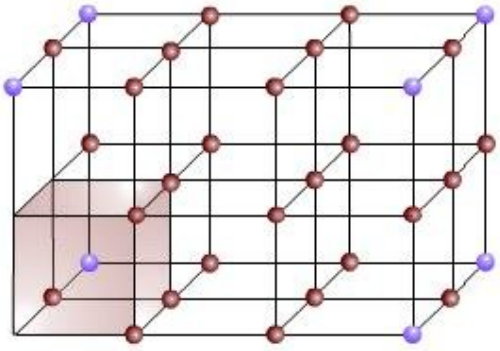
Material Science
Chapter 3 - Crystalline Structure

Engineering materials are either crystalline or no crystalline (also called amorphous materials).

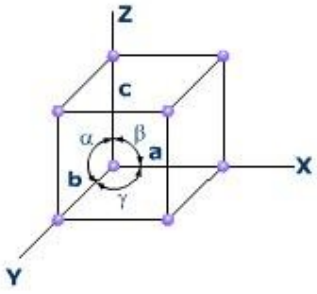
In crystalline solids, the atoms arranges itself in repeated structures, its spatial arrangement is orderly as compared to amorphous materials which are without order.

A unit cell is a group of atoms arranged in a prism shape having three sets of parallel faces . A unit cell repeats itself to form a space lattice. By describing the unit cell we can describe the solid material.

A whole network of atoms is called a space lattice.



Representation of space lattice and unit cell



Representation of dimensions of a unit cell

As in the diagram, the three lattice vectors a, b, and c gives the length of the sides and its direction in the x, y, z axis. The origin is usually an appropriately selected corner of the unit cell.

The interaxial angles are α, β and γ.

x, y, z, α, β and γ describe the unit cell and are called lattice parameters or lattice constants.

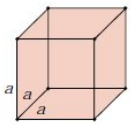
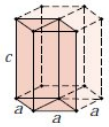
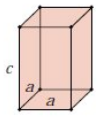
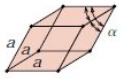
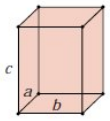
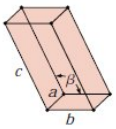
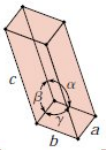
Crystal Systems and Bravais Lattice
There are seven kinds of unit cells referred to as **crystal systems**.

The seven systems can be expanded to 14 standard unit cells called the Bravais Lattice.

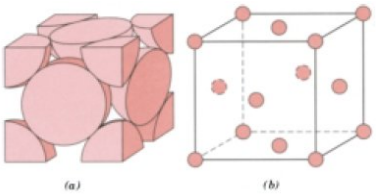
In this chapter we will discuss metallic structures in further detail. Ceramic and polymeric structures will be considered separately.

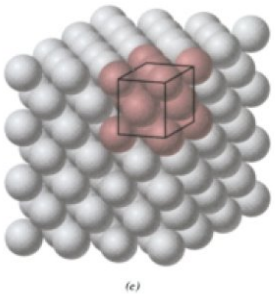
Metals have three principal structures, face centered cubic (FCC), body centered cubic (BCC) and hexagonal close packed (HCP).

Table 3.6 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

Face Centered Cubic (FCC)





The unit cell has an atom at the eight corners and atoms centered on all six faces.

The single FCC unit cell has an equivalent of 4 atoms.

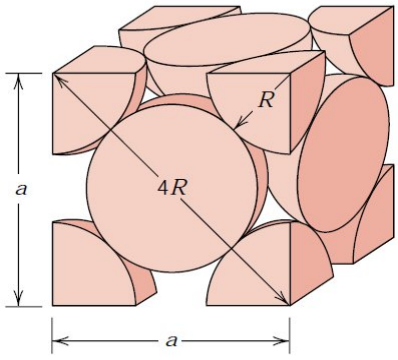
The atoms are assumed as hard spheres.

The lattice parameter **a** is the length of the cubic sides and **R** is the atomic radius.

For an FCC lattice, $$a = \frac{4R}{\sqrt{2}}$$

$$\text{Atomic Packing Factor} = \frac{\text{Volume of atoms in a BCC unit cell}}{\text{Volume of BCC unit cell}}$$

APF_{FCC} = 0.74 or 74%



Base Centered Cubic (BCC)
A unit BCC cell contains an equivalent of 2 atoms.

