CHAPTER 2

Crystal Geometry

Dr. Talaat El-Benawy

Introduction

Sc

BCC

FCC

Center atom

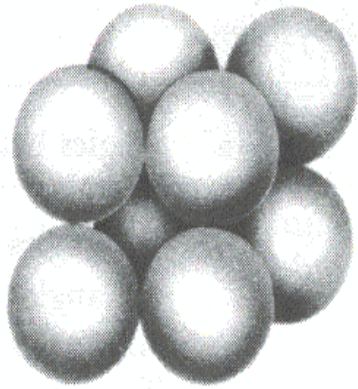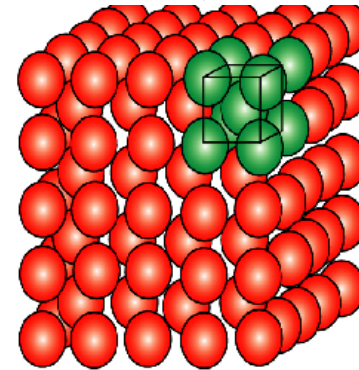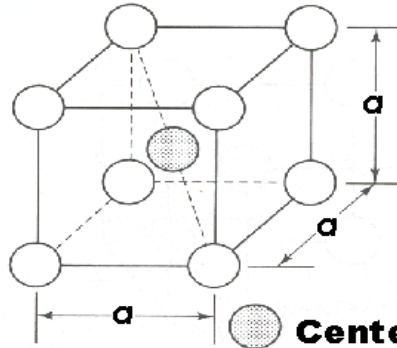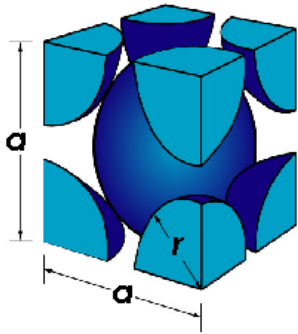Face-centered atom

4 r
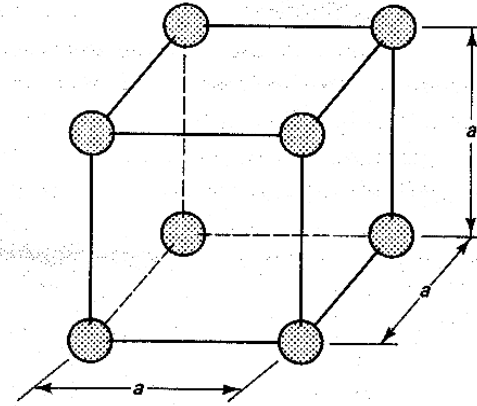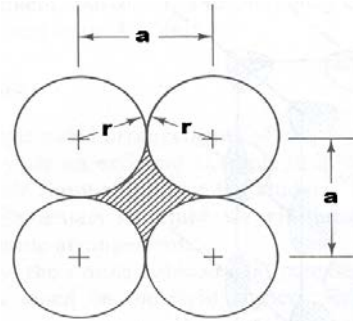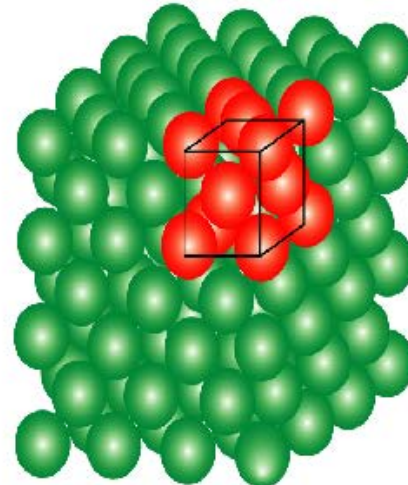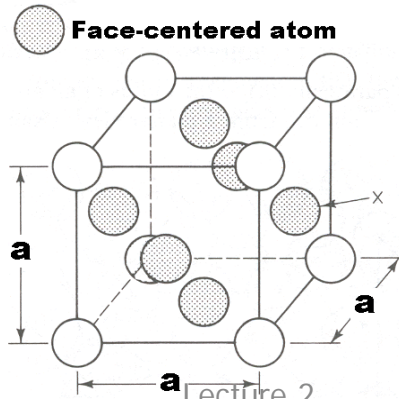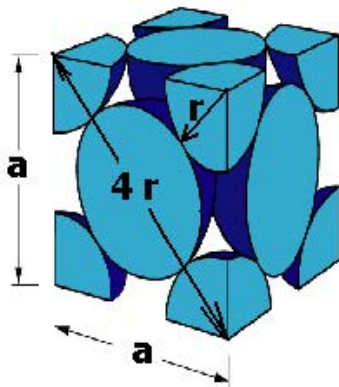
Introduction

In crystalline structure, atoms are arranging themselves in regular repetitive pattern called *lattice*. The *unit cell*, either in **BCC, FCC** or **CPH** forms, is the smallest structure unit in this pattern. It often to specify and represent some particular crystallographic points, directions and planes inside the unit cells of the crystalline lattice structure using what is so-called *Miller indices* .

In the following *Miller indices* of the cubic cell will be explained.
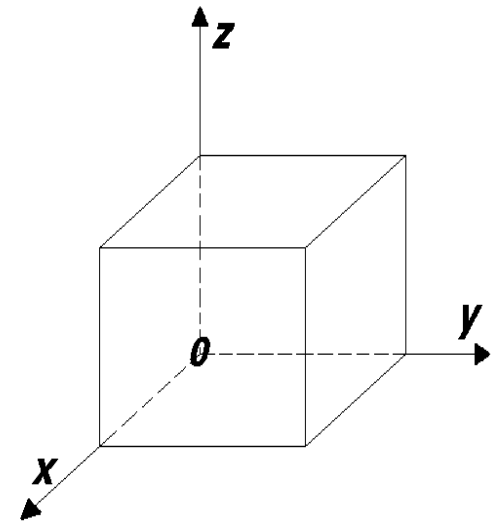
Coordinates of Points
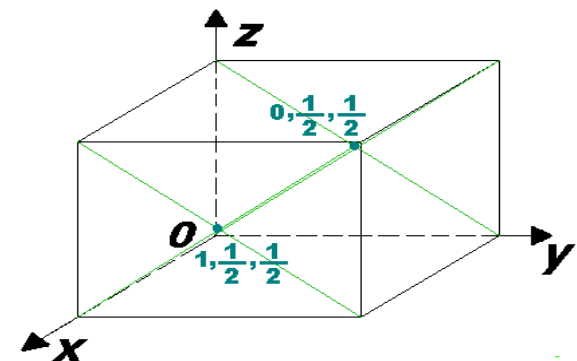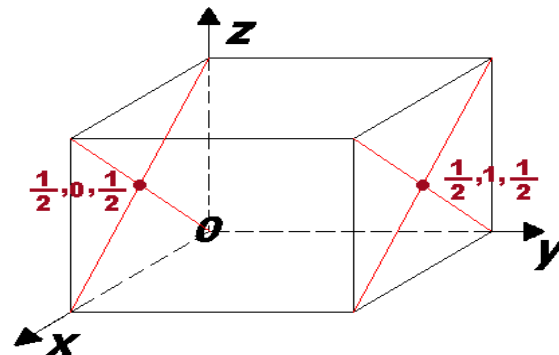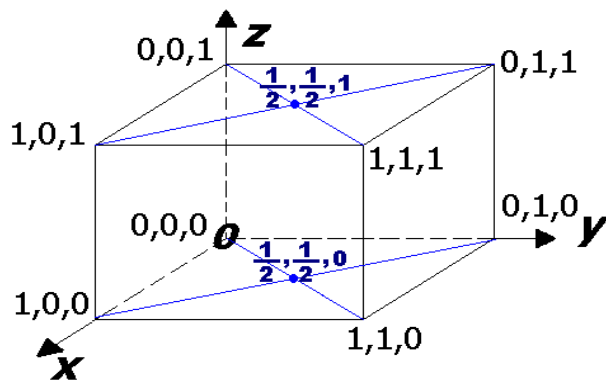
Coordinates of Directions

- **A crystallographic direction is defined as a vector line between two points.**
- **Metals are deformed in directions where *atoms are in closest contact*.**
- ***Properties of a material* may depend on the direction in the crystal.**

