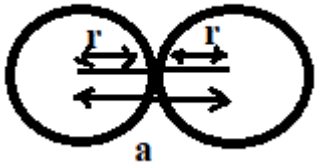
Question and Answers of Unit 3-Crystal Structure

1	Define: (i) Space lattice, (ii) Coordination number and (iii) Void space Ans: (i) The regular periodic arrangement of points in three- dimensional space such that every point has identical surroundings as that the other is called **Space lattice.** **(ii)** The **Coordination number** of an atom is the number of nearest neighbouring atoms which are simultaneously in contact with that atom. (iii) The empty space left unoccupied in a given unit cell is called **Void Space**.	3
2	Define: (i) Miller indices (ii) Unit cell. **(i)Miller indices** are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to the smallest integers. **(ii) Unit cell** is the smallest geometric building block of a space lattice having minimum volume, the repetition of which in three- dimensional space gives the entire crystal structure.	2
3	Define 1. Space lattice 2. Coordination number 3. Effective no. of atoms per unit cell 4. Atomic packing fraction. (i)The regular periodic arrangement of points in three- dimensional space such that every point has exactly identical surroundings as that the other is called **Space lattice.** (ii) The **Coordination number** of an atom is the number of nearest neighbouring atoms which are simultaneously in contact with that atom. (iii) The **Effective number of atoms per unit cell** is equal to the product of the number of atoms per lattice point and the number of lattice points per unit cell. (iv) The fraction of space occupied by atoms in a unit cell is known as **atomic packing fraction.** It is defined as the ratio of volume occupied by the atoms in a unit cell (v) to the total volume of the unit cell (V).	4
4	Define 1. Coordination number 2. Void space 3. Atomic radius. (i)The **Coordination number** of an atom is the number of nearest neighbouring atoms which are simultaneously in contact with that atom. (ii) The empty space left unoccupied in a given unit cell is called **Void Space**. (iii)**Atomic radius** is half the distance between centres of two nearest neighboring atoms in a given unit cell.	3
5	Show that FCC has a maximum atomic packing fraction compared to BCC and SC unit cell. Atomic packing fraction (APF): The fraction of space occupied by atoms in a unit cell is known as atomic packing fraction. It is defined as the ratio of volume occupied by the atoms in a unit cell (v) to the total volume of the unit cell (V). $$APF = \frac{\text{Volume of effective number of atoms in unit cell}}{\text{Total Volume of unit cell}}$$ $$= \frac{(\text{No.of atoms per unit cell})(\text{Volume of each atom})}{\text{Total Volume of unit cell}} = \frac{Zv}{V} = \frac{Z \times \frac{4}{3}\pi r^3}{a^3}$$ ---------- (1)	4

	<u>SC</u> For the SC cell, Z=1 and a = 2r, Volume of spherical atom $= v = \frac{4}{3}\pi r^3$ Total Volume of unit cell, $V = a^3$ $= (2r)^3$ $= 8r^3$ Substituting the value of Z, v and V, we get in eqn. *1* $\therefore APF = \frac{1 \times \frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6}$ $\boldsymbol{APF = 0.52}$ <u>BCC</u> For BCC, $Z = 2$ and $a = \frac{4r}{\sqrt{3}}$ Volume of spherical atom $= v = \frac{4}{3}\pi r^3$ Total Volume of unit cell, V $= a^3$ $= 64\frac{r^3}{3\sqrt{3}}$ Substituting the value of Z, v and Vin equation1, we get $\therefore APF = \frac{2 \times \frac{4}{3}\pi r^3}{64\frac{r^3}{3\sqrt{3}}} = \frac{\pi\sqrt{3}}{8}$ $\boldsymbol{APF = 0.68}$ <u>FCC</u> In case of FCC cell, $Z = 4$ and $a = 2\sqrt{2}\,r$, Total Volume of unit cell = a^3 $= (2\sqrt{2}r)^3 = 16\sqrt{2}r^3$ Volume of spherical atom, v $= \frac{4}{3}\pi r^3$ Substituting the value of Z, v and Vin equation1, we get $\therefore APF = \frac{4 \times \frac{4}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}}$ $\boldsymbol{APF = 0.74}$ From above results, we conclude that APF of FCC unit cell is greater than that of BCC and SC unit cell.	
6	Compute atomic radius for SC, BCC and FCC structure. Atomic radius is half the distance between centres of two nearest neighboring atoms in a given unit cell. **For SC unit cell**, corner atoms are in contact with each other along the edge of unit cell as shown in Fig1.  Fig.1: Determination of radius in SC cell. If 'a' is the edge of unit cell. $\boldsymbol{a = 2r}$ $\therefore r = \frac{a}{2}$ **For BCC structure**, atoms are in contact with each other *along the body diagonal AD* as shown in Fig.2,	5