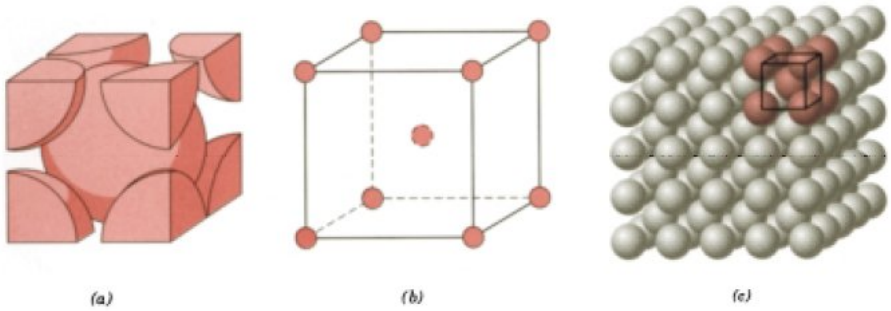
The atoms touch on another atom across the diagonal as indicated in the figure.

Hence, $a = \frac{4R}{\sqrt{3}}$ where R is the atomic radius.

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

APF_{BCC} = 0.68 or 68%

The remaining 32% is empty space.



Hexagonal Close Packed (HCP)
The isolated unit cell is called the primitive cell as in the figure below.

Atoms at “1” contribute 1/6 of an atom each. Atoms at “2” contribute $^{1}/_{12}$ of and atom each an atom at “3” is centered inside the unit cell therefore there the total number of atoms per unit cell is 2 atoms.

The ratio of height, ‘c’ of the HCP crystal to its basal side ‘a’ is called the c/a ratio. The c/a ratio for an **ideal** HCP structure consist of uniform spheres packed as tightly together as possible is 1.633. For c/a ratio higher than ideal, the atoms are elongated and for lower c/a ratio the atoms are compressed.

$APF_{HCP} = 0.74$ or 74%

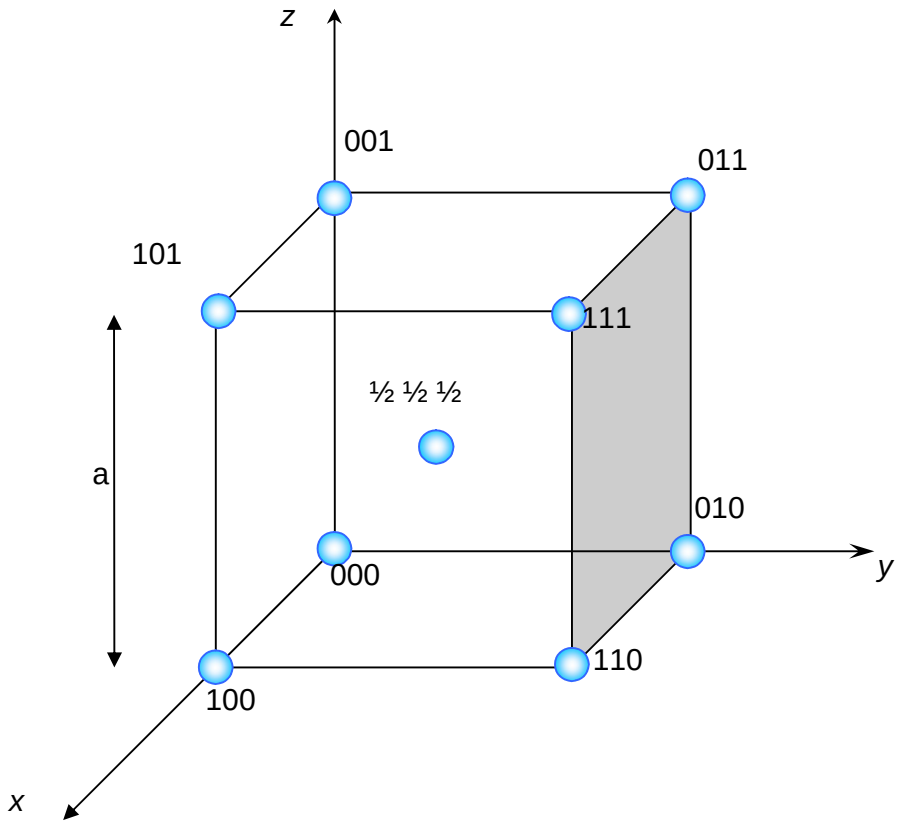
The geometry of a crystal is described by

Atom **position** in a unit cell.
The **directions** in unit cells.
The **planes** in unit cells.