The procedure for finding directions by *Miller indices* is as follows:

a) **Determine the coordinates of two points that lie on the direction.**

b) **Subtract the coordinates of the "tail" point from the coordinates of the "head" point.**

c) **Clear fractions and reduce the results obtained from the subtraction to lowest integers.**

d) **Enclose the numbers in square brackets $[x \ y \ z]$. If a negative sign is produced, represent the negative sign with a bar over the number.**

Example:

Determine the miller indices of the directions A, B and C in the figure.
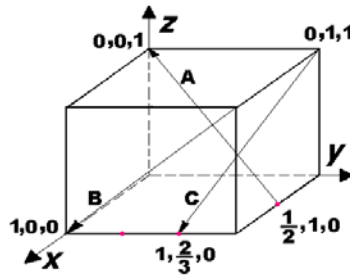
Direction A:

(a) Two points are $\frac{1}{2},1,0$ and $0,0,1$

(b) $0,0,1 - \frac{1}{2},1,0 = -\frac{1}{2},-1,1$

(c) $2(-\frac{1}{2},-1,1) = -1,-2,2$

(d) $[\bar{1}\,\bar{2}\,2]$

Direction B:

(a) Two points are $0,1,1$ and $1,0,0$
(b) $1,0,0 - 0,1,1 = 1,-1,-1$
(c) No fraction
(d) $[1\,\bar{1}\,\bar{1}]$
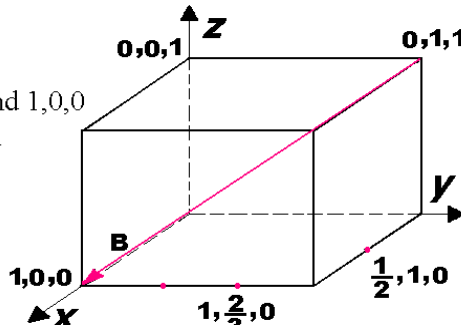
Direction C:
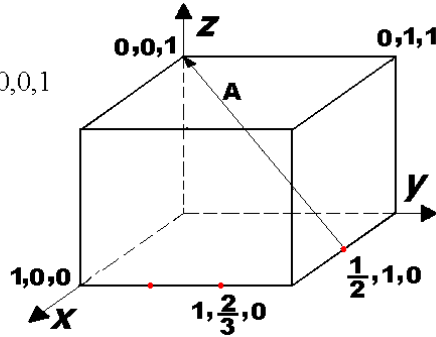
(a) Two points are $0,1,1$ and $1,\frac{2}{3},0$

(b) $1,\frac{2}{3},0 - 0,1,1 = 1,-\frac{1}{3},-1$

(c) $3(1,-\frac{1}{3},-1) = 3,-1,-3$

(d) $[3\,\bar{1}\,\bar{3}]$
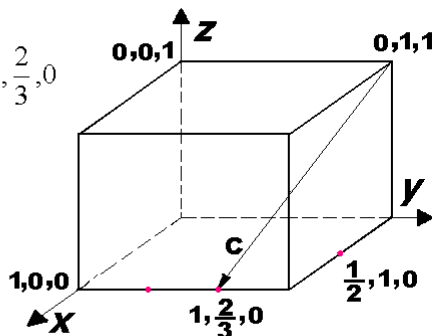
If it is required to represent direction of specified indices, the direction indices are repesented as point and the direction will be the line drawn between this point and the original point of 0,0,0 where its tail.

If the indices are higher than 1, the cleared fraction must be recalculated.

Example: Represent [122]
 - Recalculating cleared fraction is 1/2,1,1
 - Represent point 1/2,1,1 and draw
   the direction to it from original 0,0,0
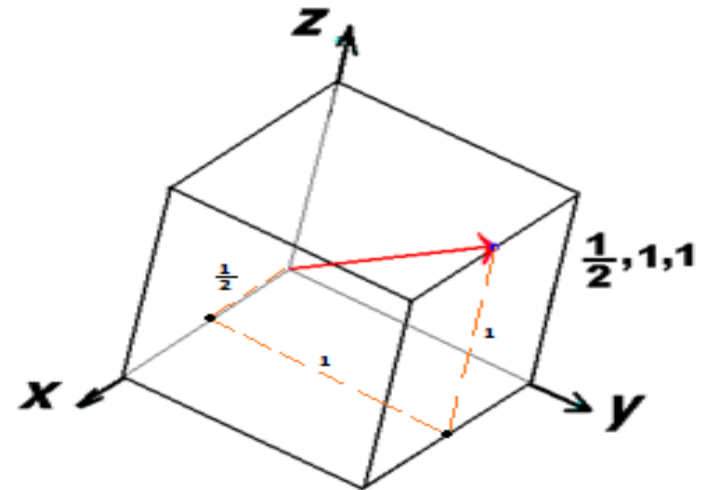
Also, for negative indices, it is preferred to move the origin point to temporary one to facilitate the direction drawing as shown in the figure for direction of as the following:

- Direction indices are $[2\,\bar{1}\,\bar{2}]$ then move the origin O in y and Z directions to eliminate the negative sign of them.

- The point of indices are 2,-1,-2

- Recalculate the fractions $\frac{1}{2}(2,-1,-2) = 1,-\frac{1}{2},-1$

- Represent the point $1,-\frac{1}{2},-1$ and draw line between this point and the temporary origin where the direction tail
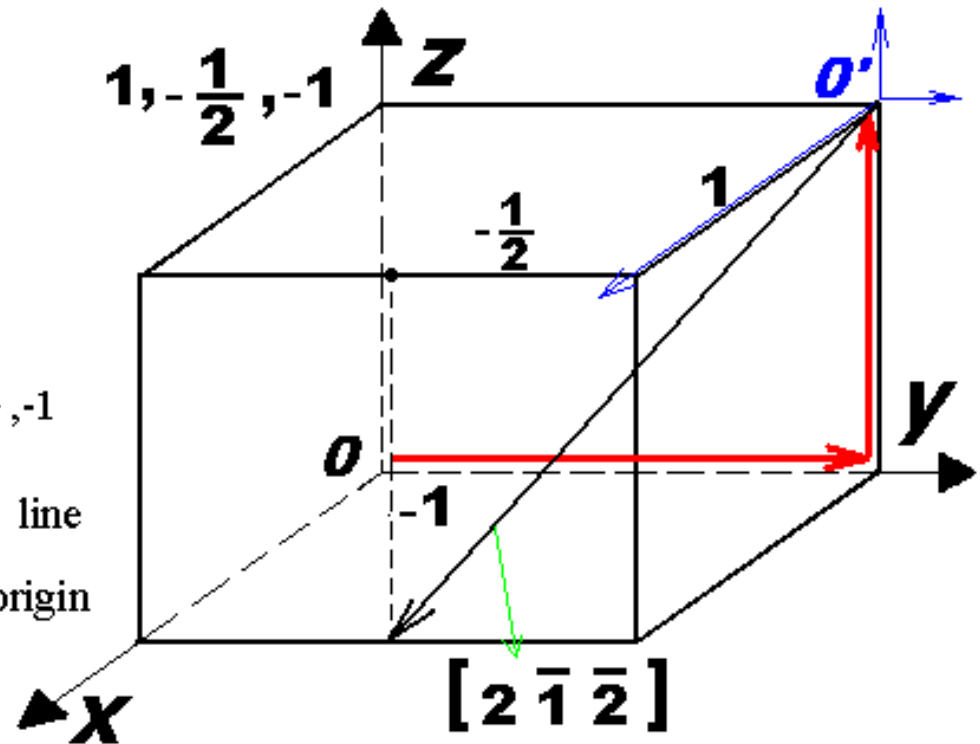
Linear Density

Linear density (LD) is defined as the fraction of the line length in particular crystallographic direction that passes through atom centers.

