

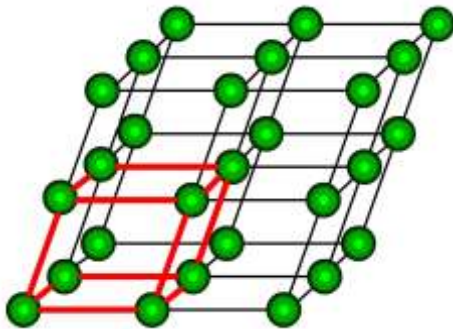
## Chapter two

## Crystal Structures

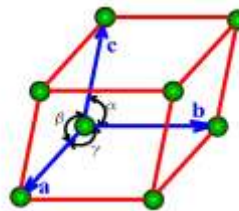
## The Space Lattice and Unit Cells:

Atoms or ions of a solid are arranged in a pattern that repeats itself in three dimensions; they form a solid that is said to have a *crystal structure*

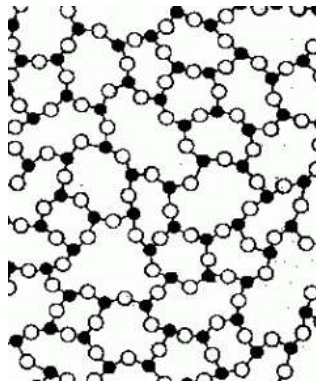
- Atoms, arranged in repetitive 3-Dimensional pattern, in long range order (LRO) give rise to *crystal structure*.
- Properties of solids depend upon crystal structure and bonding force.
- An imaginary network of lines, with atoms at intersection of lines, representing the arrangement of atoms is called *space lattice*.
- Unit cell is that block of atoms which repeats itself to form space lattice.
- **Materials arranged in short range order are called amorphous materials**



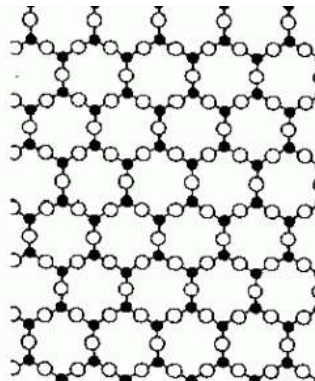
Space Lattice



Unit Cell



Amorphous



Crystal

## Crystal Systems and Bravais Lattice:

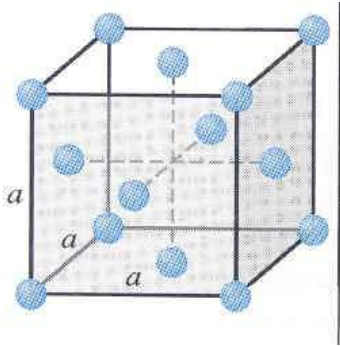
- Only seven different types of unit cells are necessary to create all point lattices. Bravais (1811–1863). French crystallographer showed that 14 standard unit cells could describe all possible lattice networks.
- There are four basic types of unit cells:
  - Simple
  - Body Centered
  - Face Centered
  - Base Centered

<i>Crystal Class</i>	<i>Axial Distances</i>	<i>Axial Angles</i>	<i>Possible Types of Unit Cells</i>	<i>Examples</i>
<b>Cubic</b>	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	Primitive, Body centred, Face centred	Copper, KCl, NaCl Zinc blende, diamond
<b>Tetragonal</b>	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	Primitive, Body centred	SnO <sub>2</sub> , White tin, TiO <sub>2</sub> , CaSO <sub>4</sub>
<b>Orthorhombic</b>	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	Primitive, Body centred, Face centred, End centred	Rhombic sulphur, KNO <sub>3</sub> , CaCO <sub>3</sub> , BaSO <sub>4</sub>
<b>Hexagonal</b>	$a = b \neq c$	$\alpha = \beta = 90^\circ$ ; $\gamma = 120^\circ$	Primitive	Graphite, Mg, ZnO, CdS
<b>Trigonal or Rhombohedral</b>	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	Primitive	(CaCO <sub>3</sub> ) Calcite, HgS (Cinnabar)
<b>Monoclinic</b>	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ$ ; $\beta \neq 90^\circ$	Primitive and End centred	Monoclinic sulphur, Na <sub>2</sub> SO <sub>4</sub> ·10H <sub>2</sub> O
<b>Triclinic</b>	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	Primitive	K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> , CuSO <sub>4</sub> ·5H <sub>2</sub> O, H <sub>3</sub> BO <sub>3</sub>

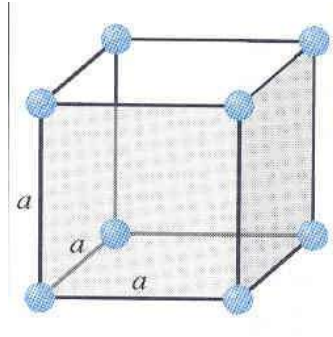
## Types of Unit Cells:

### • Cubic Unit Cell

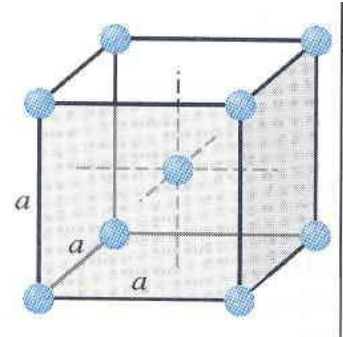
- $a = b = c$
- $\alpha = \beta = \gamma = 90^\circ$



Face centered



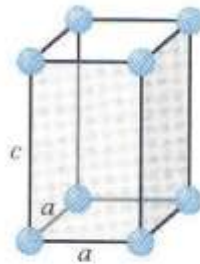
Simple



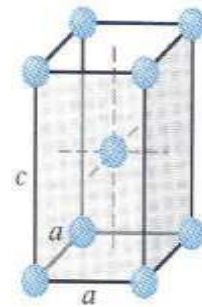
Body Centered

### • Tetragonal

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



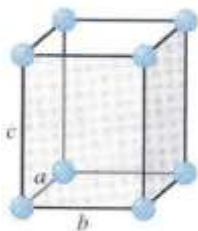
Simple



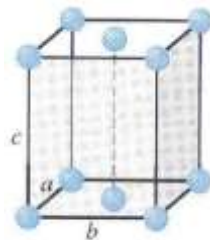
Body Centered

### Orthorhombic

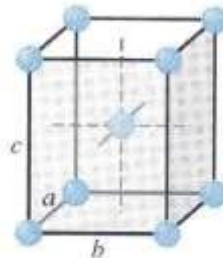
- $a \neq b \neq c$
- $\alpha = \beta = \gamma = 90^\circ$



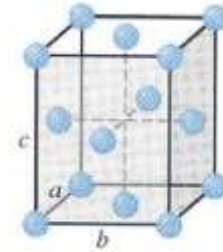
Simple



Base Centered



Body Centered

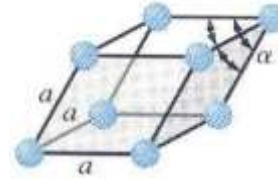


Face Centered

### Rhombohedral

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

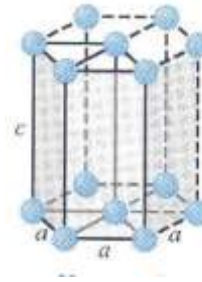
Simple



### Hexagonal

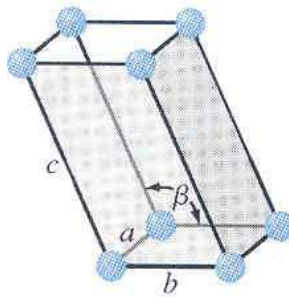
- $a = b \neq c$
- $\alpha = \beta = 90^\circ, \gamma = 120^\circ$