From the figure,

$(AD)^2 = (AC)^2 + (CD)^2$

$= (AB)^2 + (BC)^2 + (CD)^2$

$=(a)^2 + (a)^2 + (a)^2$

$= 3\,a^2$

$\therefore AD = \sqrt{3}a$ ……. (1)

But also, AD = r + 2r + r

$\therefore AD = 4\,r$ ……. (2)

From equations (1) & (2),

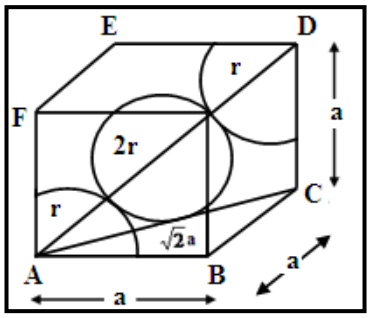


Fig.2: Determination of radius in BCC cell.

$$4\,r = \sqrt{3}a$$

$$r = \frac{\sqrt{3}a}{4}$$

For FCC structure, atoms are in contact with along face diagonal AC as shown in Fig.3.,

$(AC)^2 = (AB)^2 + (BC)^2$

$= a^2 + a^2$

$= 2\,a^2$

$AC = \sqrt{2}\,a$ ……. (1)

But also, AC = r + 2r + r

$AC = 4\,r$ ……. (2)

From equations (1) & (2) we get,

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

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

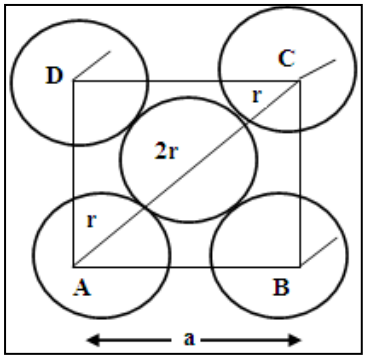


Fig3: Determination of radius in FCC cell

7	Show that FCC structure possesses maximum packing density (APF) and minimum percentage of void space among BCC and FCC.	6

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

$$= \frac{(\text{No.of atoms per unit cell})(\text{Volume of each atom})}{\text{Total Volume of unit cell}} = \frac{Zv}{V} = \frac{Z \times \frac{4}{3}\pi r^3}{a^3}$$ ---------- (1)