Example: Calculate the linear density of [100] and [110] in FCC crystal structure cells

Solution: - *For direction [100]*

Linear density $= LD$

$$LD = \frac{\text{Total line length intersecting atoms}}{\text{Direction length}} = \frac{L_i}{L} = \frac{2r}{a}$$

For FCC $a_{FCC} = \frac{4r}{\sqrt{2}} = L$; Then $LD = \frac{2r}{4r/\sqrt{2}} = 0.707$

i.e. 70.7% of the direction [100] are occupied by atoms
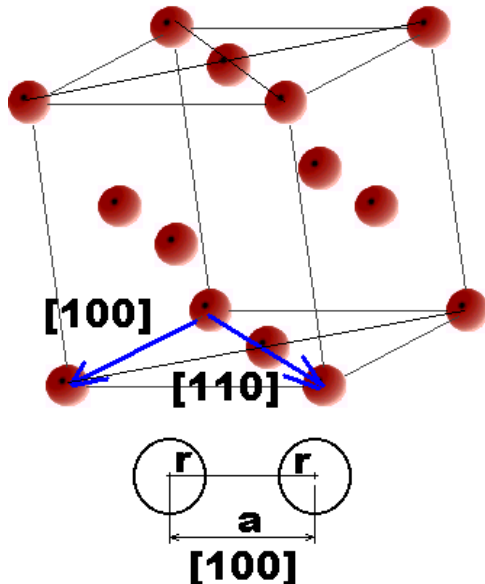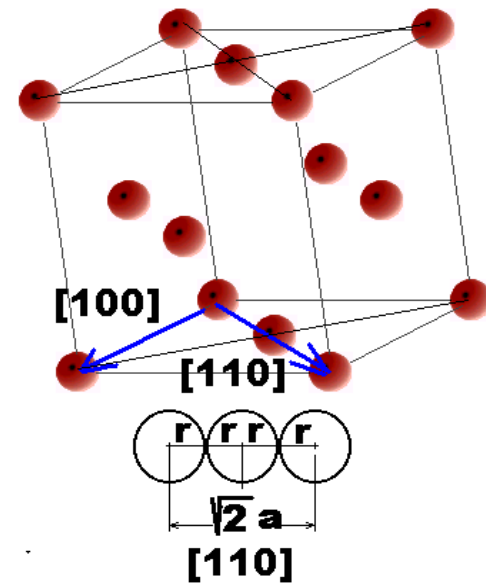

For direction [110]

Linear density $= LD$

$$LD = \frac{\text{Total line length intersecting atoms}}{\text{Direction length}} = LD = \frac{L_i}{L}$$

$L = \sqrt{2}\,a$ and $L_i = 4r$

Since $a_{FCC} = \frac{4r}{\sqrt{2}}$ $\therefore L = \sqrt{2}\,\frac{4r}{\sqrt{2}} = 4r$

$$LD = \frac{4r}{4r} = 1.0$$

i.e. 100% of the direction [110] are occupied by atoms

Coordinates of Planes

Because of the symmetry and repetitive nature of crystalline materials, their atoms are contained in planes. Identification of these planes assist our understanding for the influence of the atoms on the mechanical and/or the physical properties of crystalline materials.

Miller indices can be used to identify these planes as the following procedure:

(a) Identify the points at which the plane intercepts the x, y, and Z coordinates in terms of the number of lattice parameters. If the plane passes through the origin, the origin of the coordinate system must be moved.

(b) Take reciprocals of these intercepts $h=1/x, k=1/y, l=1/Z$.

(c) Enclose the resulting numbers in parentheses $(h\ k\ l)$. Again, negative numbers should be written with a bar over the number.

Example:
Determine Miller induces of the planes **A**, **B** and **C** in the given figures
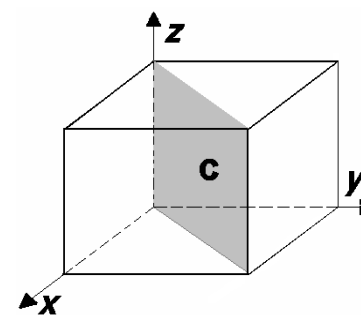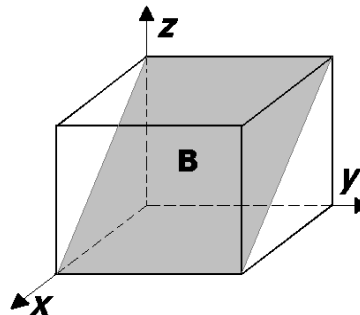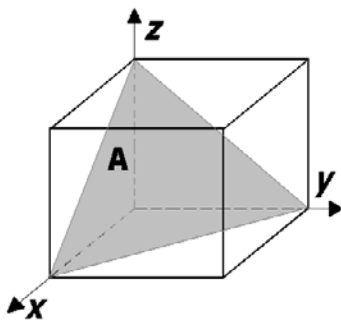
Solution:

For Plane A:

(a) x = 1, y = 1, Z = 1

(b) $h = \dfrac{1}{x} = 1, \quad k = \dfrac{1}{y} = 1, \quad l = \dfrac{1}{Z} = 1$

(c) No fraction

(d) $h = 1, k = 1, l = 1$ then the plane is (111)
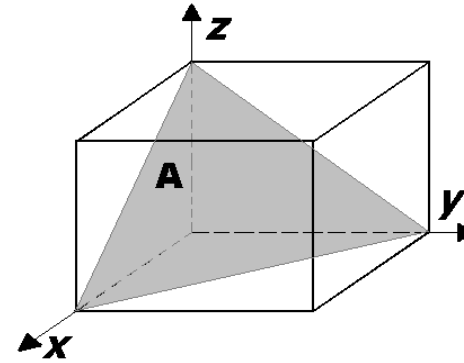
For Plane B:

(a) x = 1, y = ∞, Z = 1

(b) $h = \dfrac{1}{x} = 1, \quad k = \dfrac{1}{y} = 0, \quad l = \dfrac{1}{Z} = 1$

(c) No fraction

(d) $h = 1, k = 0, l = 1$ then the plane is (101)
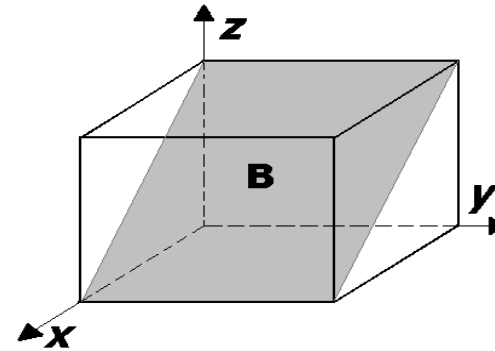
For Plane C:

(a) After moving the origin of the coordinates
x = 1, y = −1, Z = ∞

(b) $h = \dfrac{1}{x} = 1, \quad k = \dfrac{1}{y} = -1, \quad l = \dfrac{1}{Z} = 0$

(c) No fraction

(d) $h = 1, k = -1, l = 0$ then the plane is $(1\bar{1}0)$

9
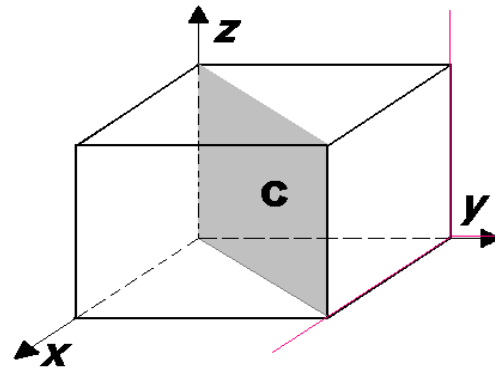
Planar Density

Planar density (PD) is simply the fraction of the total crystallographic plane area that is occupied by atoms (atoms are represented by circles); the plane must pass through an atom's center for particular atom to be included.

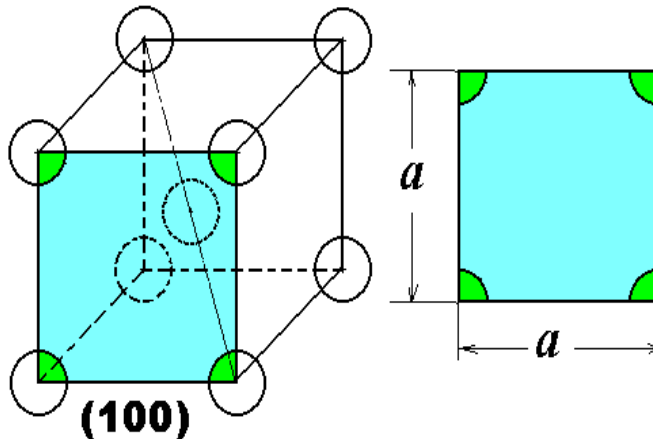**Example:** Calculate planar density of the (100) and (110) in BCC crystal structure.

