specified as condensed state and gaseous state. Solids and liquids come under condensed state. Any material whose position of constituent particles is fixed can be regarded as solids.

Solids are characterized by incompressibility, rigidity and mechanical strength. This indicates that the molecules, atoms or ions that make up as solid is closely packed. Thus in solids we will have a well ordered molecular, atomic or ionic arrangement.

In general solids can be classified into:

- Crystalline-particles are orderly arranged (long range order).
- Amorphous-particles are randomly oriented.

If the atoms or molecules are uniquely arranged in crystalline solid or liquid we call it as a crystal structure. A crystal posses long range order and symmetry. The main property of crystal structure is its periodicity. This periodicity is due to the arrangement of atoms/molecules in the lattice points. The crystal structure as a whole can be considered as the repetition of unit cell. For a given crystal structure the shape of unit cell is same but varies from crystal to crystal.

X-ray diffraction studies reveal that the constituent particles (molecules, atoms or ions) are arranged in a definite pattern in the crystal. To get the diffraction pattern the wavelength of light used must be comparable with the atomic spacing.

Lattice

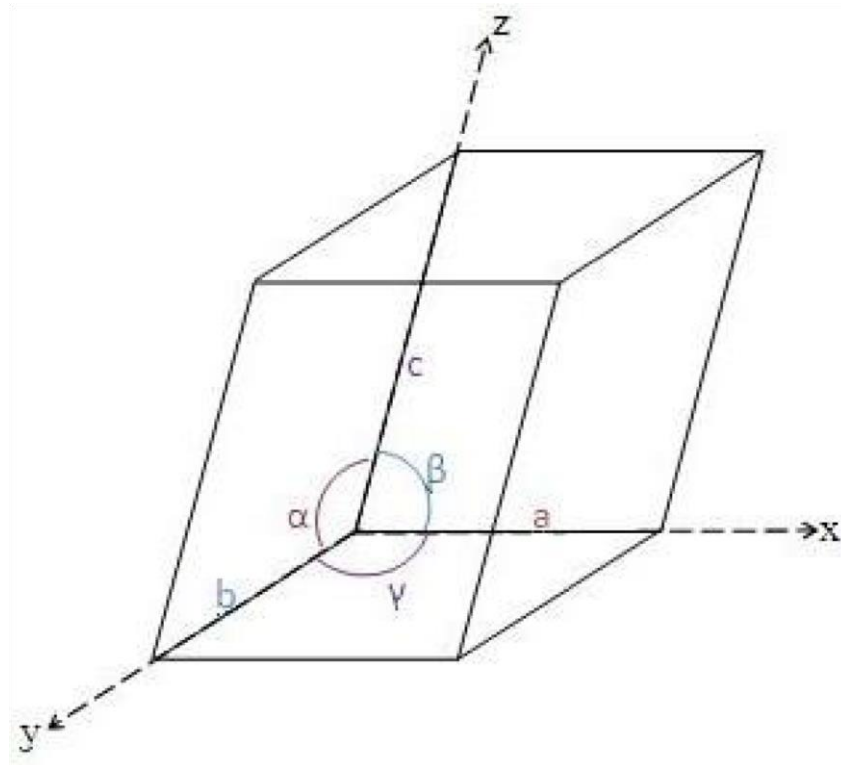
A crystal structure is formed only when the group of atoms is arranged identically at the lattice point. The group of atoms or molecules is called a basis. Lattice point is actually an imaginary concept.

In other way, we can say that,

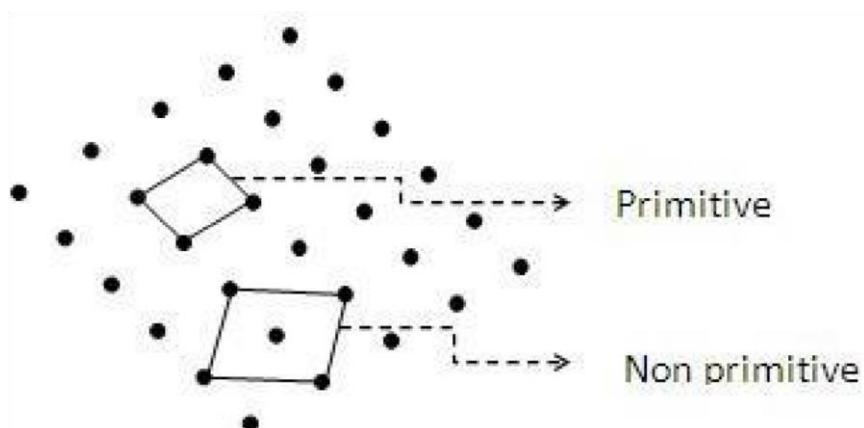
Lattice + Basis=crystal structure

Line joining any two points is a translation in lattice. Two non-collinear translation leads to a plane lattice and three non coplanar translation leads to a space lattice.