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<th>SC</th>
<th>BCC</th>
<th>FCC</th>
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<tr>
<td>For the SC cell, Z=1 and a = 2r,
Volume of spherical atom
$= v = \frac{4}{3}\pi r^3$
Total Volume of unit cell,
$V = a^3$
$= (2r)^3$
$= 8r^3$
Substituting the value of Z, v and V, we get in eqn. 1
$\therefore APF = \frac{1 \times \frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6}$
$\boldsymbol{APF = 0.52}$
Void space% = (1-APF) ×100
= (1-0.52) ×100
= 48%</td>
<td>For BCC, $Z = 2$ and $a = \frac{4r}{\sqrt{3}}$
Volume of spherical atom
$= v = \frac{4}{3}\pi r^3$
Total Volume of unit cell, V
$= a^3$
$= 64\frac{r}{3\sqrt{3}}^3$
Substituting the value of Z, v and V, we get
$\therefore APF = \frac{2 \times \frac{4}{3}\pi r^3}{64\frac{r}{3\sqrt{3}}^3} = \frac{\pi\sqrt{3}}{8}$
$\boldsymbol{APF = 0.68}$
Void space% = (1-APF) ×100
= (1-0.68) ×100
= 32%</td>
<td>In case of FCC cell,
$Z = 4$ and $a = 2\sqrt{2}\,r$,
Total Volume of unit cell = a^3
$= (2\sqrt{2}r)^3 = 16\sqrt{2}r^3$
Volume of spherical atom, v
$= \frac{4}{3}\pi r^3$
Substituting the value of Z, v and V, we get
$\therefore APF = \frac{4 \times \frac{4}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}}$
$\boldsymbol{APF = 0.74}$
Void space% = (1-APF) ×100
= (1-0.74) ×100
= 26%</td>
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From above results, we conclude that FCC structure possesses maximum packing density (APF) and minimum percentage of void space compared to BCC and FCC.
</td><td></td></tr>
<tr><td>8</td><td>Calculate the atomic radii and packing fractions for Body Centred and Face Centred Cubic Unit Cell.
Ans. As given in earlier questions.</td><td>4</td></tr>
<tr><td>9</td><td>Define Miller Indices. What are the steps of finding miller indices?
