5.2 Unit Cell

The unit cell is a smallest geometric volume containing one or more atoms arranged in three dimension. And also, it is called fundamental building block of a crystal structure.

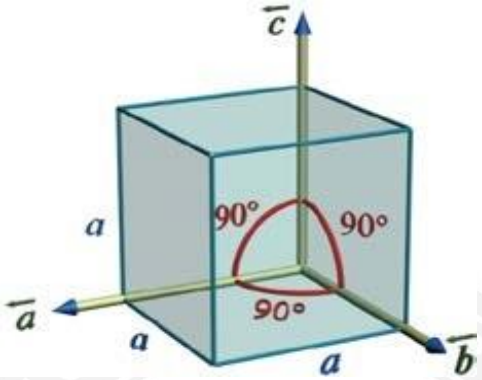

Fig 5.2.1- Unit Cell

Primitive cell

Primitive cell is the smallest volume unit cell which contains the lattice points at the corner only.

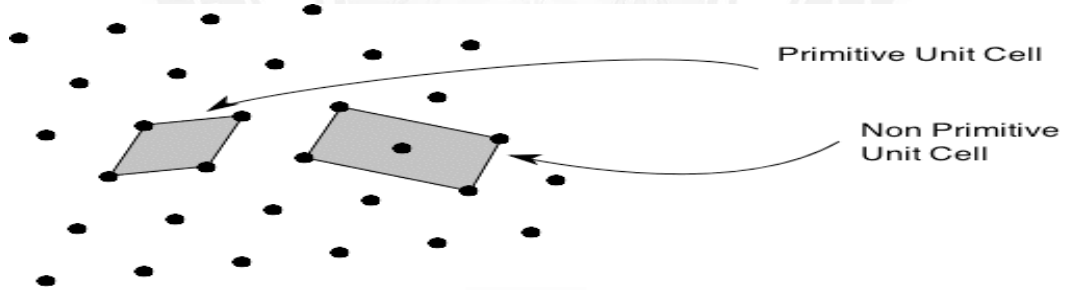

Fig 5.2.2- Primitive cell

Lattice Constant

The distance between any two successive lattice points along any three dimensional directions is called lattice constant.

Parameters determining the Crystal structure of Materials

Let us discuss some of the important parameters which are used to describe the crystal structure.

Number of atoms per unit cell or Effective number

The total number of atoms present in or shared by a unit cell is known as number of atoms per unit cell.

Atomic radius

Atomic radius is defined as half of the distance between any two nearest neighbour atoms which have direct contact with each other, in a crystal of a pure element. It is usually expressed in terms of cube edge *a*.

Co-ordination number

Co-ordination number is the number of nearest neighbouring atoms to a particular atom. Or Co- ordination number is the number of nearest neighbours directly surrounding a given atom.

Atomic packing factor or packing density or density of packing

Atomic packing factor is defined as the ratio between the volumes occupied by the total number of atoms per unit cell (*u*) to the total volume of the unit cell (*v*).

$$\text{APF} = \frac{U}{V}$$

Where,

u - Total number of atoms per unit cell X volume of one atom

v - Total volume of the unit cell

Seven Crystal Systems

Based on the fundamental translation vector and interfacial angle, the crystal classified in to seven types. They are,

1. ***Cubic***
2. ***Triclinic***
3. ***Monoclinic***
4. ***Orthorhombic***
5. ***Tetragonal***
6. ***Rhombohedral***

7. Hexagonal.

Sr. No.	Crystal System	Axial length of Unit Cell	Inter axial angles	Number of Lattice in the system
1	Cubic	$a=b=c$	$\alpha=\beta=\gamma=90^0$	3
2	Tetragonal	$a=b\neq c$	$\alpha=\beta=\gamma=90^0$	2
3	Orthorhombic	$a\neq b\neq c$	$\alpha=\beta=\gamma=90^0$	4
4	Monoclinic	$a\neq b\neq c$	$\alpha=\beta=90^0\neq\gamma$	2
5	Triclinic	$a\neq b\neq c$	$\alpha\neq\beta\neq\gamma\neq90^0$	1
6	Trigonal	$a=b=c$	$\alpha=\beta=\gamma<120^0,\neq90^0$	1
7	Hexagonal	$a=b\neq c$	$\alpha=\beta=90^0$, and $\gamma=120^0$	1

Bravais Space Lattice

A three dimensional space lattice is generated by repeated translation of three non-coplanar vectors *a, b* and *c*. There are only fourteen distinguishable ways of arranging points in three dimensional spaces. These fourteen space lattices are known as Bravais space lattices. The different Bravais space lattices and their crystal systems are listed in given table.

Crystal System	**Bravais Space Lattices**	**Symbols**	
Cubic	Simple	P	3
	Body Centred	I	

	Face Centred	F	
Triclinic	Simple	P	1
Monoclinic	Simple	P	2
	Base Centred	C	
Orthorhombic	Simple	P	4
	Base Centred	C	
	Body Centred	I	
	Face Centred	F	
Tetragonal	Simple	P	2
	Body Centred	I	
Rhombohedral	Simple	P	1
Hexagonal	Simple	P	1