Unit cell

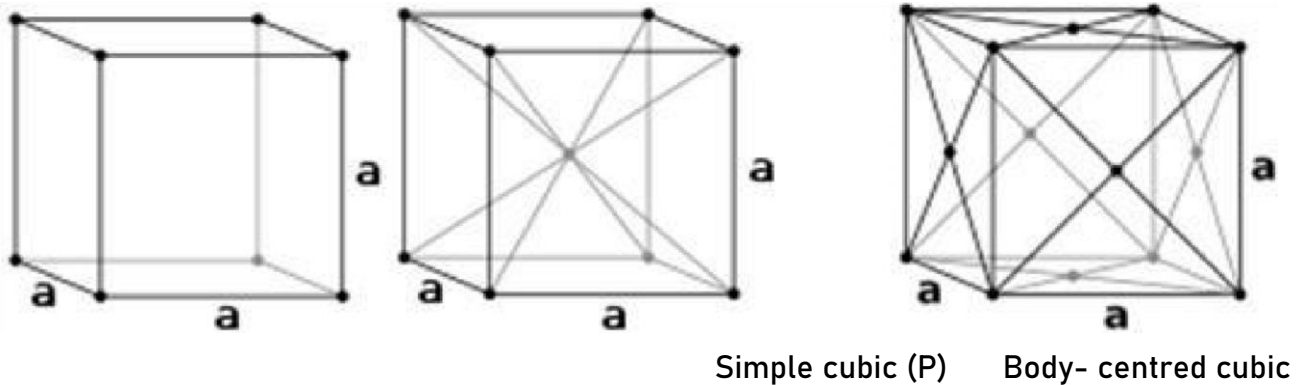


Unit cell can be considered as the building block of a crystal. It has the same symmetry as the entire crystal. When we arrange the unit cell in 3D, we get the bulk crystal. In other words it can be described as the smallest volume which when repeated in all direction gives the crystal. The three edges a , b , c along the axis and angle between them α , β and γ is termed as lattice parameters. In 3D it is better to consider a parallelepiped as unit cell.



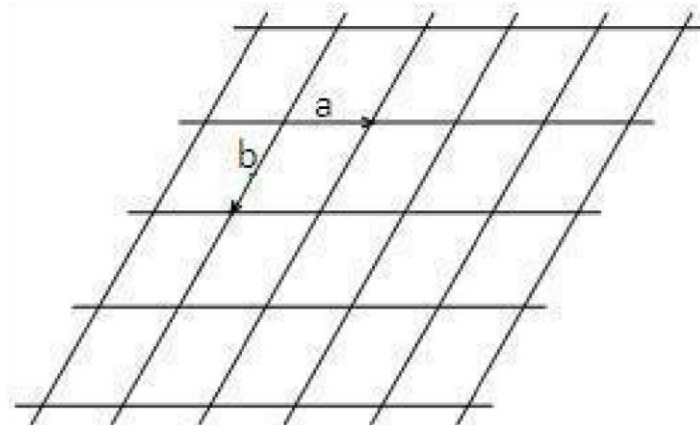
Unit cell can be of primitive as well as non primitive type. A primitive cell is a minimum volume unit cell and has only one lattice point in it and the latter contains more than one.

In the given figure below, simple cube is a primitive cell. No. of atoms per unit cell is one for it. The rest two are non primitive. No. of atoms per unit cell is 2 and 4 respectively.



(I) Face centered cubic (F)

Bravais Lattice in Two dimension-Plane lattice



In general, number of lattices obtained is unlimited since there is no restriction to the length a , b of the lattice translations and on angle ϕ between them. Such a lattice for arbitrary a , b and ϕ is known as oblique lattice. This oblique lattice is invariant under rotation of $2\pi/n$ (with $n=1$ and 2). It can also be made invariant under rotation of $2\pi/n$ with $n=3, 4$ and 6 .