Definition: "Miller indices are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to the smallest integers".
4.8.1. STEPS TO FIND OUT MILLER INDICES
The Miller indices of crystallographic axes are determined using the following steps:
Step 1: Determine the intercepts made by the plane on crystallographic axes. The intercepts are expressed as integral multiples of the axial lengths.
Step 2: Take the reciprocals of the integers of the intercepts.
Step 3: Reduce the reciprocals into the smallest set of integers h, k and l by multiplying each reciprocal with LCM of their denominator.
Step 4: Enclose the integers in parenthesis without commas (h k l).
For example: -In a crystal, let a lattice plane cut the intercepts at 2a, 1b, 2c along x, y, z axes, where a, b, c are primitive vectors of the unit cell.
Solution:
Step 1: - The intercepts are (2a, 1b, 2c). The integers are 2, 1, 2
Step 2: – The reciprocal of intercepts are $\frac{1}{2}, \frac{1}{1}, \frac{1}{2}$
Step 3: - Multiplying by LCM we get 1, 2, 1</td><td>3</td></tr>
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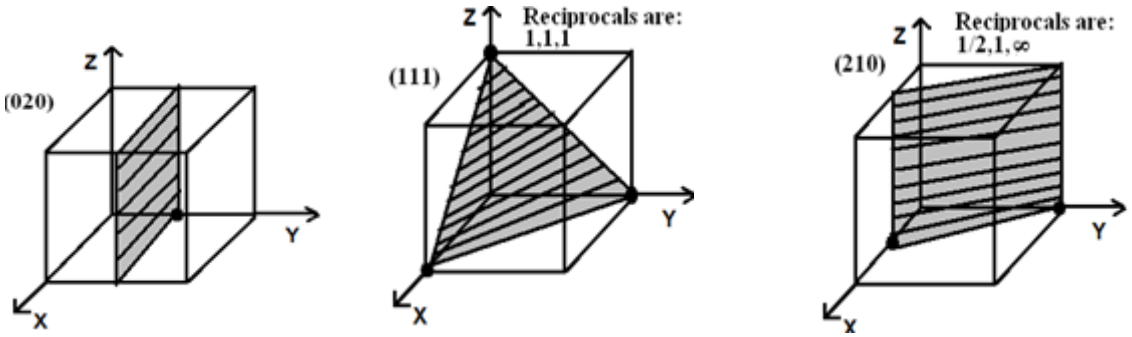
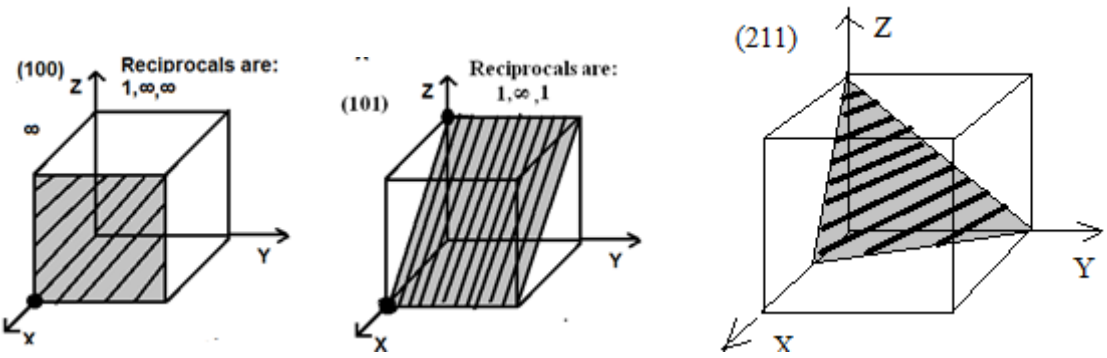
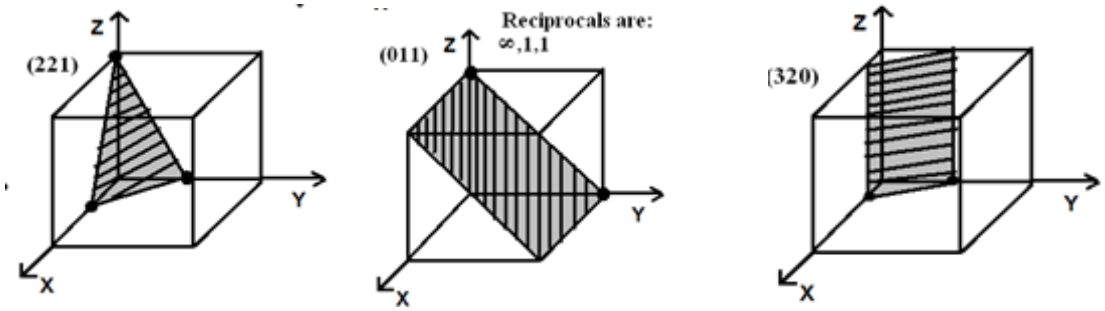
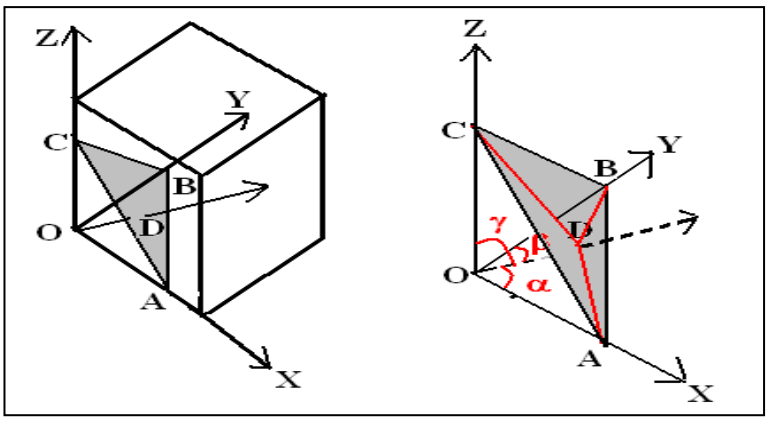
	Step 4: - The miller indices of the given plane are (121)	
10	Draw crystal planes in cubic crystal for Miller Indices (020), (111) and (210). 	3
11	Draw the planes for miller indices (100), (101) and (211) in a cubic crystal. 	3
12.	Draw crystal planes in a cubic crystal for given Miller Indices: (221), (001) and (320). 	3
13.	Derive the relation between lattice constant (a), Interplanar spacing (d) and Miller indices (hkl). Consider two parallel crystallographic planes of a cubic crystal structure having miller indices (**hkl**).  Fig. : Determination of inter planar distance in a cubic crystal	3