Simple

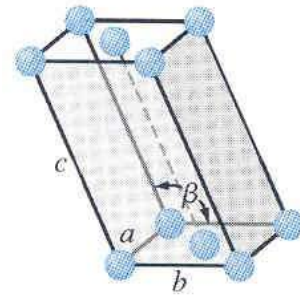


### Monoclinic

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

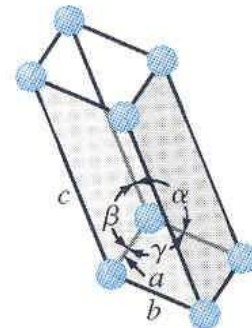


Simple



Base Centered

- **Triclinic**
- $a \neq b \neq c$
- $\alpha \neq \beta \neq \gamma$



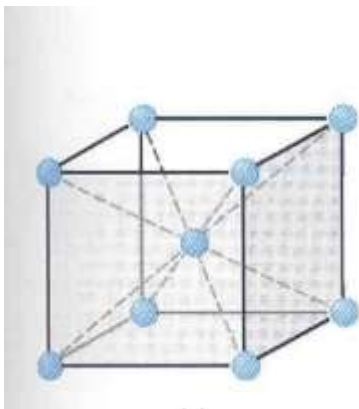
Simple

## ➤ Principal Metallic Crystal Structures

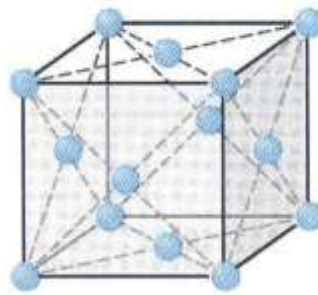
- 90% of the metals have Body Centered Cubic (BCC), Face Centered Cubic (FCC) and Hexagonal Close Packed (HCP) crystal structure.
- HCP is denser version of simple hexagonal crystal structure.
- Most metals crystallize in these dense-packed structures because energy is released as the atoms come closer together and bond more tightly with each other.
- The cube side of the unit cell of body-centered cubic iron, for example, at room temperature is equal to  $0.287 \times 10^{-9}$  m, or 0.287 nanometer (nm). Therefore, if unit cells of pure iron are lined up side by side, in 1 mm there will be

$$1 \text{ mm} \times \frac{1 \text{ unit cell}}{0.287 \text{ nm} \times 10^{-6} \text{ mm/nm}} = 3.48 \times 10^6 \text{ unit cells}$$

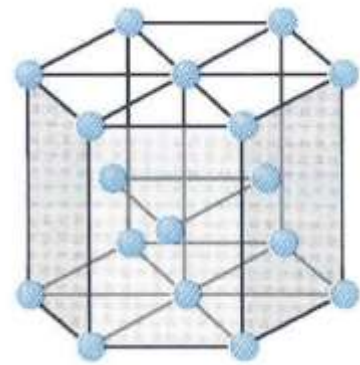
- The distance between the atoms (interatomic distance) in crystal structures can be determined experimentally by x-ray diffraction analysis.
- For example, the interatomic distance between two aluminum atoms in a piece of pure aluminum at 20°C is 0.2862 nm.
- The radius of the aluminum atom in the aluminum metal is assumed to be half the interatomic distance, or 0.143 nm.



**BCC Structure**



**FCC Structure**



**HCP Structure**

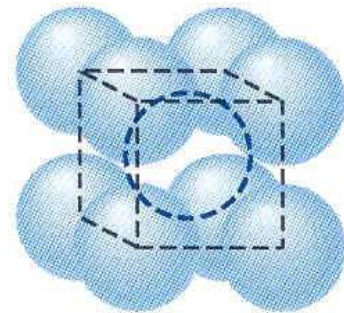
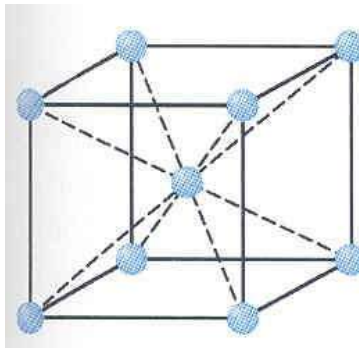
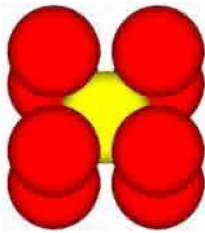
### Body Centered Cubic (BCC) Crystal Structure:

- Represented as one atom at each corner of cube and one at the center of cube.
  - Each central atom has 8 nearest neighbors.
  - Therefore, *coordination number* is 8.

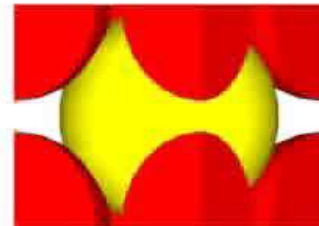
The coordination number, CN = the number of closest neighbors to which an atom is bonded = number of touching atoms

Examples:-

- Chromium ( $a=0.289 \text{ nm}$ )
- Iron ( $a=0.287 \text{ nm}$ )
- Sodium ( $a=0.429 \text{ nm}$ ) , where  $a$  is the lattice constant.



- Each of these cells has the equivalent of two atoms per unit cell.
- One complete atom is located at the center of the unit cell,
- and an eighth of a sphere is located at each corner of the cell, making the equivalent of another atom
- Therefore each unit cell has  $(8 \times 1/8) + 1 = 2$  atoms
- In the BCC unit cell, atoms contact each other at cube diagonal
- Therefore, lattice constant  $a = \frac{4R}{\sqrt{3}}$

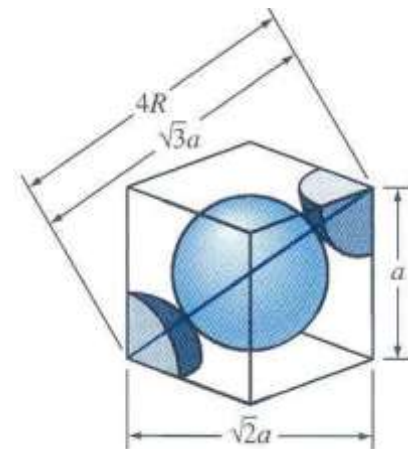


Example:

Iron at  $20^\circ\text{C}$  is BCC with atoms of atomic radius  $0.124 \text{ nm}$ . Calculate the lattice constant ( $a$ ) for the cube edge of the iron unit cell.

$\sqrt{3}a = 4R$  Where  $R$  is the radius of the iron atom.

Therefore  $a = \frac{4R}{\sqrt{3}} = \frac{4(0.124 \text{ nm})}{\sqrt{3}} = 0.2864 \text{ nm}$





### Atomic Packing Factor of BCC Structure:

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

$$V_{\text{atoms}} = 2 \left( \frac{4\pi R^3}{3} \right) = 8.373 R^3$$

$$V_{\text{unit cell}} = a^3 = \left( \frac{4R}{\sqrt{3}} \right)^3 = 12.32 R^3$$

$$\text{Therefore APF} = \frac{8.723 R^3}{12.32 R^3} = 0.68$$

**Thus**, 68 percent of the volume of the BCC unit cell is occupied by atoms and the remaining 32 percent is empty space.

### Example:

Calculate the atomic packing factor (APF) for the BCC unit cell, assuming the atoms to be hard spheres.

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

Since there are two atoms per BCC unit cell, the volume of atoms in the unit cell of radius  $R$  is

$$V_{\text{atoms}} = (2) \left( \frac{4}{3} \pi R^3 \right) = 8.373 R^3$$

The volume of the BCC unit cell is

$$V_{\text{unit cell}} = a^3$$

where  $a$  is the lattice constant.