For Plane (100):

$$PD = \frac{\text{Total atoms area that occupied the plane}}{\text{Plane area}} = \frac{A_c}{A_p}$$

For BCC $a_{BCC} = \frac{4r}{\sqrt{3}}$ Then $A_p = a^2 = \left(\frac{4r}{\sqrt{3}}\right)^2$ also $A_c = 4 \times \frac{\pi r^2}{4}$

$$PD = \frac{A_c}{A_p} = \frac{4 \times \dfrac{\pi r^2}{4}}{\left(\dfrac{4r}{\sqrt{3}}\right)^2} = 0.589 \equiv 58.9\%$$

i.e. **58.9%** of the plane (100) are occupied by atoms

(100)

For Plane (110):

$$PD = \frac{\text{Total atoms area that occupied the plane}}{\text{Plane area}}$$

$$PD = \frac{A_c}{A_p}$$

From Figure $A_p = \sqrt{2}\, a^2$, also $a_{BCC} = \frac{4r}{\sqrt{3}}$,

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

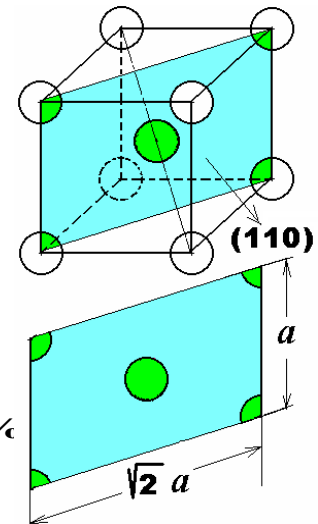Plane (110) contains four quarter atoms in the corners and one circle in the center.

$$A_c = 4 \times \frac{\pi r^2}{4} + \pi r^2$$

$$PD = \frac{A_c}{A_p} = \frac{4 \times \dfrac{\pi r^2}{4} + \pi r^2}{\sqrt{2}\left(\dfrac{4r}{\sqrt{3}}\right)^2}$$

$$= \frac{2\pi r^2}{\sqrt{2}\left(\dfrac{16}{3}\right)r^2}$$

$$= 0.833 \quad \text{i.e.} \quad PD = 83.3\%$$

i.e. **83.3%** of the plane (110) are occupied by atoms

(110)

Interplanar Relationship

The spacing between planes in a crystalline material is very important when discussing deformation or machining behavior of crystalline materials.

Separation distance (d) between crystal planes (A and B), is analyzed by X-ray through the diffraction of an angle θ X-ray beam when certain geometrical conditions are met.

The difference between *ray 1* **and** *ray 2* **equals to the distance** *SQT* **that could equal one wavelength** (λ) **or a multiple of it** (*n*λ). **When all the** *X-rays* **are in phase as they leave the crystal and are detected, the following condition exists:**

Difference between ray 1 and ray 2 = $n\lambda = 2\,\mathbf{d}\,sin\,\theta$

Where *n* represents an integer number of the wave lengths: 1, 2, … and so on.

This equation is commonly termed *Bragg's law*. In practice, the value of *n* is typically taken to be **1** because the diffracted beam is usually weaker when more than one wavefront is present.
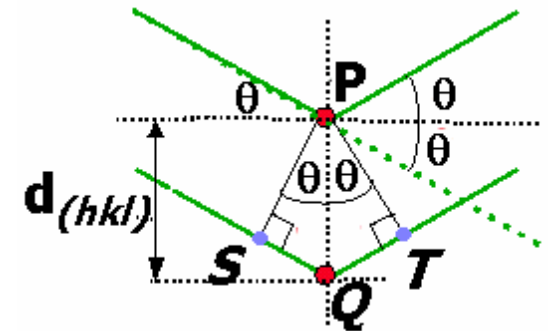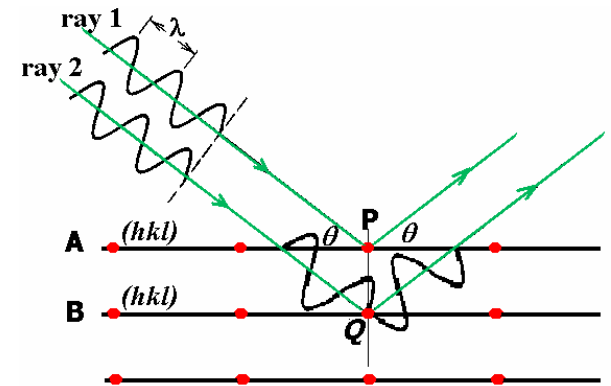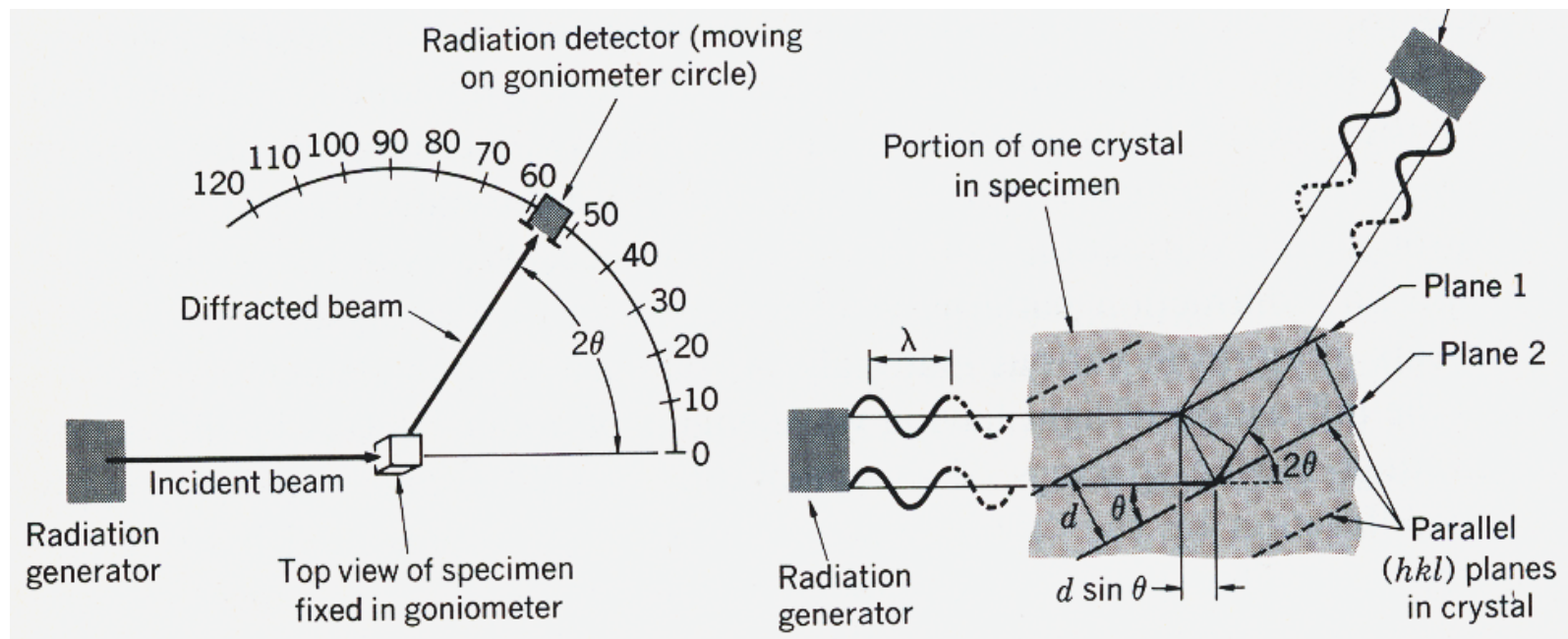
How to define distance between planes (d)

Interplanar spacing **d** corresponding to cubic
and hexagonal crystal structure

Crystal structure system	Interplanar spacing $d_{(hkl)}$
Cubic (BCC & FCC)	$d_{(hkl)} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$