	Let one of the planes be passing through origin 'O' and the next plane ABC makes intercepts OA, OB and OC along the three crystallographic axes X, Y and Z respectively as shown in fig. Then the interceps on axes X, Y, Z respectively will be $\mathrm{OA} = \frac{a}{h}, \quad \mathrm{OB} = \frac{b}{k} \quad \text{and} \quad \mathrm{OC} = \frac{c}{l}$ Since, for a cubic crystal, $a = b = c$ $\mathrm{OA} = \frac{a}{h}, \quad \mathrm{OB} = \frac{b}{k} \quad \text{and} \quad \mathrm{OC} = \frac{c}{l}$ Where '**a**' is lattice constant of the cubic crystal. Draw a perpendicular OD from origin to the second plane, such that OD is the interplanar distance. Let the interplanar distance OD be equal to 'd' and the direction cosines of OD cos α, cos β and cos γ. $\angle \mathrm{ODA} = \angle \mathrm{ODB} = \angle \mathrm{ODC} = 90°$. In right angled triangle ΔODA, $\angle \mathrm{ODA} = 90°$ and $\angle \mathrm{DOA} = \alpha$, hence $\cos\alpha = \frac{OD}{OA} = \frac{d}{\frac{a}{h}} = \frac{dh}{a}$ $\cos\beta = \frac{OD}{OB} = \frac{d}{\frac{a}{k}} = \frac{dk}{a}$ $\cos\gamma = \frac{OD}{OC} = \frac{d}{\frac{a}{l}} = \frac{dl}{a}$ By law of direction cosines, the sum of the squares of directional cosines of a line is equal to unity. Thus, $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$ $\therefore \left(\frac{\mathrm{dh}}{\mathrm{a}}\right)^2 + \left(\frac{\mathrm{dk}}{\mathrm{a}}\right)^2 + \left(\frac{\mathrm{dl}}{\mathrm{a}}\right)^2 = 1$ $\frac{\mathrm{d}^2}{\mathrm{a}^2}(\mathrm{h}^2 + \mathrm{k}^2 + \mathrm{l}^2) = 1$ $\mathrm{d}^2 = \frac{\mathrm{a}^2}{(\mathrm{h}^2 + \mathrm{k}^2 + \mathrm{l}^2)}$ $\therefore \boldsymbol{d_{hkl}} = \frac{\boldsymbol{a}}{\sqrt{(\boldsymbol{h^2 + k^2 + l^2})}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.31)$	
14.	Obtain an expression for interplanar spacing between two adjacent planes of Miller indices (hkl) in a cubic crystal. Same answer as given above.	4
15	Derive Bragg's law of X-Ray diffraction. Why are X-rays used to study diffraction in crystals? Consider a set of parallel Bragg's plane MN, PQ and RS separated by interplanar distance 'd' as shown in fig. 4.20. Let a beam of monochromatic x-rays of wavelength '**λ**' represented by AB and DE be incident on these planes. The scattered beam emerges from the atoms of the planes PQ and RS along BC and EF respectively.	4

