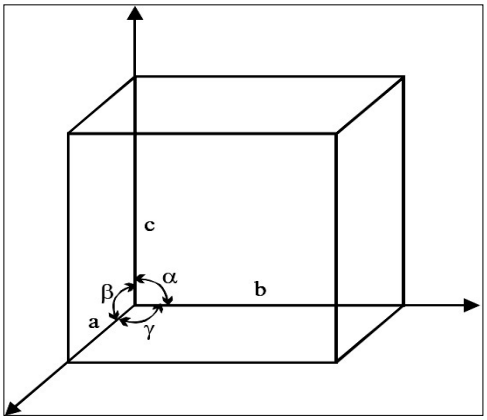
THE SOLID STATE

UNIT CELLS AND CRYSTAL LATTICES

UNIT CELL AND CRYSTAL LATTIC: -

UNIT CELL (U.C.)

Unit cell of the crystalline substance is defined as the smallest repeating unit which shows the complete geometry of the crystalline substance. For e.g., brick in wall. A unit cell is the smallest picture of the whole crystal. A unit cell is characterized by the edge lengths a, b and c along the three edges of the unit cell and the angles α, β and γ between the pair of edges bc; ca and ab respectively.



Characteristics of a Unit Cell:

1. Its dimensional along the three edges, a, b and c. These edges may or may not be mutually perpendicular.
2. Angles between the edges, a (between b and c) b (between a and c) and g (between a and b).
3. Each unit cell has characteristic relation between a, b and c or a, b, and g to give rise different types of unit cell

Thus, a unit cell is characterised by six parameters, a, b, c, a, b, and g. These parameters of a typical unit cell are shown in figure.

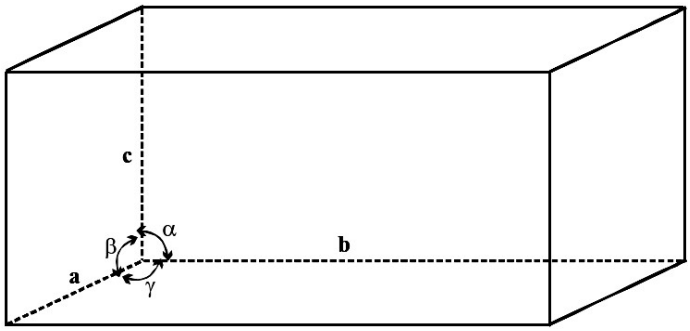


Illustration of parameters of a unit cell

A unit cell may also be defined as a 1D, 2D, 3D three-dimensional group of lattice points that generates the whole lattice by repetition or stacking.

Note: - Generally, most symmetrical and smallest volume unit cell is selected.

1-Dimensional space lattice:

Uniformly separated lattice point in 1-D

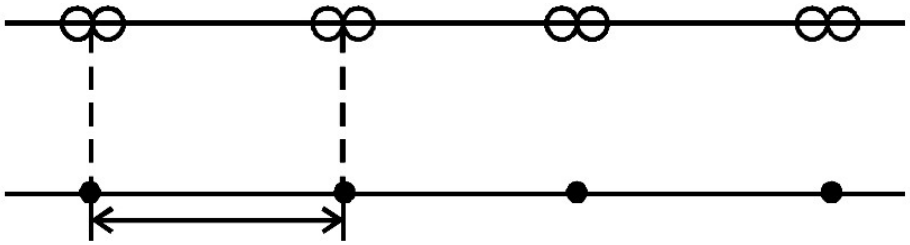
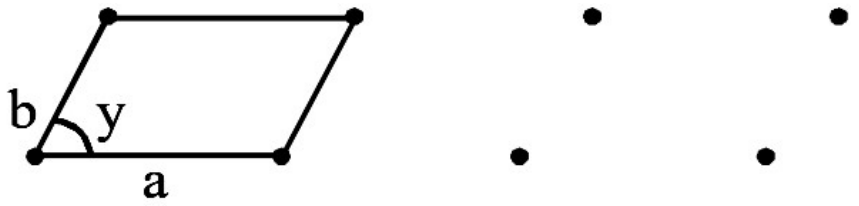


Figure: - only one parameter is required → distance between two lattice point.

2-D Lattice:

Regular arrangement of point in plane 3 parameter required → Two edge lengths & angle between these two edges.



Parallelogram

We can only shift the unit cell parallel not rotate it.