Don't forget that $n \lambda = 2 \, d \, sin \, \theta$

X-Ray Diffraction apparatus

1. *Laud method:* **variable λ and fixed θ**

2. *Rotating crystal method*: **fixed λ and variable *θ***

3. *Powder method:* **fixed λ and variable *θ***

Primary-beam slits

X-ray tube

Tube shield support

Specimen holder

Goniometer dials

Diffracted-beam slits

Scintillation counter
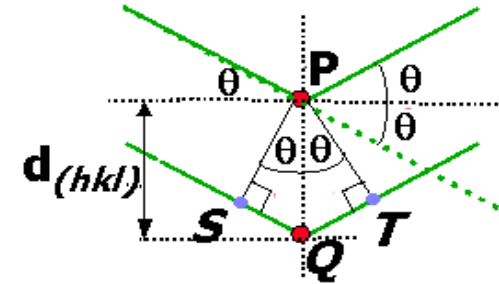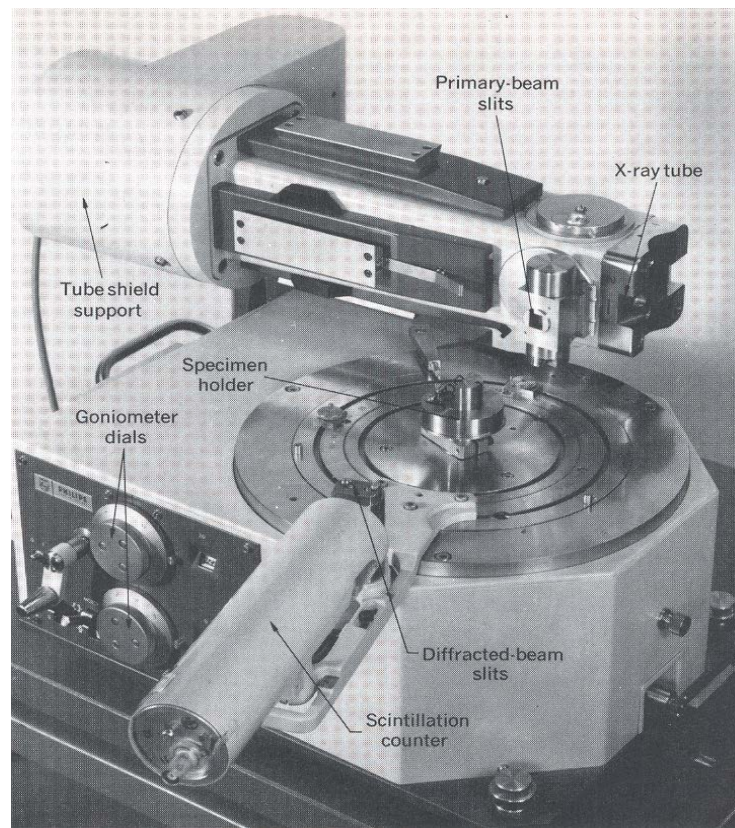
X-Ray diffraction of Powdered FCC lead sample

Intensity

(111)

(200)

(220)

(311)

(222)

(400)

(331)

(420)

(422)

Diffraction angle 2θ
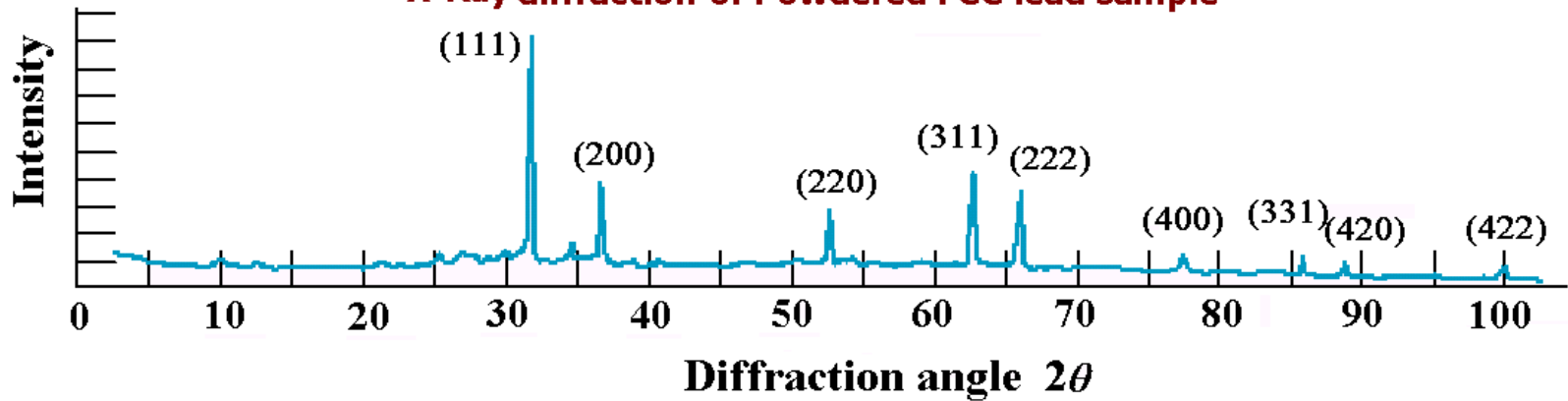
Solved Example

Ex(1) A diffraction analysis experiment is performed on a sample of BCC crystal structure on the plane (110). It is required to calculate the atom radius (r) and density (ρ) of the sample. Given that the wavelength (λ) of the first order (n=1) X-ray, equals 1.54 Å, the incidence angle of the X-ray $\theta = 19.3°$ and the atomic weight of the sample A = 92.9 g/mol

Solution:

Given: - BCC structure then $n = 2$ and $a = \dfrac{4}{\sqrt{3}} r$, $V = a^3$, $A = 92.9\,gram/mol$

- Plane to be diffracted is (110),

- Diffraction beam : $\lambda = 1.54 \overset{o}{A}$, $n = 1$ and $\theta = 19.3°$

$$n\lambda = 2\,d\sin\theta$$
$$1\times 1.54 = 2\times d\times \sin(19.3)$$

$$\boxed{d = 2.3297 \overset{o}{A}}$$

$$d_{(hkl)} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{(110)} = \dfrac{a}{\sqrt{(1)^2 + (1)^2 + (0)^2}} = 2.3297$$

$$\therefore \boxed{a = 3.295 \overset{o}{A}}$$
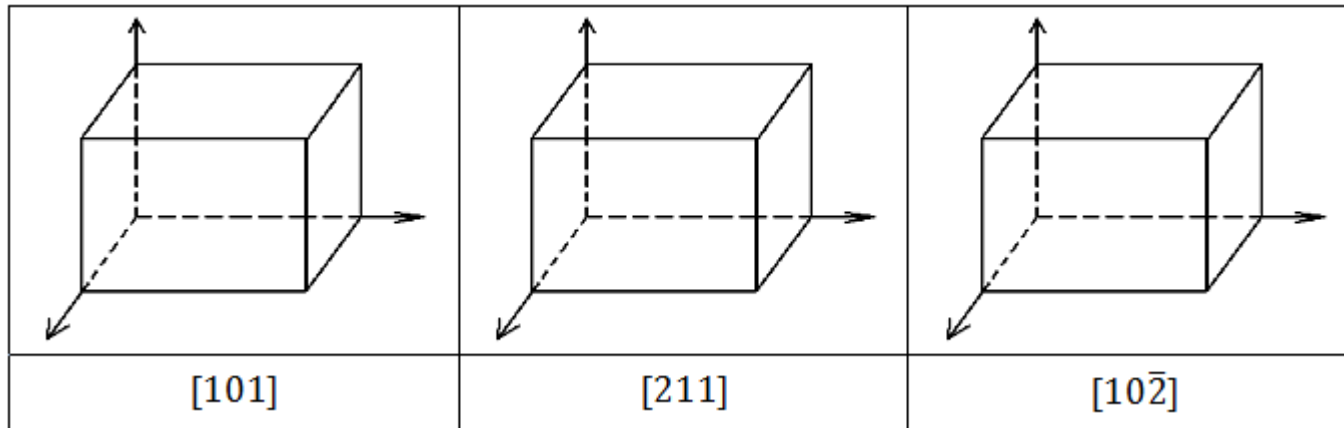
$$\because a = \dfrac{4}{\sqrt{3}} r = 3.295$$