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4R}{\sqrt{3}}$$

$$V_{\text{unit cell}} = a^3 = 12.32 R^3$$

$$\text{APF} = \frac{8.373 R^3}{12.32 R^3} = 0.68$$

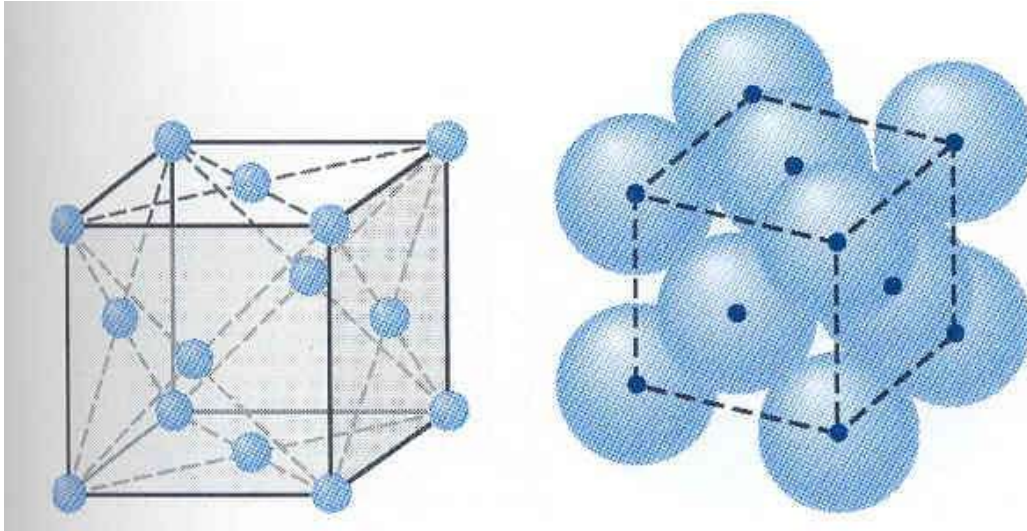
### Face Centered Cubic (FCC) Crystal Structure:

- FCC structure is represented as one atom each at the corner of cube and at the center of each cube face.
- Coordination number for FCC structure is 12

Atomic Packing Factor is 0.74 for the closest packing possible of “spherical atoms.”

### Examples:-

- Aluminum ( $a = 0.405 \text{ nm}$ )
- Gold ( $a = 0.408 \text{ nm}$ )

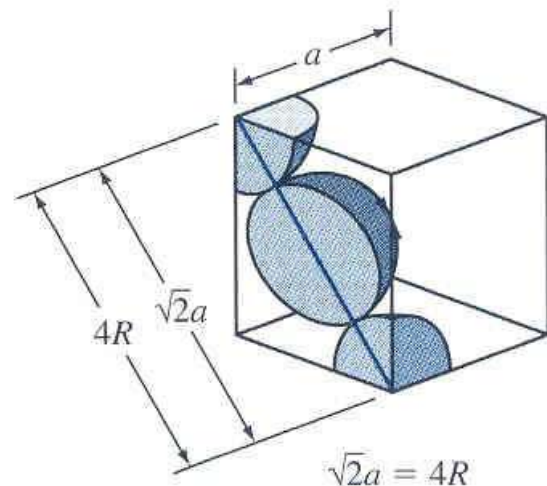


Each unit cell has eight octants ( $8 \times 1/8$ ) atom at corners and six half-atoms at the center of six faces.

- Therefore each unit cell has  $(8 \times 1/8) + (6 \times 1/2) = 4$  atoms

- Atoms contact each other across cubic face diagonal

Therefore, lattice constant  
 $\sqrt{2}a = 4R$  or  $a = \frac{4R}{\sqrt{2}}$

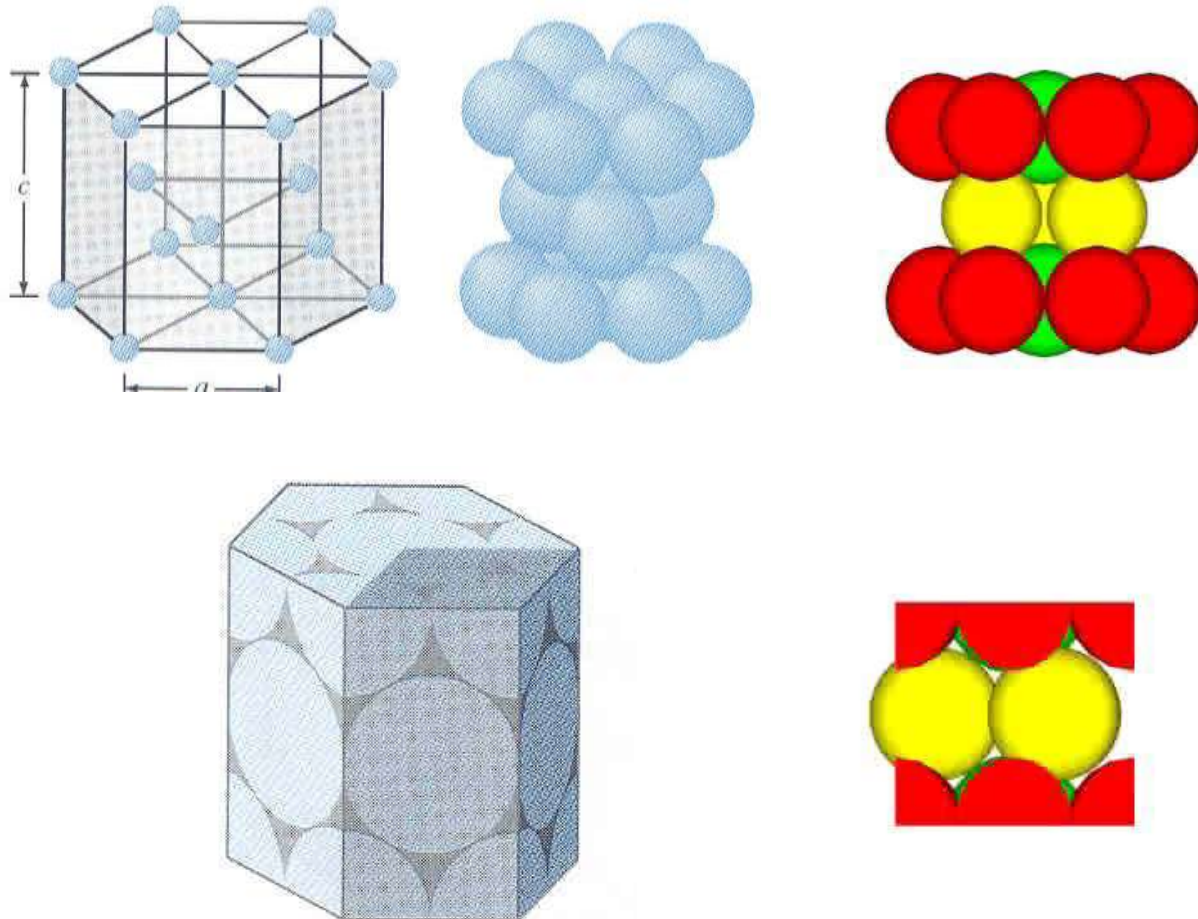


### Hexagonal Close-Packed Structure:

- The HCP structure is represented as an atom at each of 12 corners of a hexagonal prism, 2 atoms at top and bottom face and 3 atoms in between top and bottom face.
- Atoms attain higher APF by attaining HCP structure than simple hexagonal structure.



- $APF = 0.74$  the same as that for the FCC crystal structure since in both structures the atoms are packed as tightly as possible.
- In both the HCP and FCC crystal structures each atom is surrounded by 12 other atoms, and thus both structures have a coordination number of 12



- Each atom has six  $\frac{1}{6}$  Atoms at each of top and bottom layer,
- Two half atoms at top and bottom layer and 3 full atoms at the middle layer.
- Therefore each HCP unit cell has  $(2 \times 6 \times \frac{1}{6}) + (2 \times \frac{1}{2}) + 3 = 6$  atoms
- The ratio of the height  $c$  of the hexagonal prism of the HCP crystal structure to its basal side  $a$  is called the  $c/a$  ratio
- The  $c/a$  ratio for an ideal HCP crystal structure consisting of uniform spheres packed as tightly together as possible is 1.633
- cadmium and zinc have  $c/a$  ratios higher than ideality (elongated)
- magnesium, cobalt, zirconium, titanium, and beryllium have  $c/a$  ratios less than the ideal ratio (compressed)

• **Examples:-**

- Zinc ( $a = 0.2665 \text{ nm}$ ,  $c/a = 1.85$ )
- Cobalt ( $a = 0.2507 \text{ nm}$ ,  $c/a = 1.62$ )
- Ideal  $c/a$  ratio is 1.633.