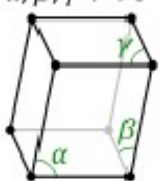
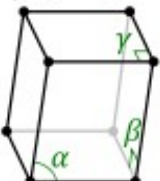
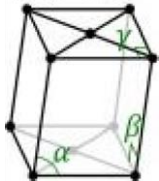
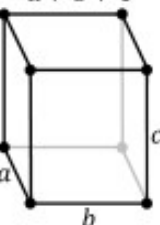
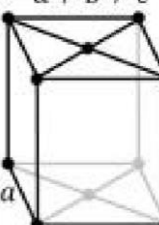
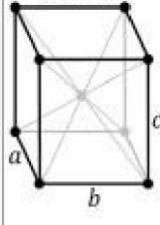
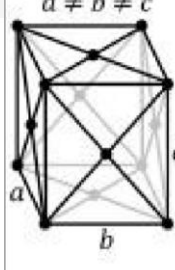
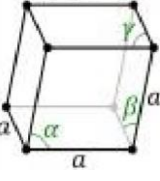
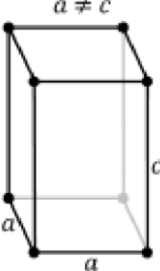
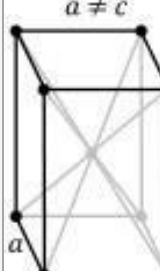
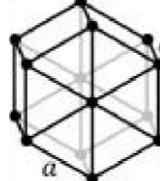
For $a=b$ and $\phi=90^\circ$, we get square lattice $a \neq b$
 and $\phi=90^\circ$, rectangular $a=b$ and $\phi \neq 90^\circ$, rhombus
 $a=b$ and $\phi=120^\circ$, hexagonal

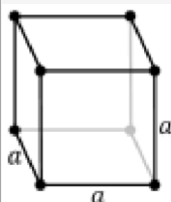
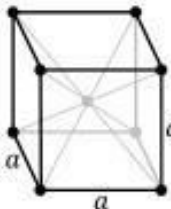
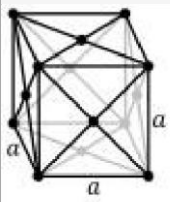
Bravais Lattice in Three dimension-Space lattice

Based on the lattice parameters a , b , c , α , β and γ and applying the restrictions as above, only 14 types of lattices are possible in three dimensions. One general (triclinic) and thirteen special. Only seven different systems of axis are found to be sufficient to represent all Bravais lattice. This fourteen space lattice is divided into seven crystal systems.

They are triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic.

Serial No :	Lattice Systems	Simple	Base - centered	Body - centered	Face - centered	Example
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1	triclinic(none)					$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{K}_2\text{Cr}_2\text{O}_7$
2)	monoclinic(1diad)	$\alpha, \beta, \gamma \neq 90^\circ$  $\alpha \neq 90^\circ$ $\beta, \gamma = 90^\circ$ 	$\alpha \neq 90^\circ$ $\beta, \gamma = 90^\circ$ 			$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$, FeSO_4 , Na_2SO_4
3	orthorhombic(3 perpendicular diads)	$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 	KNO_3 , BaSO_4
4	rhombohedral(1 triad)	$\alpha = \beta = \gamma \neq 90^\circ$ 				As, Sb, Bi
5	tetragonal(1 tetrad)	$a \neq c$ 		$a \neq c$ 		TiO_2 , SnO_2 , NiSO_4
6	hexagonal (1 hexad)					SiO_2 , Zn, Mg, Cd

7	cubic(4 triads)				Au, Cu, NaCl
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Atomic packing Fraction (APF)