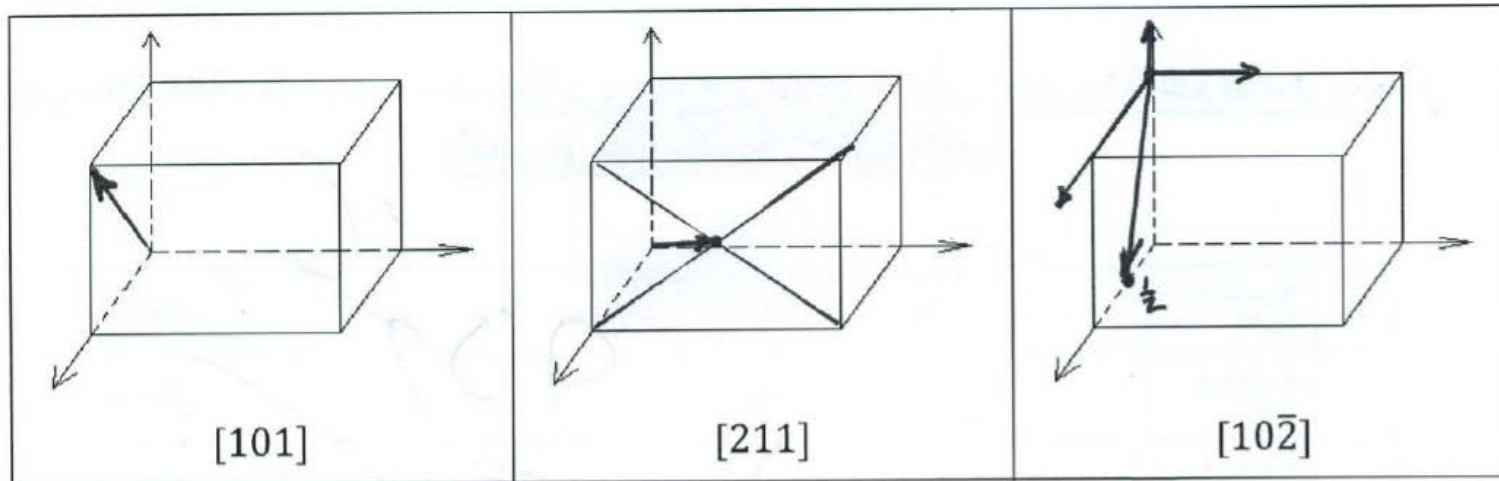$$\therefore \boxed{r = 1.43 \overset{o}{A}}$$

$$\rho = \dfrac{A \times n}{N_A \times a^3} = \dfrac{92.9 \times 2}{6.023\times 10^{23} \times (3.295\times 10^{-8})^3}$$

$$\therefore \boxed{\rho = 8.623\ gram/cm^3}$$

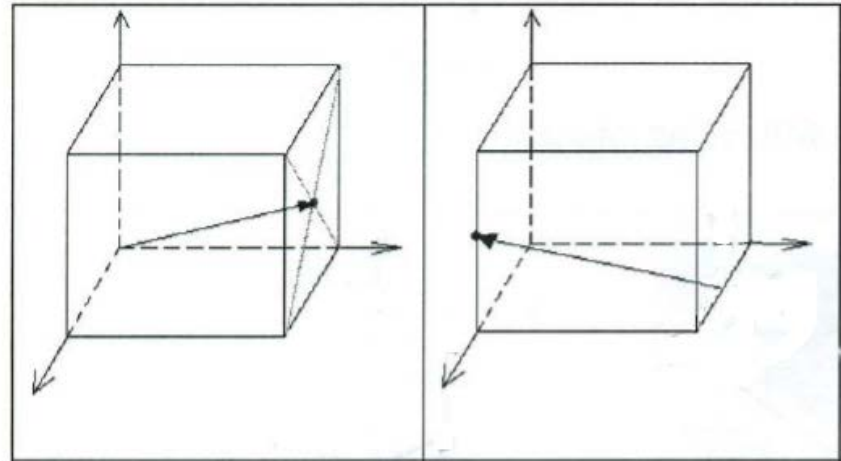# Ex(2) Within a cubic unit cell, sketch the following directions

| [101] | [211] | [10$\bar{2}$] |

Solution:

| [101] | [211] | [10$\bar{2}$] |

- [101] → 1,0,1
- [211] → (2,1,1)$\frac{1}{2}$ ≡ 1,$\frac{1}{2}$,$\frac{1}{2}$
- [10$\bar{2}$] → (1,0,-2)$\frac{1}{2}$ ≡ $\frac{1}{2}$,0,-1 → غير نقطة محور (يبدأ من z)
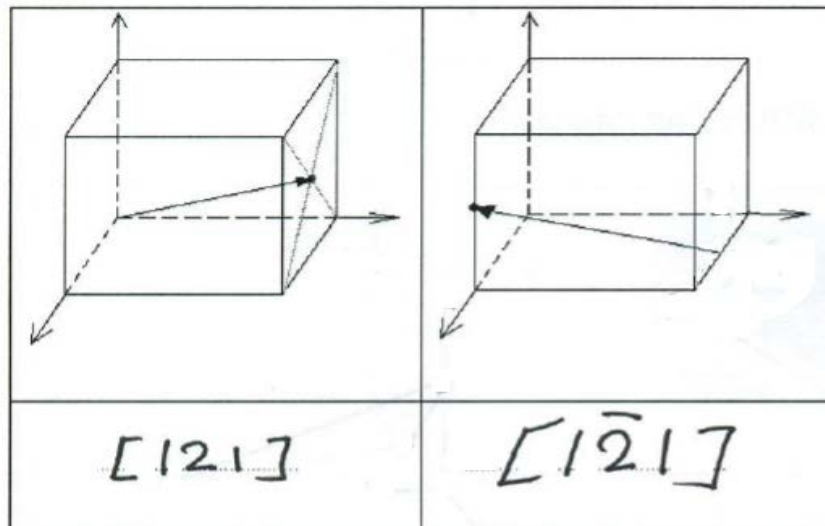
Ex(3) Determine the indices for the directions shown in the following cubic unit cell:
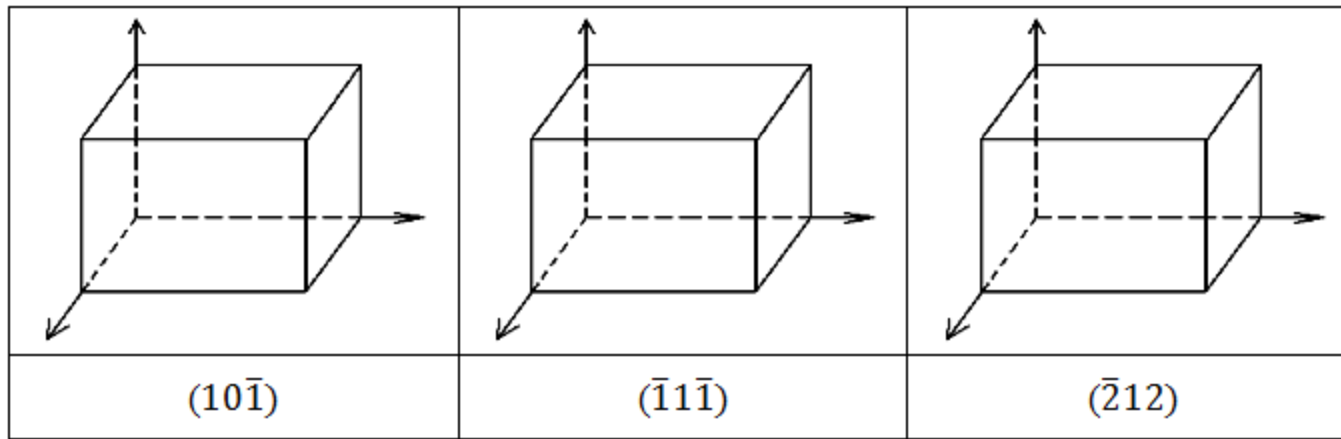

Solution:

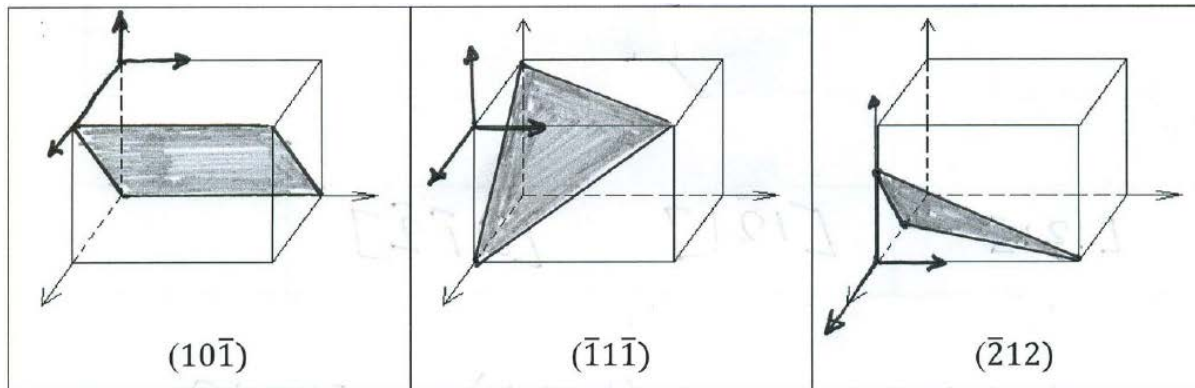$$-\frac{1}{2}, 1, \frac{1}{2} - 0, 0, 0 \equiv \left(\frac{1}{2}, 1, \frac{1}{2}\right) \frac{*2}{} \equiv [1\,2\,1]$$

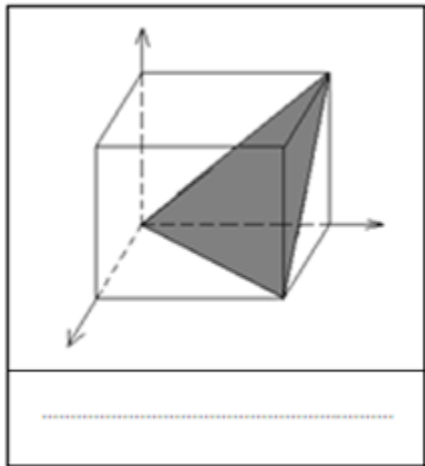$$-1, 0, \frac{1}{2} - \frac{1}{2}, 1, 0 \equiv \left(\frac{1}{2}, -1, \frac{1}{2}\right) *2 = [1\,\bar{2}\,1]$$

| [1 2 1] | [1 $\bar{2}$ 1] |

Ex(4) Sketch within a cubic unit cell the following planes:

$(10\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{2}12)$

Solution:

$(10\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{2}12)$

Ex(5) Determine the Miller indices for the plane shown:

Solution:

$$(1\bar{1}1)$$
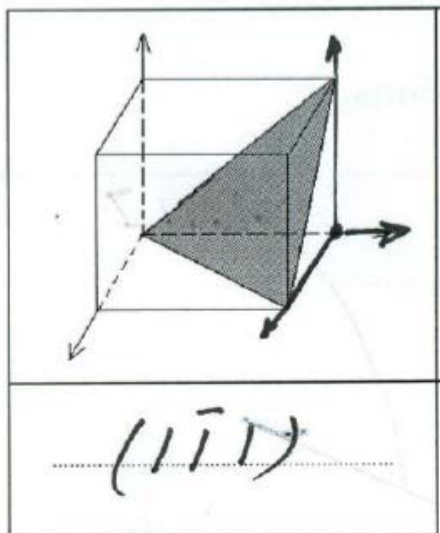
Ex(6) Calculate linear density for FCC [100] and [111] directions.
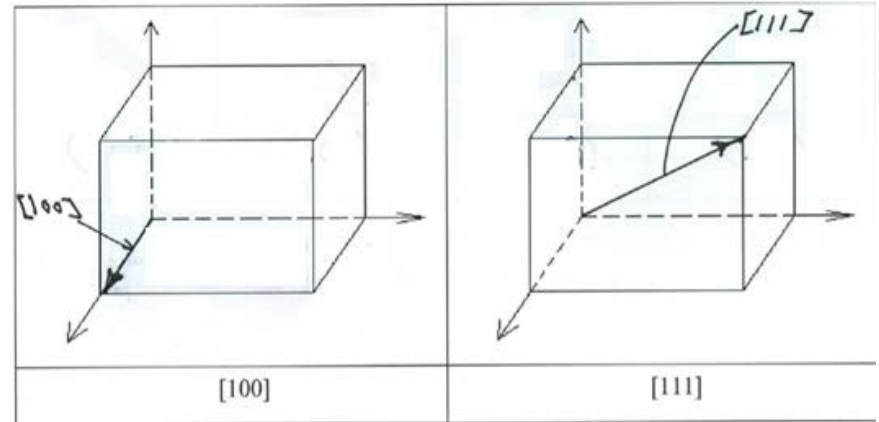
Solution:

| [100] | [111] |

For Direction [100]

For FCC

$$a = \frac{4}{\sqrt{2}} r$$

$$LD = \frac{2r}{a} = \frac{2r}{\frac{4}{\sqrt{2}}r}$$

$$\therefore LD = 0.707$$

$$LD\% = 70.7\%$$

For Direction [111]

For FCC

$$a = \frac{4}{\sqrt{2}} r$$

$$\sqrt{3}a$$
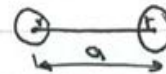
$$LD = \frac{2r}{\sqrt{3}a} = \frac{2r}{\sqrt{3} \cdot \frac{4}{\sqrt{2}}r}$$

$$LD = 0.408$$

$$LD\% = 40.8\%$$

Ex(7) Calculate linear density for FCC [100] and [111] directions.

Solution:

| [100] | [111] |

For Direction [100]	For Direction [111]

For Direction [100]

For FCC

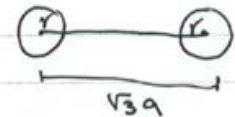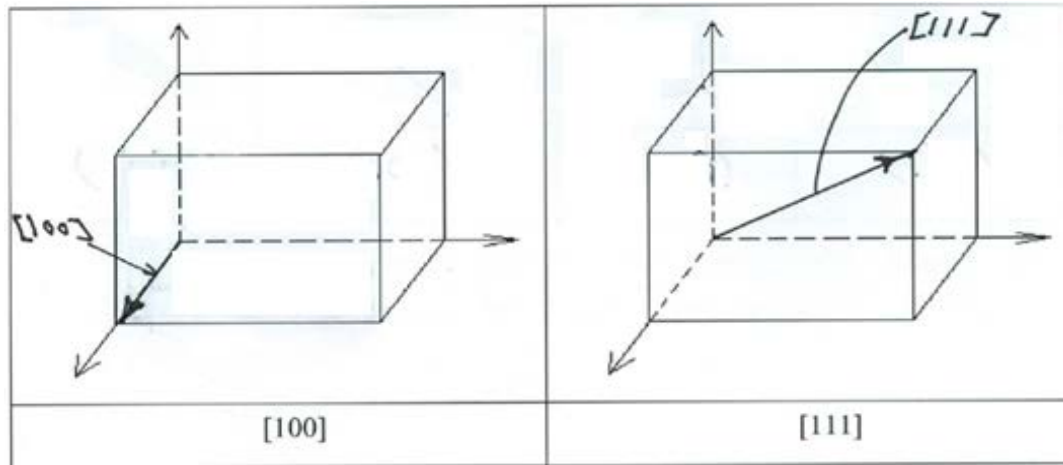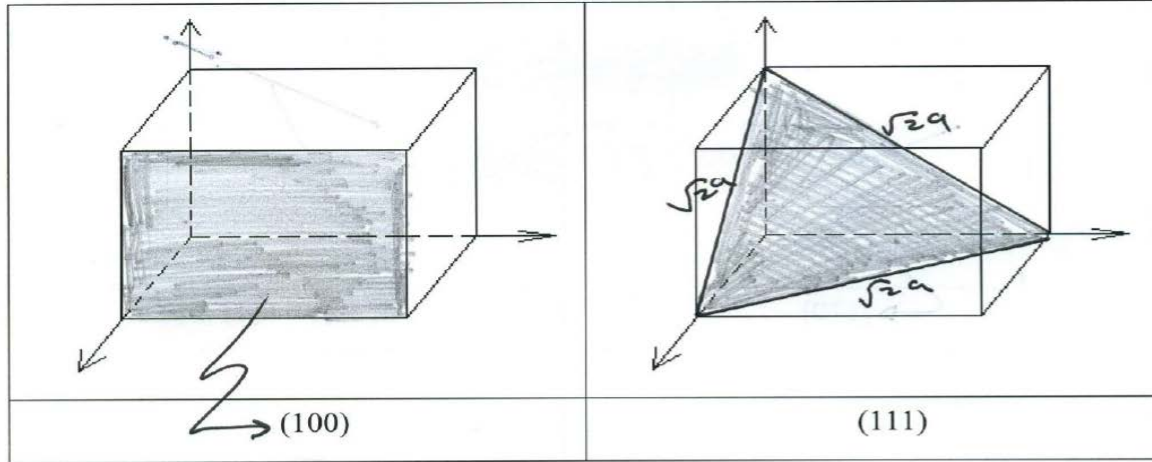$a = \dfrac{4}{\sqrt{2}} r$