Example:

Calculate the volume of the zinc crystal structure unit cell by using the following data: pure zinc has the HCP crystal structure with lattice constants  $a = 0.2665 \text{ nm}$  and  $c = 0.4947 \text{ nm}$ .

■ **Solution**

The volume of the zinc HCP unit cell can be obtained by determining the area of the base of the unit cell and then multiplying this by its height (Fig. ).

The area of the base of the unit cell is area  $ABDEFG$  of Fig.  $a$  and  $b$ . This total area consists of the areas of six equilateral triangles of area  $ABC$  of Fig.  $b$ . From Fig.  $c$ ,

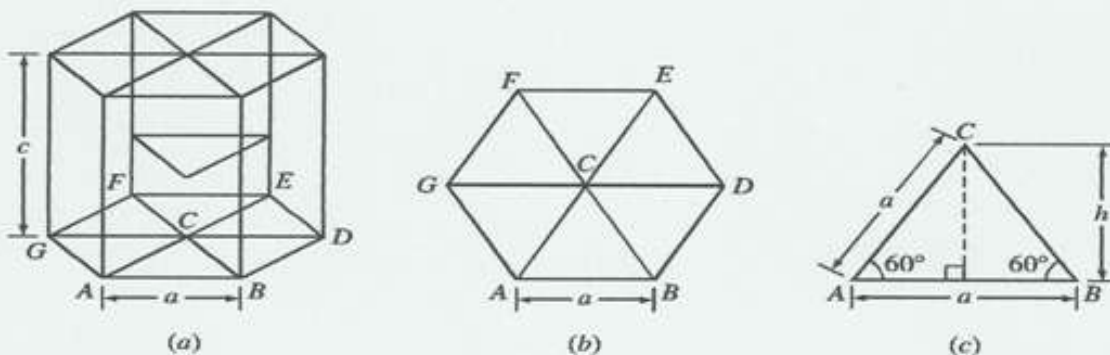
$$\begin{aligned} \text{Area of triangle } ABC &= \frac{1}{2}(\text{base})(\text{height}) \\ &= \frac{1}{2}(a)(a \sin 60^\circ) = \frac{1}{2}a^2 \sin 60^\circ \end{aligned}$$

From Fig.  $b$ ,

$$\begin{aligned} \text{Total area of HCP base} &= (6) \left( \frac{1}{2}a^2 \sin 60^\circ \right) \\ &= 3a^2 \sin 60^\circ \end{aligned}$$

From Fig.  $a$ ,

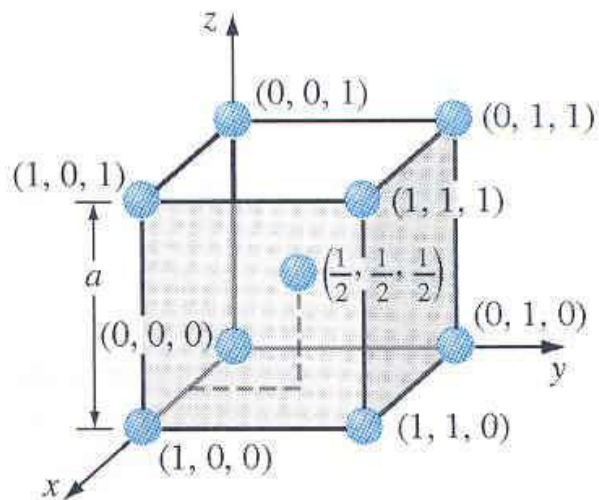
$$\begin{aligned} \text{Volume of zinc HCP unit cell} &= (3a^2 \sin 60^\circ)(c) \\ &= (3)(0.2665 \text{ nm})^2(0.8660)(0.4947 \text{ nm}) \\ &= 0.0913 \text{ nm}^3 \end{aligned}$$



Diagrams for calculating the volume of an HCP unit cell. (a) HCP unit cell. (b) Base of HCP unit cell. (c) Triangle  $ABC$  removed from base of unit cell.

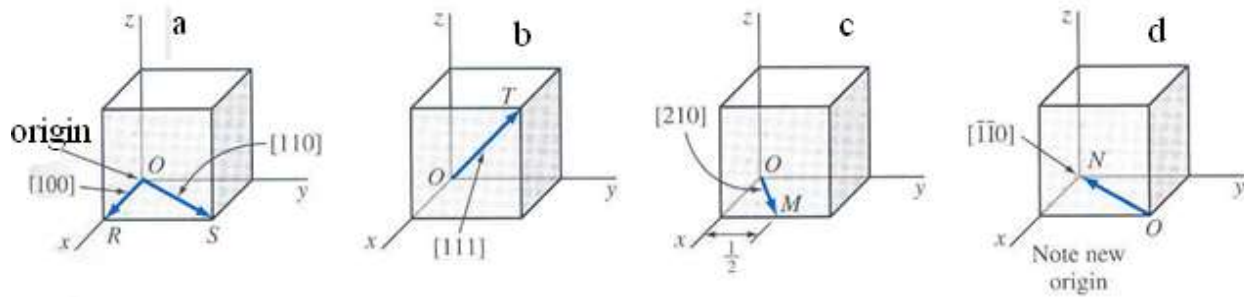
## Atom Positions in Cubic Unit Cells:

- Cartesian coordinate system is used to locate atoms.
- In a cubic unit cell
  - Positive y axis is the direction to the right.
  - Positive x axis is the direction coming out of the paper.
  - Positive z axis is the direction towards top.
  - Negative directions are to the opposite of positive directions.
- Atom positions are located using unit distances along the axes.
  - The position coordinates for the atoms in the BCC unit cell are shown in Fig. below.
  - The atom positions for the eight corner atoms of the BCC unit cell are  $(0, 0, 0)$   $(1, 0, 0)$   $(0, 1, 0)$   $(0, 0, 1)$   $(1, 1, 1)$   $(1, 1, 0)$   $(1, 0, 1)$   $(0, 1, 1)$
  - The center atom in the BCC unit cell has the position coordinates  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
  - For simplicity sometimes only two atom positions in the BCC unit cell are specified which are  $(0, 0, 0)$  and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$



## Directions in Cubic Unit Cells:

- In cubic crystals, *Direction Indices* are vector components of directions resolved along each axis, resolved to smallest integers.
- Direction indices are position coordinates of unit cell where the direction vector emerges from cell surface, converted to integers.



### Procedure to Find Direction Indices:

1. Produce the direction vector till it emerges from surface of cubic cell
2. Determine the coordinates of point of emergence and origin
3. Subtract coordinates of point of Emergence by that of origin
4. Are all are integers?
  - a. If No, Convert them to smallest possible integer by multiplying by an integer, then go to b.
  - b. If Yes, Are any of the direction vectors negative?
    - i. If Yes, Represent the indices in a square bracket without comas with a  $\bar{\phantom{x}}$  over negative index (Eg:  $[1\bar{2}1]$ )
    - ii. If No, Represent the indices in a square bracket without comas (Eg:  $[212]$ )

The position coordinates of the direction vector  $OM$  (Fig.c) are  $(1, 1/2, 0)$ , and since the direction vectors must be integers, these position coordinates must be multiplied by 2 to obtain integers. Thus, the direction indices of  $OM$  become  $2(1, 1/2, 0) = [210]$ .

The position coordinates of the vector  $ON$  (Fig. d) are  $(-1, -1, 0)$ . A negative direction index is written with a bar over the index. Thus, the direction indices for the vector  $ON$  are  $[\bar{1}\bar{1}0]$ . Note that to draw the direction  $ON$  inside the cube the origin of the direction vector had to be moved to the front lower-right corner of the unit cube (Fig. d)

The letters  $u, v, w$  are used in a general sense for the direction indices in the  $x, y$ , and  $z$  directions, respectively, and are written as  $[uvw]$ . It is also important to note that *all parallel direction vectors have the same direction indices*.