Position

To locate an atom position in a unit cell we use rectangular *x*, *y*, and *z* axes.

We use unit distances to locate atoms along the x, y, and z axes, anything in between is given as a fraction

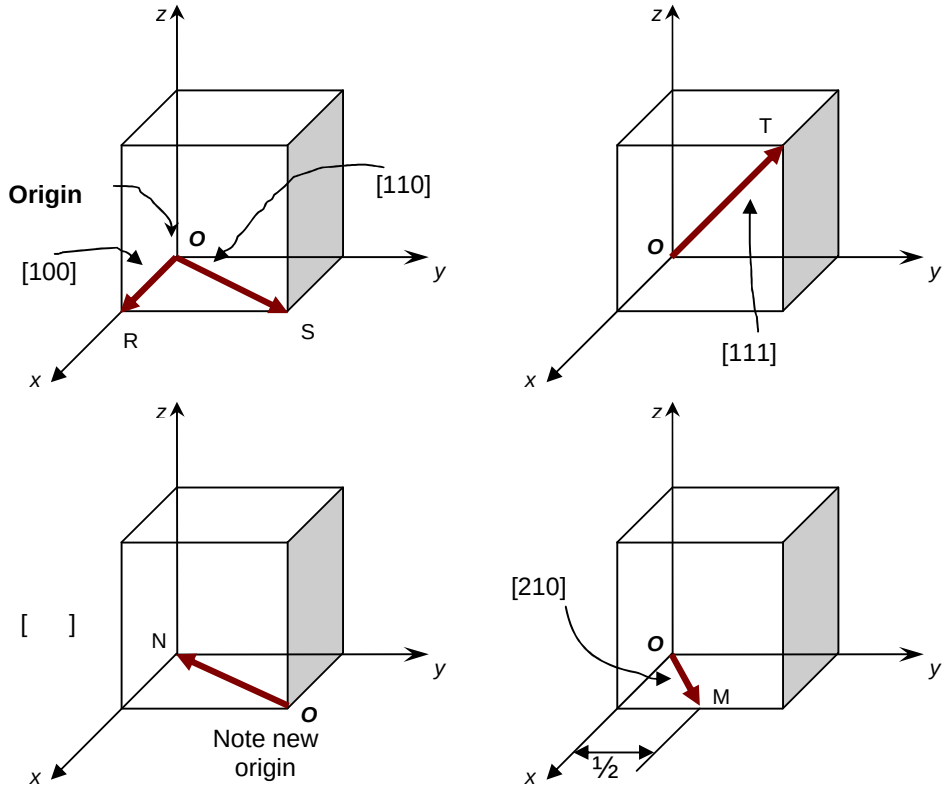


Direction

Directions are drawn from an origin selected within a unit cell. It is usually at a corner.

They are written in square brackets and they must be written as smallest integers.

Negative directions are written with a bar over.



Planes

The Miller notation system is used to identify crystal planes in cubic crystal structure.

The Miller indices of a crystal plane are defined as the reciprocal of the fraction intercepts that the plane makes with the axes x, y and z of the three non-parallel edges of the cubic unit cell.

Procedure:

- Choose an origin or a plane that does not intersect the origin 000.
- Determine where the planes intercept the x, y and z axis.
- Form the reciprocal of these intercepts
- Clear the fractions and the smallest set of whole numbers are the Miller indices (hkl). They are enclosed in parentheses and not separated by commas.

In crystal planes, the distance between two closest parallel planes with the same miller indices is given by:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Volume, Planar and Linear Density

Polymorphism or Allotropy