$LD = \dfrac{2r}{a} = \dfrac{2r}{\frac{4}{\sqrt{2}}r}$

$\therefore LD = 0.707$

$LD\% = 70.7\%$

For Direction [111]

For FCC

$a = \dfrac{4}{\sqrt{2}} r$

$\sqrt{3}a$

$LD = \dfrac{2r}{\sqrt{3}a} = \dfrac{2r}{\sqrt{3} * \frac{4}{\sqrt{2}} r}$

$LD = 0.408$

$LD\% = 40.8\%$

Ex (8) Calculate planar density expressions for FCC (100) and (111) planes

Solution:

(100)

(111)

For Plane (100)

For FCC $\quad a = \dfrac{4}{\sqrt{2}} r$
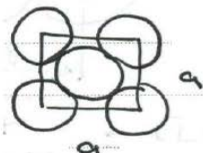
$$PD = \frac{4 \frac{\pi r^2}{4} + \pi r^2}{a^2}$$
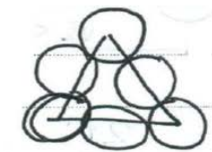
$$= \frac{2\pi r^2}{\left(\frac{4}{\sqrt{2}}\right)^2 r^2}$$

$$= 0.785$$

$$\therefore PD\% = 78.5\%$$

For Plane (111)

For FCC $\quad a = \dfrac{4}{\sqrt{2}} r$

$$PD = \frac{3 \frac{\pi r^2}{8} + 3 \frac{\pi r^2}{2}}{\frac{1}{2} \sqrt{2}a \times \frac{\sqrt{3}}{2} \sqrt{2}a}$$

$$= \frac{(0.5 + 1.5)\pi r^2}{\frac{\sqrt{3}}{2} \left(\frac{4}{\sqrt{2}}\right)^2 \times r^2}$$

$$= 0.907$$

$$PD\% \quad 90.7\%$$

Home Work

Problem 1
The metal rhodium has an FCC crystal structure. If the **angle of diffraction** for the (311) set of planes occurs at ٣٨° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute:
(a) the interplanar spacing for this set of planes, and
(b) the atomic radius for a rhodium atom.

Problem 2
X-ray diffraction analysis experiment of the first order is performed for an FCC element, calculate the **incidence angle (θ)** of the diffraction X-ray beam that will indicate plane (100). Given that the available X-ray wavelength λ = 4.0 Å, element atomic weight and density are 26.9 g/mol and 2.6 g/cm³, respectively.
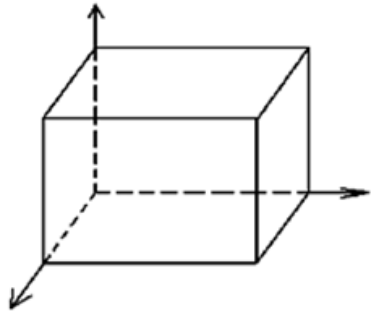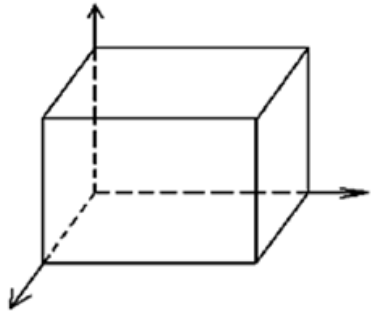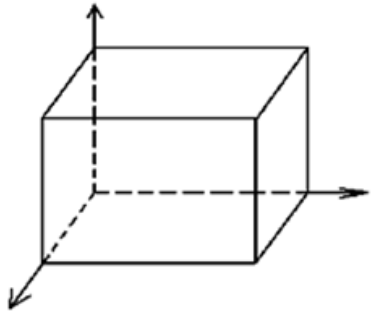
Problem 3
The metal niobium has a BCC crystal structure. If the **angle of diffraction** for the (211) set of planes occurs at 76° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1659 nm is used, compute:
(a) the interplanar spacing for this set of planes, and
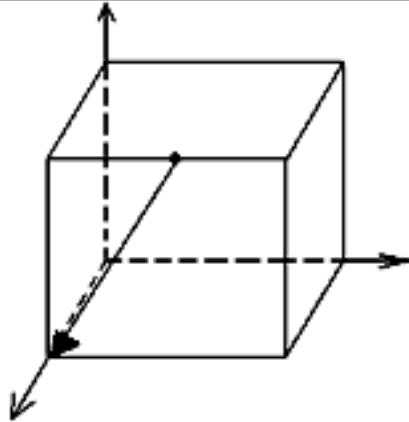**(b)** the atomic radius for the niobium atom
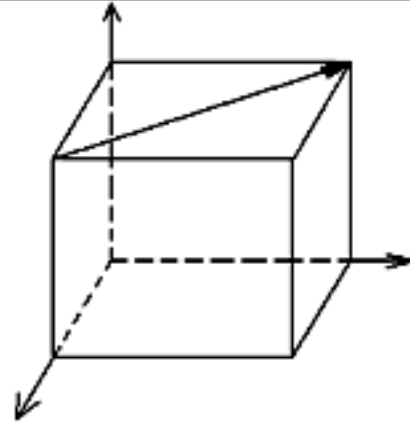
Problem 4
Within a cubic unit cell, sketch the following directions:

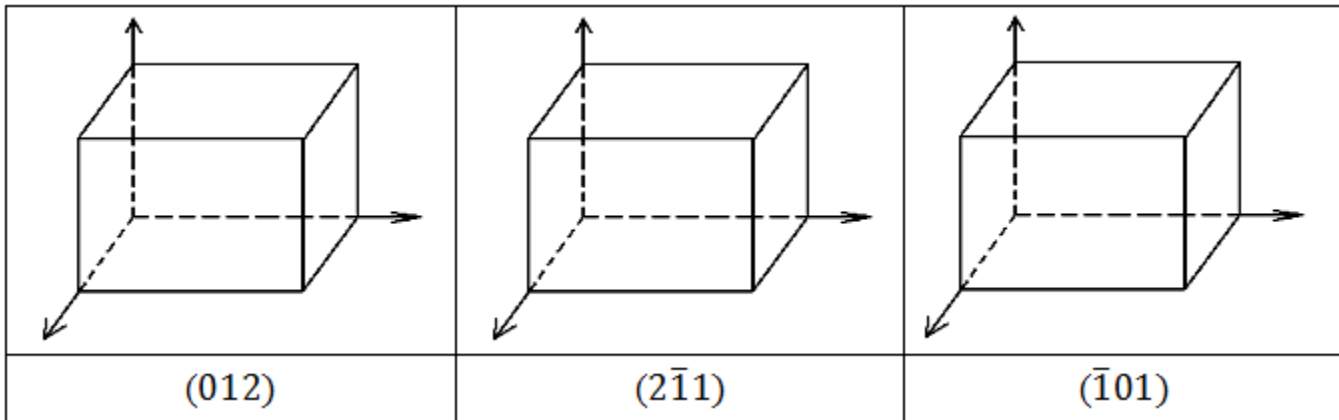|		
$[\bar{1}1\bar{1}]$	$[\bar{2}12]$	$[30\bar{1}]$

Problem 5
Determine the indices for the directions shown
in the following cubic unit cell:

Problem 6
Sketch within a cubic unit cell the following planes:

| (012) | (2Ī1) | (Ī01) |

Problem 7
Determine the Miller indices for the planes shown in the following unit cells:

Problem 8
Calculate linear density expressions for BCC [110] and [111] directions.

| [110] | [111] |

For Direction [110]

For Direction [111]

Problem 9
Calculate planar density expressions for BCC (100) and (110) planes.

| (100) | (110) |

| For Plane (100) | For Plane (110) |