Directions are said to be *crystallographically equivalent* if the atom spacing along each direction is the same. For example, the following cubic edge directions are crystallographic equivalent directions:

$$[100], [010], [001], [0\bar{1}0], [00\bar{1}], [\bar{1}00] \equiv \langle 100 \rangle$$

Equivalent directions are called *indices of a family or form*. The notation  $\langle 100 \rangle$  is used to indicate cubic edge directions collectively. Other directions of a form are the cubic body diagonals  $\langle 111 \rangle$  and the cubic face diagonals  $\langle 110 \rangle$ .

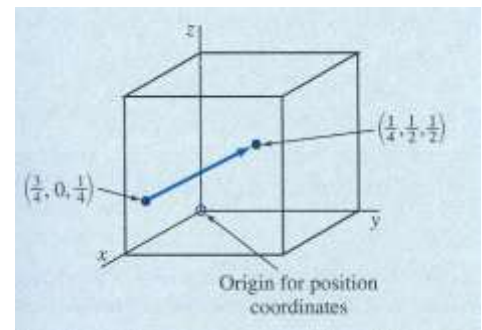
Example:

Determine direction indices of the given vector. Origin coordinates are  $(3/4, 0, 1/4)$ . Emergence coordinates are  $(1/4, 1/2, 1/2)$ .

Subtracting origin coordinates from emergence coordinates,  
 $(1/4, 1/2, 1/2) - (3/4, 0, 1/4) = (-1/2, 1/2, 1/4)$

Multiply by 4 to convert all fractions to integers  
 $4 \times (-1/2, 1/2, 1/4) = (-2, 2, 1)$

Therefore, the direction indices are  $[\bar{2} \ 2 \ 1]$



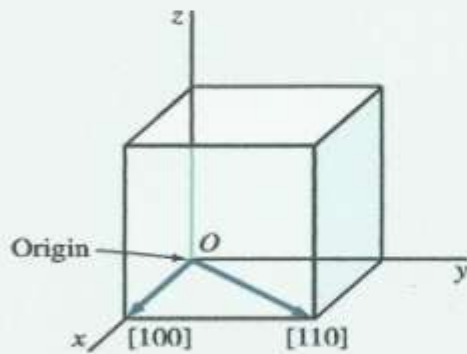


Draw the following direction vectors in cubic unit cells:

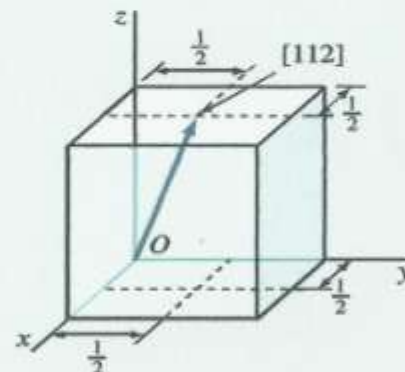
- (a)  $[100]$  and  $[110]$
- (b)  $[112]$
- (c)  $[\bar{1}10]$
- (d)  $[\bar{3}2\bar{1}]$

■ **Solution**

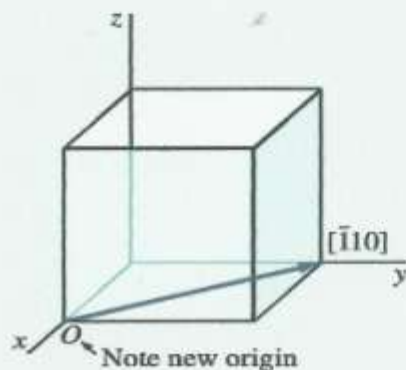
- (a) The position coordinates for the  $[100]$  direction are  $(1, 0, 0)$  (Fig. 3.12a). The position coordinates for the  $[110]$  direction are  $(1, 1, 0)$  (Fig. 3.12a).
- (b) The position coordinates for the  $[112]$  direction are obtained by dividing the direction indices by 2 so that they will lie within the unit cube. Thus they are  $(\frac{1}{2}, \frac{1}{2}, 1)$  (Fig. 3.12b).
- (c) The position coordinates for the  $[\bar{1}10]$  direction are  $(-1, 1, 0)$  (Fig. 3.12c). Note that the origin for the direction vector must be moved to the lower-left front corner of the cube.
- (d) The position coordinates for the  $[\bar{3}2\bar{1}]$  direction are obtained by first dividing all the indices by 3, the largest index. This gives  $-1, \frac{2}{3}, -\frac{1}{3}$  for the position coordinates of the exit point of the direction  $[\bar{3}2\bar{1}]$ , which are shown in Fig. 3.12d.



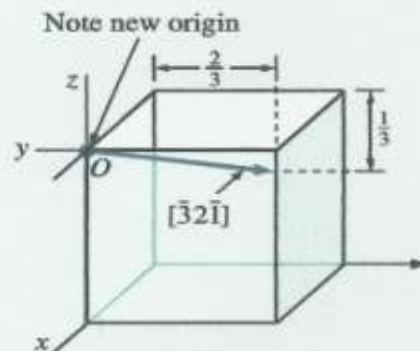
(a)



(b)



(c)



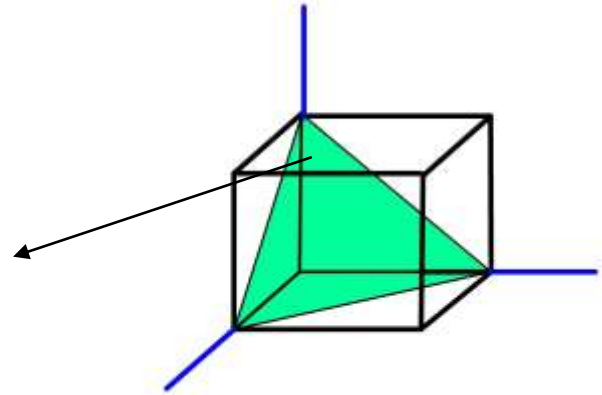
(d)



**Miller Indices:**

- Miller Indices are used to refer to specific lattice planes of atoms.
- They are reciprocals of the fractional intercepts (with fractions cleared) that the plane makes with the crystallographic x,y and z axes of three nonparallel edges of the cubic unit cell.

Miller Indices = (111)

**Miller Indices – Procedure:**

1. Choose a plane that does not pass through origin
2. Determine the x,y and z intercepts of the plane
3. Find the reciprocals of the intercepts
4. Fractions?
  - a. If Yes, Clear fractions by multiplying by an integer to determine smallest set of whole numbers, then go to b
  - b. If No, Place a 'bar' over the Negative indices
5. Enclose in parenthesis (hkl) where h,k,l are miller indices of cubic crystal plane for x,y and z axes. Eg: (111)

- Interplanar spacing between parallel closest planes with same miller indices is given by

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

Where  $d_{hkl}$  = interplanar spacing between parallel closest planes with Miller indices  $h$ ,  $k$ , and  $l$

$a$  = lattice constant (edge of unit cube)

$h, k, l$  = Miller indices of cubic planes being considered

Example:

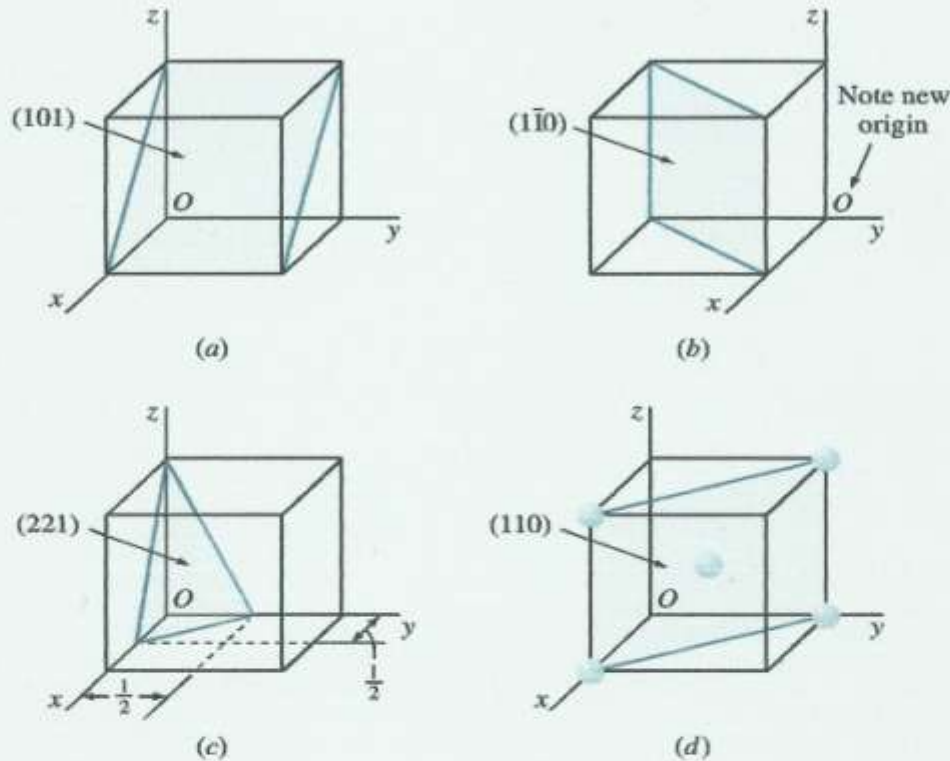
Copper has an FCC crystal structure and a unit cell with a lattice constant of 0.361 nm. What is its interplanar spacing  $d_{220}$ ?

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.361}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.128 \text{ nm}$$

Draw the following crystallographic planes in cubic unit cells:

- (a) (101)    (b)  $(1\bar{1}0)$     (c) (221)  
 (d) Draw a (110) plane in a BCC atomic-site unit cell, and list the position coordinates of the atoms whose centers are intersected by this plane.

### ■ Solutions



**Figure EP3.7**

Various important cubic crystal planes.

- (a) First determine the reciprocals of the Miller indices of the (101) plane. These are  $1, \infty, 1$ . The (101) plane must pass through a unit cube at intercepts  $x = 1$  and  $z = 1$  and be parallel to the  $y$  axis.
- (b) First determine the reciprocals of the Miller indices of the  $(1\bar{1}0)$  plane. These are  $1, -1, \infty$ . The  $(1\bar{1}0)$  plane must pass through a unit cube at intercepts  $x = 1$  and  $y = -1$  and be parallel to the  $z$  axis. Note that the origin of axes must be moved to the lower-right back side of the cube.
- (c) First determine the reciprocals of the Miller indices of the (221) plane. These are  $\frac{1}{2}, \frac{1}{2}, 1$ . The (221) plane must pass through a unit cube at intercepts  $x = \frac{1}{2}$ ,  $y = \frac{1}{2}$ , and  $z = 1$ .
- (d) Atom positions whose centers are intersected by the (110) plane are  $(1, 0, 0)$ ,  $(0, 1, 0)$ ,  $(1, 0, 1)$ ,  $(0, 1, 1)$ , and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . These positions are indicated by the solid circles.

## Planes and Directions in Hexagonal Unit Cells:

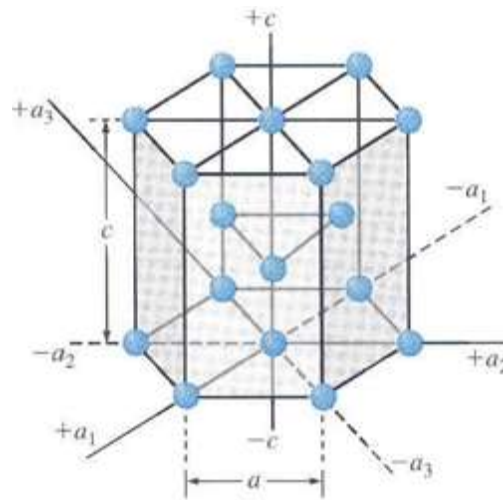
- Four indices are used (hkil) called as *Miller-Bravais* indices.

There are three basal axes,  $a_1$ ,  $a_2$ , and  $a_3$ , which make  $120^\circ$  with each other. The fourth axis or  $c$  axis is the vertical axis located at the center of the unit cell.

- Four axes are used ( $a_1$ ,  $a_2$ ,  $a_3$  and  $c$ ).

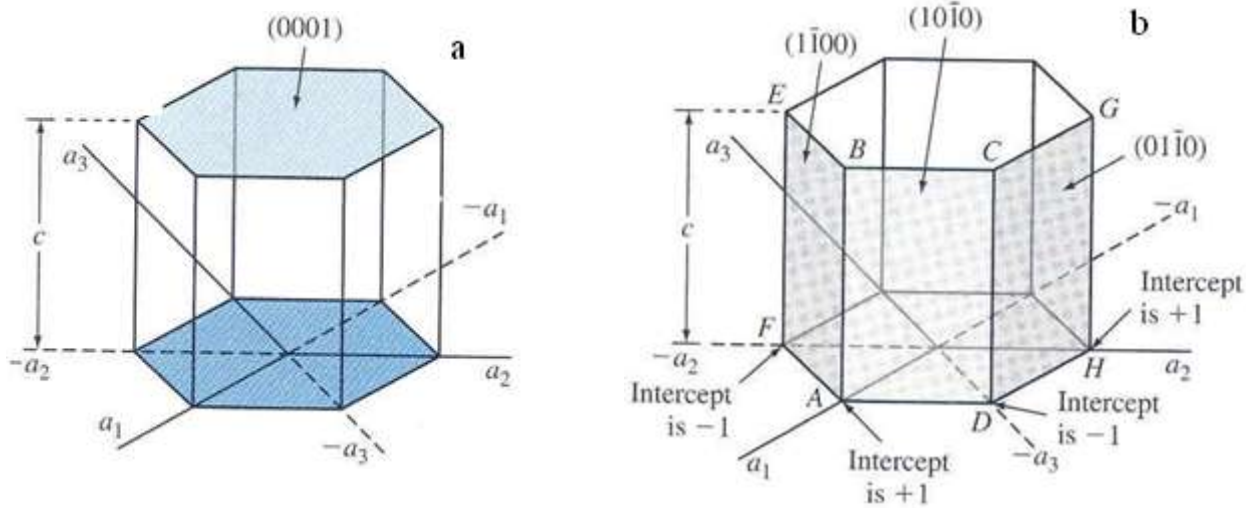
The  $a$  unit of measurement along the  $a_1$ ,  $a_2$ , and  $a_3$  axes is the distance between the atoms along these axes and is indicated in Figure below. The unit of measurement along the  $c$  axis is the height of the unit cell.

- Reciprocal of the intercepts that a crystal plane makes with the  $a_1$ ,  $a_2$ ,  $a_3$  and  $c$  axes give the  $h$ ,  $k$ ,  $i$  and  $l$  indices respectively.



- **Basal Planes:** - The basal planes of the HCP unit cell are very important planes for this unit cell and are indicated in Fig. *a*.