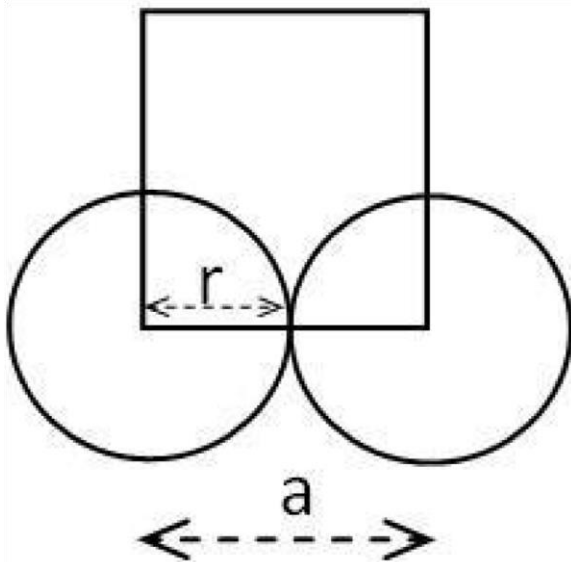
Atomic packing fraction mainly gives us an idea about the arrangement of atoms/ions in solids. It will give the efficiency with which the available space is being filled by atoms.

Packing fraction is defined as the ratio of volume of atoms occupying the unit cell to the volume of unit cell.

$$APF = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$$

Examples:

1. Simple Cubic



Consider a cube of side 'a'. Atoms of radius 'r' is placed at the corner. So that length of cube $a=2r$.

$$\text{Volume of atoms in unit cell} = \frac{1 \times \frac{4}{3}\pi r^3}{3}$$

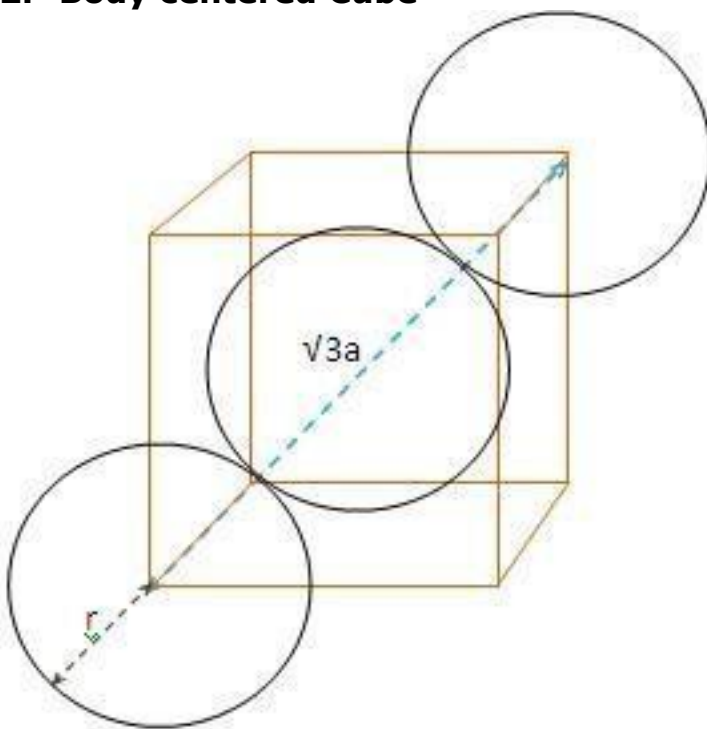
In a simple cubic structure, the atoms occupies at the eight corners. An atom at the corner is equally shared by 8 unit cells. So the contribution of one atom to a unit cell is $1/8$. Therefore the no. of atoms per unit cell is $(1/8)*8$ (corner atoms) = 1.

$$a^3 = (2r)^3 = 8r^3$$

Volume of unit cell =

$$APF = \frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6} = 52\%$$

2. Body centered Cube



Consider a cube of side 'a', and atoms of radius 'r' are placed at corners and at the body centre. Length of body diagonal, $\sqrt{3}a = 4r$.

$$\text{Volume of atoms in unit cell} = \frac{\frac{4}{3}\pi r^3}{3} = \frac{4\pi r^3}{3}$$

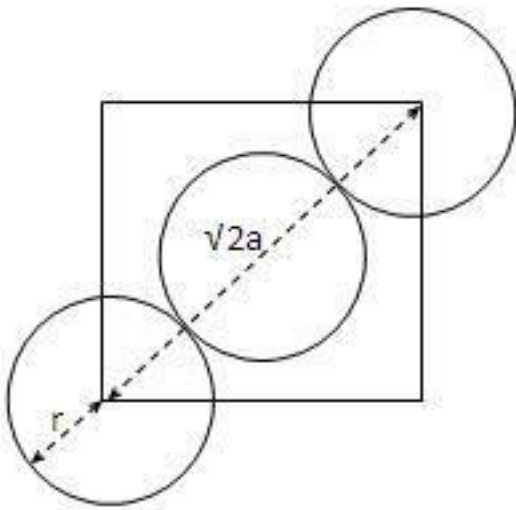
In a body centered cube, there will be one atom at the centre along with 8 corner atoms. This corner atom is shared by 8 unit cell and the atom at the centre is not a shared one. Therefore no. of atoms per unit cell = $(1/8)*8$ (corner atoms) + 1(body centre) = 2.