(i) Square unit cell ® a = b, g = 90º

(ii) Rectangle unit cell ® a ¹ b, g = 90º

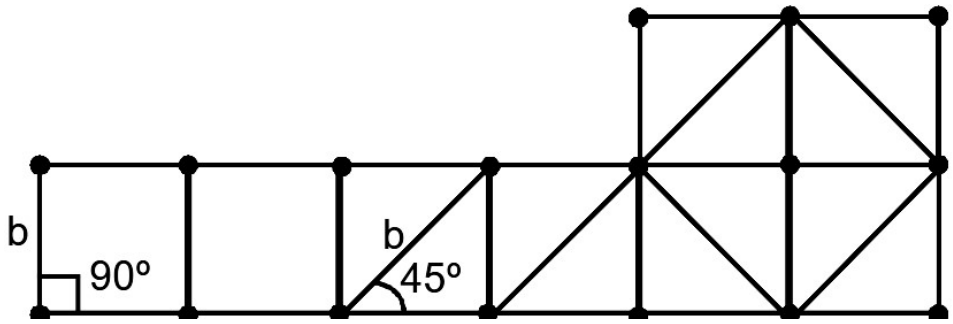
(iii) Hexagonal unit cell ® a = b, g = 60º

(iv) Rhombic unit cell ® a = b, g ¹ 90º & g ¹ 60º

(v) Parallelogram ® a ¹ b, g ¹ 90º

Most symmetrical ® square unit cell.

Square unit cell:



Figure

Primitive unit cell:

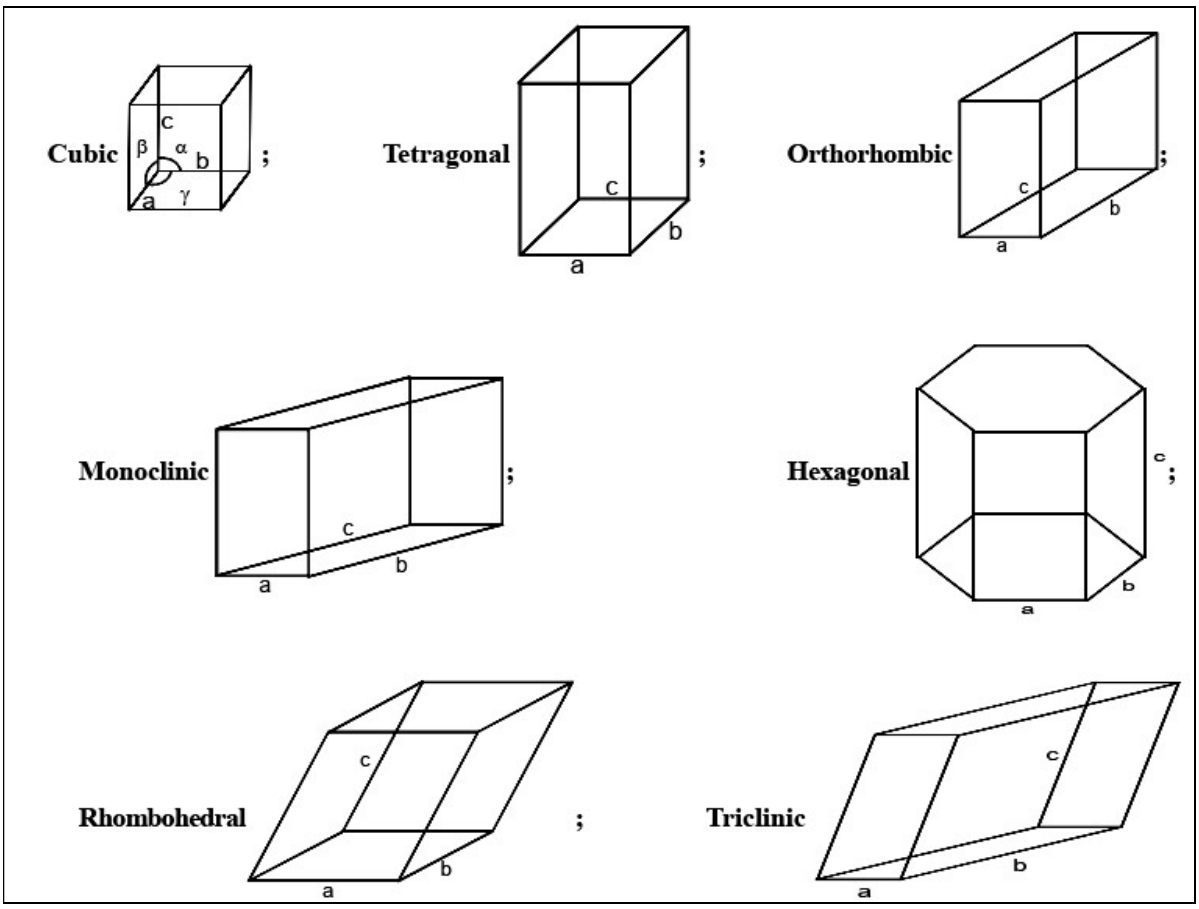
Unit cell having lattice point only at the corner.