- Since the basal plane on the top of the HCP unit cell in Fig. *a* is parallel to the  $a_1$ ,  $a_2$ , and  $a_3$  axes, the intercepts of this plane with these axes will all be infinite.
- Thus  $a_1 = \infty$ ,  $a_2 = \infty$ ,  $a_3 = \infty$   
 $c = 1$ , since the top basal plane intersects the  $c$  axis at unit instance.
- Taking the reciprocals of these intercepts gives the Miller-Bravais indices for the HCP basal plane
- Therefore; (hkil) = (0001) Or the HCP basal plane is (0001)



### • Prism Planes:-

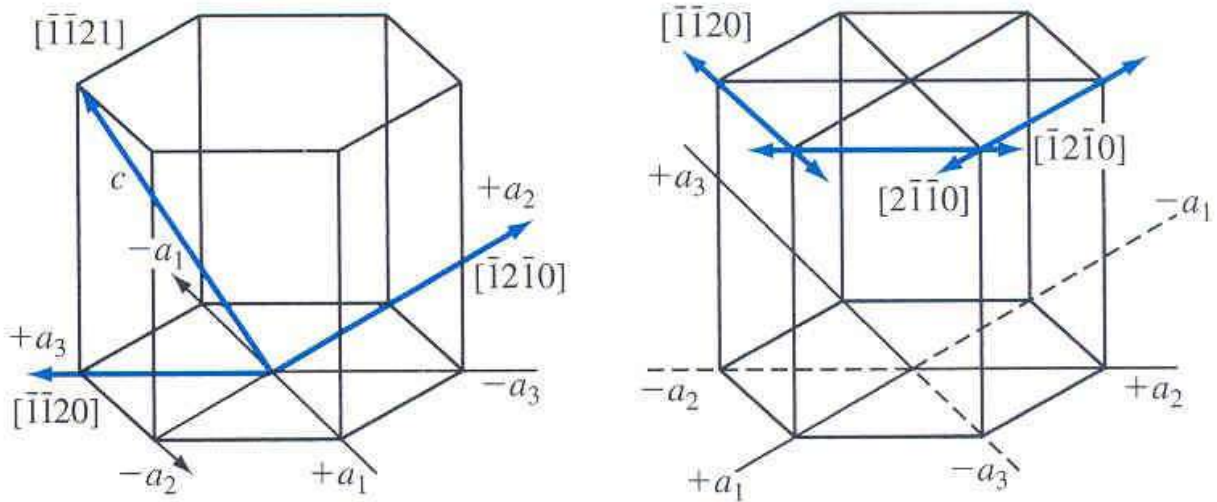
- For the front prism plane ABCD, in figure b
- Intercepts are  $a_1 = 1$ ,  $a_2 = \infty$ ,  $a_3 = -1$ ,  $c = \infty$ . Or  $(hkli) = (10\bar{1}0)$
- Similarly, the ABEF prism plane of Fig. b has the indices  $(1\bar{1}00)$
- The DCGH plane the indices  $(01\bar{1}0)$ .
- All HCP prism planes can be identified collectively as the  $\{10\bar{1}0\}$  family of planes.

### Directions in HCP Unit Cells:

- Directions in HCP unit cells are also usually indicated by 4 indices  $[uvtw]$ .
- $u, v, t$  and  $w$  are lattice vectors in  $a_1$ ,  $a_2$ ,  $a_3$  and  $c$  directions respectively.

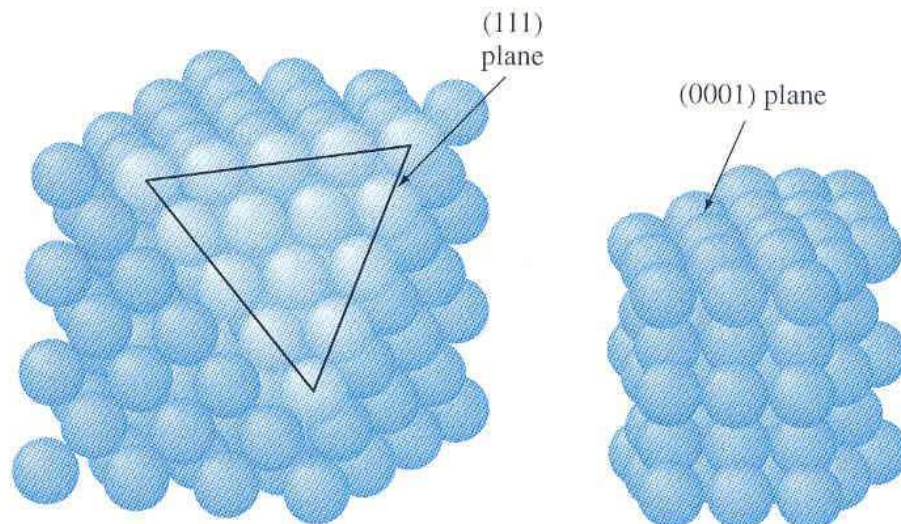
### • Example:-

For  $a_1$ ,  $a_2$ ,  $a_3$  directions, the direction indices are  $[2\bar{1}\bar{1}0]$ ,  $[\bar{1}2\bar{1}0]$  and  $[\bar{1}\bar{1}20]$  respectively.

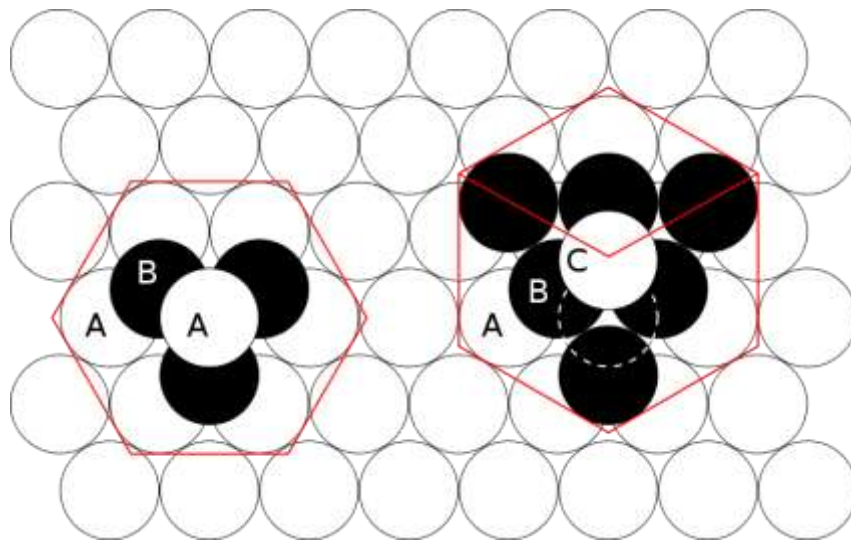
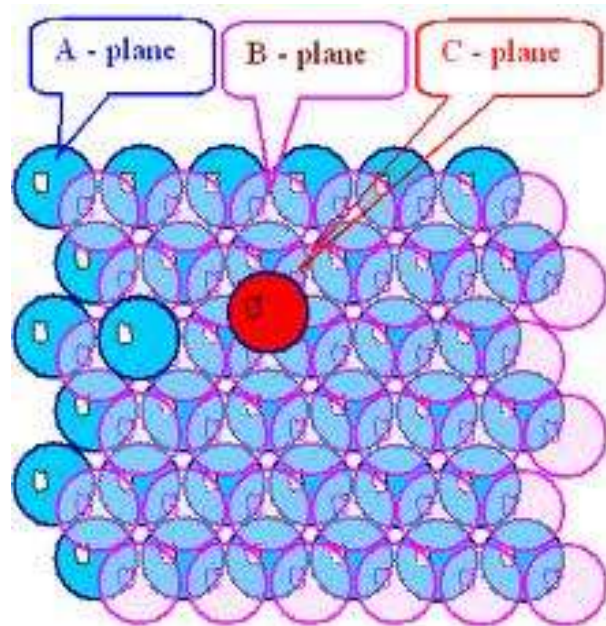


### Comparison of FCC and HCP crystals:

- Both FCC and HCP are close packed structures. That is, their atoms, which are considered approximate “spheres,” are packed together as closely as possible so that an atomic packing factor of 0.74 is attained.
- FCC crystal is close packed in (111) plane while HCP is close packed in (0001) plane as shown in Fig. below.







The hcp lattice (left) and the fcc lattice (right). The outline of each respective Bravais lattice is shown in red. The letters indicate which layers are the same. There are two "A" layers in the hcp matrix, where all the spheres are in the same position. All three layers in the fcc stack are different. Note the fcc stacking may be converted to the hcp stacking by translation of the upper-most sphere, as shown by the dashed outline.



## Volume Density:

A value for the volume density of a metal can be obtained by using the equation

$$\text{Volume density of metal} = \rho_v = \frac{\text{mass/unit cell}}{\frac{\text{volume}}{\text{unit cell}}}$$

Copper has an FCC crystal structure and an atomic radius of 0.1278 nm. Assuming the atoms to be hard spheres that touch each other along the face diagonals of the FCC unit cell as shown in Fig. 3.7, calculate a theoretical value for the density of copper in megagrams per cubic meter. The atomic mass of copper is 63.54 g/mol.