$$a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3$$

Volume of unit cell

$$APF = \frac{\frac{8\pi r^3}{3}}{\frac{64r^3}{(3\sqrt{3})}} = \frac{\sqrt{3}\pi}{8} = 68\%$$

3. Face centered Cube



Consider a cube of length 'a' and atoms of radius 'r' are placed at the corners as well as at the face centre. Length of face diagonal $\sqrt{2}a=4r$.

$$\text{Volume of unit cell} = \frac{4}{3} \pi r^3 = \frac{16}{3} \pi r^3$$

In a face centered cube, each face possess one atom along with 8 corner atoms. The atoms at the faces are equally shared by two unit cell. Corner atoms by 8 unit cells. So the no. of atoms per unit cell is $=(1/8)*8(\text{corner}$

atoms) $+(1/2)*6(\text{atoms at face})=4$.

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

Volume of unit cell

$$APF = \frac{\frac{16}{3} \pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\pi}{3\sqrt{2}} = 74\%$$

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Crystal Structure

Theory
 Procedure
 Self Evaluation
 Simulator
 Assignment
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 Feedback

The simulator displays a 3D model of a cubic crystal lattice. The unit cell is a cube with red spheres at the corners. The axes are labeled a , b , and c . The angles between the axes are labeled α , β , and γ . The lattice is semi-transparent, showing the internal structure.

Menu

Select Lattice Type:

Select SubType:

Lattice Transparency: 35 (0 to 100 slider)

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a=b=c$

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Crystal Structure

Theory
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The simulator displays a 3D model of a hexagonal crystal lattice. The unit cell is a hexagonal prism with red spheres at the corners. The axes are labeled a , b , and c . The angles between the axes are labeled α , β , and γ . The lattice is semi-transparent, showing the internal structure.

Menu

Select Lattice Type:

Select SubType:

Lattice Transparency: 35 (0 to 100 slider)

Measurements

$\alpha=\beta=90^\circ, \gamma=120^\circ$
 $a=b \neq c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type

Select SubType

Lattice Transparency 35

Measurements

$\alpha \neq 90^\circ \beta = \gamma = 90^\circ$
 $a \neq b \neq c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type

Select SubType

Lattice Transparency 35

Measurements

$\alpha \neq \beta \neq \gamma \neq 90^\circ$
 $a \neq b \neq c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type
Orthorhombic

Select SubType
Face Centered

Lattice Transparency 35
0 50.00 100

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a \neq b \neq c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type
Orthorhombic

Select SubType
Body Centered

Lattice Transparency 35
0 50.00 100

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a \neq b \neq c$

Crystal Structure



The diagram shows a 3D tetragonal unit cell. The vertical axis is labeled 'c', and the two horizontal axes are labeled 'a' and 'b'. The angles between the axes are labeled α , β , and γ . The cell is colored with green, yellow, and pink faces.

Menu

Select Lattice Type

Select SubType

Lattice Transparency 35

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a=b \neq c$

Crystal Structure



The diagram shows a 3D tetragonal unit cell. The vertical axis is labeled 'c', and the two horizontal axes are labeled 'a' and 'b'. The angles between the axes are labeled α , β , and γ . The cell is colored with green, yellow, and pink faces.

Menu

Select Lattice Type

Select SubType

Lattice Transparency 35

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a=b \neq c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type
Cubic

Select SubType
Simple

Lattice Transparency 35
0 50.00 100

Measurements

$\alpha=\beta=\gamma=90^\circ$
 $a=b=c$

Crystal Structure



Crystal Structure

Menu

Select Lattice Type
Monoclinic

Select SubType
Base Centered

Lattice Transparency 35
0 50.00 100

Measurements

$\alpha \neq 90^\circ \beta=\gamma=90^\circ$
 $a \neq b \neq c$