Non-Primitive or centered unit cell:

Unit cell having lattice point at corner as well as with in the unit cell.

3-D-Lattice

Seven Primitive unit cells in crystals



CO-ORDINATION NUMBER

The number of nearest particles around a specific particle in a given crystalline substance is called as co-ordination number of that crystalline substance.

PACKING EFFICIENCY OR PACKING DENSITY (P.E.)

Packing efficiency is defined as the ratio of volume occupied by the atoms to the total volume of the crystalline substance i.e., packing efficiency is equal to-

P.E.= $\frac{\textit{Volume occupied by atoms present in a crystal}}{\textit{Volume of crystal}}$

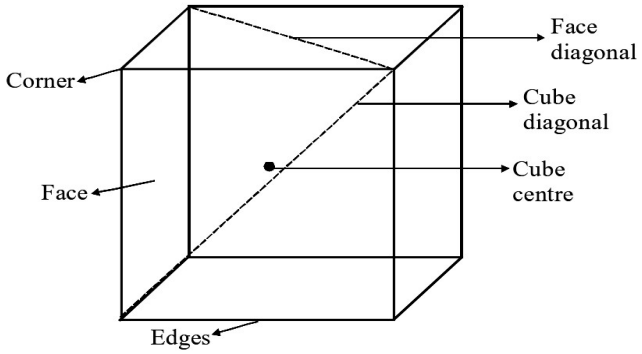
P.E.= $\frac{\textit{Volume occupied by atoms present in a crystaVolume occupied by atoms present in unit cell}}{\textit{Volume of Unit Cell}}$

P.E. = $\frac{n \times \left(\frac{4}{3}\right)\pi r^3}{V}$

Where n = number of atoms present in unit cell

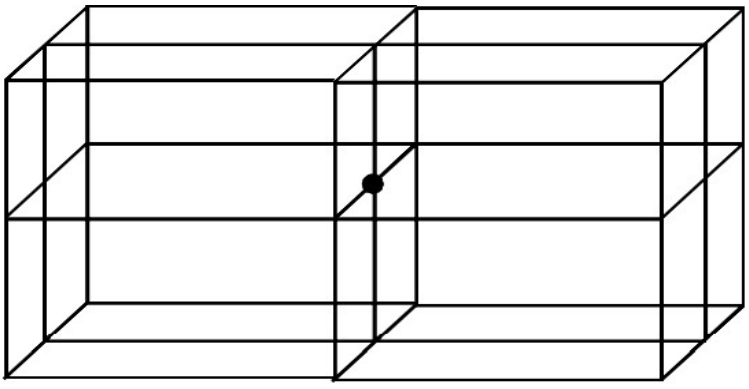
GEOMETRY OF A CUBE

Number of corners	=	8
Number of faces	=	6
Number of edges	=	12
Number of cube centre	=	1
Number of cube diagonals	=	4
Number of face diagonals	=	12

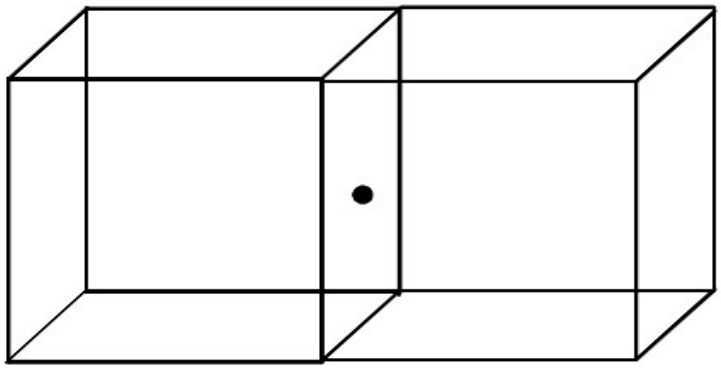


Contribution of an atom at different sites of cube:

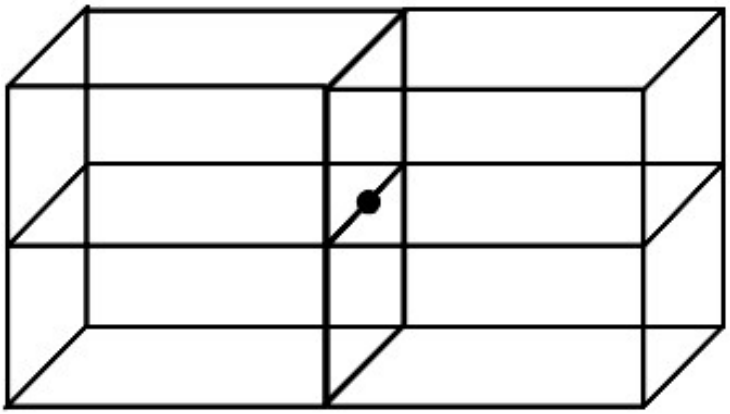
A corner of a cube is common in 8 cubes. So, the part of $\frac{1}{8}$ an atom is present at this corner of cube.



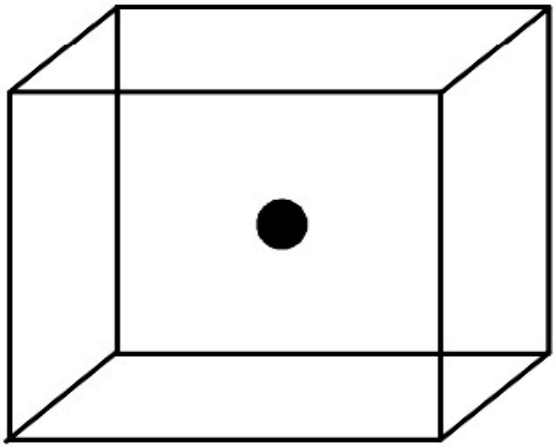
A face of a cube is common is 2 cubes. So $\frac{1}{2}$ the part of an atom is present at the face of a cube.



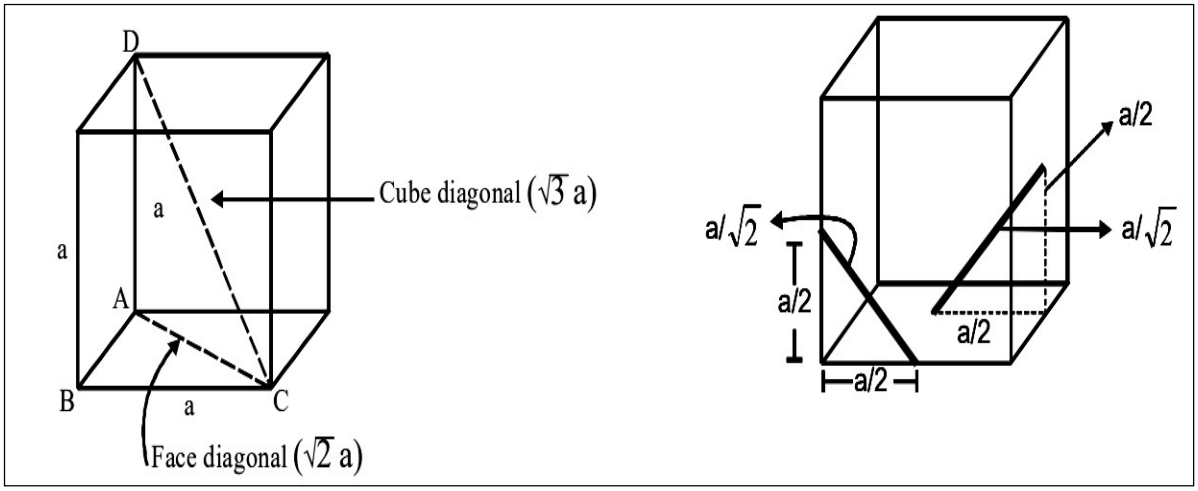
An edge of a cube is common in four cubes, so $\frac{1}{4}$ the part of the atom is present at the edge of a cube



A cube centre is not common in any another cube, so one complete atom is present at the cube centre.



Length of face diagonal and cube diagonal



Distance between
2 adjacent face centres $=\frac{a}{\sqrt{2}}$

Distance between
2 adjacent edge centre $=\frac{a}{\sqrt{2}}$

Consider the triangle ABC, with the help of pathogroups theorem

AC = $\sqrt{AB^2+BC^2}=\sqrt{a^2+a^2}=\sqrt{2a}$ (length of face diagonal.)