### ■ Solution

For the FCC unit cell,  $\sqrt{2}a = 4R$ , where  $a$  is the lattice constant of the unit cell and  $R$  is the atomic radius of the copper atom. Thus

$$a = \frac{4R}{\sqrt{2}} = \frac{(4)(0.1278 \text{ nm})}{\sqrt{2}} = 0.361 \text{ nm}$$

$$\text{Volume density of copper} = \rho_v = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} \quad (3.5)$$

In the FCC unit cell there are four atoms/unit cell. Each copper atom has a mass of  $(63.54 \text{ g/mol})/(6.02 \times 10^{23} \text{ atoms/mol})$ . Thus the mass  $m$  of Cu atoms in the FCC unit cell is

$$m = \frac{(4 \text{ atoms})(63.54 \text{ g/mol})}{6.02 \times 10^{23} \text{ atoms/mol}} \left( \frac{10^{-6} \text{ Mg}}{\text{g}} \right) = 4.22 \times 10^{-28} \text{ Mg}$$

The volume  $V$  of the Cu unit cell is

$$V = a^3 = \left( 0.361 \text{ nm} \times \frac{10^{-9} \text{ m}}{\text{nm}} \right)^3 = 4.70 \times 10^{-29} \text{ m}^3$$

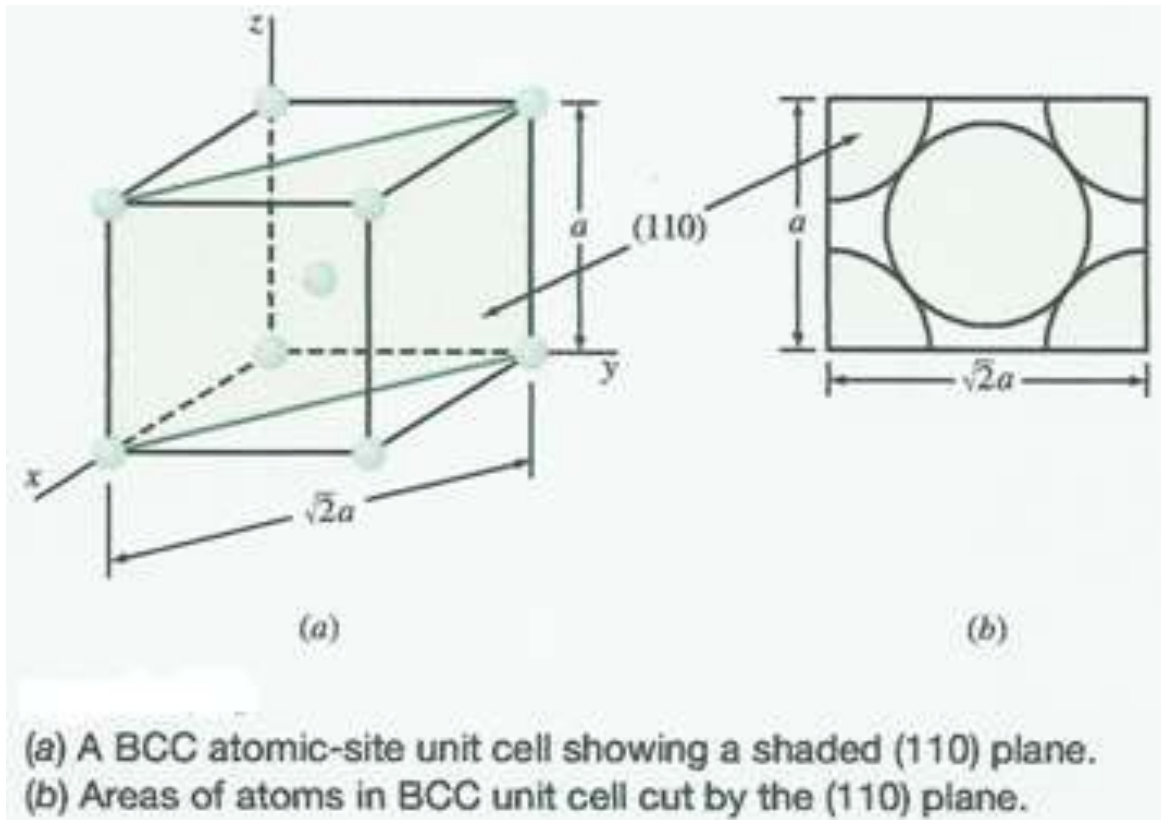
Thus the density of copper is

$$\rho_v = \frac{m}{V} = \frac{4.22 \times 10^{-28} \text{ Mg}}{4.70 \times 10^{-29} \text{ m}^3} = 8.98 \text{ Mg/m}^3 \quad (8.98 \text{ g/cm}^3) \ll$$

## Planar Atomic Density:

Is defined as the number of atoms per unit area that are centered on a given crystallographic plane. The *planar atomic density* is calculated by using the relationship

$$\text{Planar atomic density} = \rho_p = \frac{\text{No. of atoms centered on the plane}}{\text{Area of the plane}}$$



the (110) plane intersects the centers of five atoms, but the equivalent of only two atoms is counted since only one-quarter of each of the four corner atoms is included in the area inside the unit cell.

Calculate the planar atomic density  $\rho_p$  on the (110) plane of the  $\alpha$  iron BCC lattice in atoms per square millimeter. The lattice constant of  $\alpha$  iron is 0.287 nm.

### ■ Solution

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

The equivalent number of atoms intersected by the (110) plane in terms of the surface area inside the BCC unit cell is shown in Fig. 3.22 and is

$$1 \text{ atom at center} + 4 \times \frac{1}{4} \text{ atoms at four corners of plane} = 2 \text{ atoms}$$

The area intersected by the (110) plane inside the unit cell (selected area) is

$$(\sqrt{2}a)(a) = \sqrt{2}a^2$$

Thus the planar atomic density is

$$\begin{aligned} \rho_p &= \frac{2 \text{ atoms}}{\sqrt{2}(0.287 \text{ nm})^2} = \frac{17.2 \text{ atoms}}{\text{nm}^2} \\ &= \frac{17.2 \text{ atoms}}{\text{nm}^2} \times \frac{10^{12} \text{ nm}^2}{\text{mm}^2} \\ &= 1.72 \times 10^{13} \text{ atoms/mm}^2 \end{aligned}$$

### Linear Atomic Density:

Is defined as the number of atoms per unit length whose centers lie on the direction vector of a given crystallographic direction. *Atomic density* is calculated by using the relationship

$$\text{Linear atomic density} = \rho_l = \frac{\text{no. of atomic diam. intersected by selected length of line in direction of interest}}{\text{selected length of line}}$$

Calculate the linear atomic density  $\rho_l$  in the  $[110]$  direction in the copper crystal lattice in atoms per millimeter. Copper is FCC and has a lattice constant of 0.361 nm.

### ■ Solution

The atoms whose centers the  $[110]$  direction intersects are shown in Fig. 3.23. We shall select the length of the line to be the length of the face diagonal of the FCC unit cell, which is  $\sqrt{2}a$ . The number of atomic diameters intersected by this length of line are  $\frac{1}{2} + 1 + \frac{1}{2} = 2$  atoms. Thus using Eq. 3.7, the linear atomic density is

$$\begin{aligned}\rho_l &= \frac{2 \text{ atoms}}{\sqrt{2}a} = \frac{2 \text{ atoms}}{\sqrt{2}(0.361 \text{ nm})} = \frac{3.92 \text{ atoms}}{\text{nm}} \\ &= \frac{3.92 \text{ atoms}}{\text{nm}} \times \frac{10^6 \text{ nm}}{\text{mm}} \\ &= 3.92 \times 10^6 \text{ atoms/mm} \quad \blacktriangleleft\end{aligned}$$