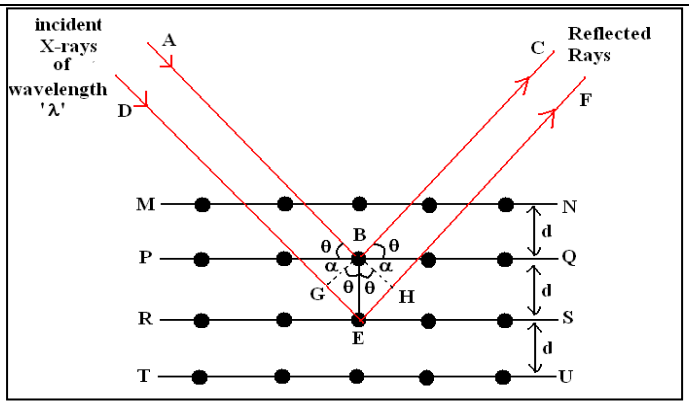


Fig.: Diffraction of X-rays

From the geometry of the fig., the path-difference Δ between the reflected rays BC and EF is,

$$\Delta = GE + EH \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

$$\angle ABG = \theta + \alpha = 90° \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

BE is normal to the plane PQ,

$$\therefore \angle PBE = \alpha + \angle GBE = 90° \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

From eqns. (2) and (3), we get,

$$\angle GBE = \theta$$

Similarly, $\angle EBH = \theta$

Now, In Δ BGE, $\sin\theta = \frac{GE}{BE} = \frac{GE}{BE}$

But, $BE = d$

$\therefore GE = d\sin\theta$

Similarly, in Δ EBH,

$EH = d\sin\theta$

$\therefore$ The path difference, $\Delta = GE + EH = d\sin\theta + d\sin\theta$

$$\Delta = 2\,d\sin\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.35)$$

The rays BC and EF will **interfere constructively** only when, their path difference $\Delta = n\lambda$,

where, n = 1, 2, 3,.....is the order of reflection.

$$\therefore \mathbf{2\,d\sin\theta = n\lambda} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.36)$$

This equation is Bragg's law, where θ is the called glancing angle of reflection.

Why are X-rays used to study diffraction in Crystals?

X rays have wavelength(~1Å) which is comparable to that of interatomic spacing. The condition of diffraction gets satisfied hence X-rays used to study diffraction in crystals.

16.	Derive Bragg's law of X-ray diffraction in crystals. State any one application of it. Derivation as given above. Application: It is used to determine crystal structure.	4
17.	State and derive Bragg's law of X-Ray diffraction. Why it is not useful in amorphous solids?	4

	W.H. Bragg and W. L. Bragg derived a simple relationship between the wavelength of incident monochromatic X-rays (λ) to the angular position of the scattered beams (θ) and the interplanar distance in the crystal (d) as $2d\sin\theta = n\lambda$ where, n is the order of reflection, This, relationship is called as Bragg's law. Derivation: As given in Q.no.15. Why it is not useful in amorphous solids? Amorphous solids have irregular arrangement of atoms. Hence the diffraction pattern obtained using amorphous solids is not a proper one compared to that obtained with crystals where there is regular three-dimensional periodic arrangement of atoms.	
18.	Calculate the effective number of atoms per unit cell in SC, BCC and FCC unit cells.	3
19.	In a cubic lattice, prove that: $\boldsymbol{d_{hkl} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}}$ where d_{hkl} is the interplanar distance, a is lattice constant and h, k, l are the Miller Indices. Answer is same as that for question no.13	3
20.	Aluminium has FCC structure. Its density is 2700 kg /m^3. Calculate the unit cell dimension and the atomic diameter. The atomic weight of Aluminium = 26.98. **Given:** For FCC structure, Z=4 Density (ρ) =2700 kg/m^3 Atomic weight M =26.98 $N_A = 6.023\times10^{26}$ atoms /k mol Unit cell dimension a=? Atomic diameter =? **Solution**: $\text{Density}(\rho) = \frac{ZM}{N_A a^3}$ $2700 = \frac{4 \times 26.98}{6.023 \times 10^{26} \times a^3}$ $a^3 = \frac{4 \times 26.98}{6.023 \times 10^{26} \times 2700} = 6.636 \times 10^{-29}$ $a = 4.049 \times 10^{-10} m = 4.049 Å$ For FCC structure, $r = \frac{a}{2\sqrt{2}} \times 4.049 Å = 1.4315 Å$ Atomic diameter $= 2r = 2 \times 1.4315\ Å = 2.863\ Å$	3
21.	X-ray with a wavelength of 1.54A^o is used to calculate the spacing of plane (200) in Aluminium. The Bragg's angle for this reflection is 22.4^0. What is the size of the unit cell of the Aluminium crystal? **Given:** (h k l) = (2 00), $\lambda = 1.54\ Å$, $n = 1, \quad \theta = 22.4°$, Find, a = ?	3