Consider the triangle DAC, with the help of Pythagoras theorem

$DC=\sqrt{DA^2+AC^2}$

$\sqrt{a^2+\left(\sqrt{2a}\right)^2}$

$\sqrt{3a}$ (Length of cube diagonal)

TYPES OF UNIT CELL: -

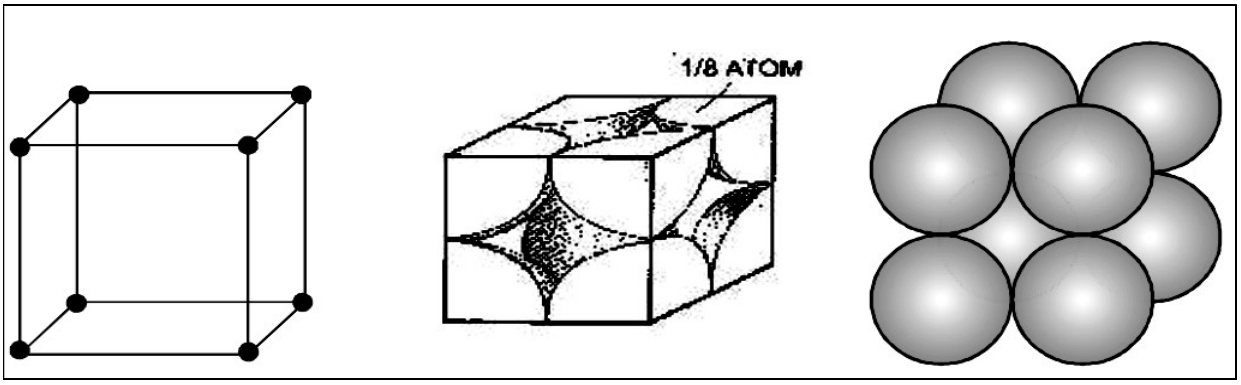
TYPE OF UNIT CELL (BRAVAIS LATTICE)

The distance between successive lattice planes of the same type is called the spacing of planes or interplanar distance between the planes. On the basis of this aspect,
the lattices may be divided in following classes:

- Simple/Primitive/Basic Unit cell
- Body centered cubic (b.c.c.) cell
- Face centered cubic (f.c.c.) cell
- End Centered Unit Cell

SIMPLE/PRIMITIVE/BASIC UNIT CELL: -

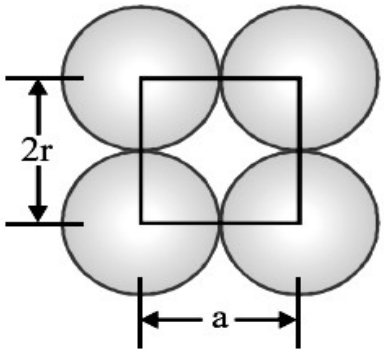
A unit cell having lattice point only at corners called as primitive or simple unit cell. i.e., in this case there is one atom at each of the eight corners of the unit cell considering an atom at one corner as the centre, it will be found that this atom is surrounded by six equidistant neighbors (atoms) and thus the co-ordination number will be six. If 'a' is the side of the unit cell, then the distance between the nearest neighbors shall be equal to 'a'



(a) Relationship between edge length 'a' and atomic radius 'r' :

$a = 2r$

i.e. $r = \frac{a}{2}$ (One face of SCC)



(b) Number of atoms present in unit cell:

In this case one atom or ion lies at each corner. Hence simple cubic unit cell contains a total of $\frac{1}{8} \times 8 = 1$ atom or ion/unit cell.

(c) Packing efficiency (P. E.):

$$\text{P.E.} = \frac{\text{Volume occupied by atoms present in unit cell}}{\text{Volume of unit cell}} = \frac{n \times \frac{4}{3}\pi r^3}{V} \qquad \left[\because \text{Volume of atom} = \frac{4}{3}\pi r^3\right]$$

For SCC: $$\text{P.E.} = \frac{1 \times \frac{4}{3} \times \pi \times \left(\frac{a}{2}\right)^3}{a^3} \qquad [\because r = \frac{a}{2} \text{ and } V = a^3, n = 1]$$

$$= \frac{\pi}{6} = 0.524 \quad \text{or} \quad 52.4\,\%$$