	Solution: From Bragg's Law, $2d\sin\theta = n\lambda$ For n = 1, $2d\sin\theta_1 = \lambda$ $\therefore d = \frac{\lambda}{2\sin\theta_1} = \frac{1.54\text{ Å}}{2\times\sin 22.4^0} = 2.020\text{Å}$ Since $d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$ Hence $a = d\times\sqrt{(h^2+k^2+l^2)}$ $= 2.020\text{Å}\times\sqrt{(2^2+0^2+0^2)} = 2.020\text{Å}\times 2 = 4.040\text{ Å}$	
22.	The density of copper is 8980 kg / m^3 and unit cell dimension is 3.61 Å. Atomic weight of copper is 63.54. (i)Determine crystal structure (ii) Calculate atomic radius. **Given:** Density (ρ) = 8980 kg/m^3 Atomic weight of Cu= M = 63.54 $N_A = 6.023\times10^{26}$ atoms /k mol Unit cell dimension a=**3.61** Å = 3.61×10^{-10}m Atomic radius =? Crystal structure =? $d_{110} = ?$ **Solution**: Density(ρ) $= \frac{ZM}{N_A a^3}$ $8980 = \frac{Z\times 63.54}{6.023X10^{26}\times(3.61\times10^{-10})^3}$ $Z = \frac{6.023\times10^{26}X(3.61\times10^{-10})^3\times 8980}{63.54} = 4$ Since Z=4, Cu has FCCstructure. For fcc structure, $r = \frac{3.61\text{Å}}{2\sqrt{2}} = 1.276\text{Å}$	4
23.	X- rays of unknown wavelength give first-order Bragg reflection at glancing angle 20º with (212) planes of copper having F.C.C. structure. Find the wavelength of X-rays if the lattice constant for copper is 3.615 Å. **Ans.Given:** a = 3.615 Å Miller indices (h k l) = (212), θ =20°, Order of reflection n=1 Wavelength of X − rays = λ =? **Solution**: $d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$ $d_{(212)} = \frac{3.615\text{Å}}{\sqrt{(2^2+1^2+2^2)}} = 1.205\text{ Å}$ According to Bragg's law, $2d\sin\theta = n\lambda$ For n = 1, $2\times 1.205\text{ Å}\times\sin 20° = \lambda$ $\lambda = 0.842\text{ Å}$	4

24.	Sodium crystallizes in a cubic lattice. The edge of the unit cell is 4.3 A. The density of sodium is 963 kg/m^3, its atomic weight being 23. What type of unit cell does sodium form? **Ans. Given:** Density **(**ρ) $= 963\ kg/m^3$ Atomic weight of Na= M = 23 N_A =6.023X10^{26} atoms /kmol Unit cell dimension a =**4.3** Å =4.3× 10^{-10}m Type of unit cell sodium forms =? **Solution**: Density (ρ) $= \frac{ZM}{N_A a^3}$ $$\rho = \frac{Z \times 23}{6.023 \times 10^{26} \times (4.3 \times 10^{-10})^3}$$ $$Z = \frac{6.023 \times 10^{26} \times (4.3 \times 10^{-10})^3 \times 963}{23} = 2$$ Since Z =2, Sodium forms BCC structure.	3
25.	Find the spacing of (2 1 2) and (0 3 0) planes in a FCC crystal having lattice constant 5 Å and also find radius. **Ans. Given:** a=5Å $d_{(212)}$ =?, $d_{(030)}$ =?and atomic radius 'r'=? **Solution**: $d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$ $$d_{(212)} = \frac{5Å}{\sqrt{(2^2+1^2+2^2)}} = 1.66\ Å$$ $$d_{(030)} = \frac{5Å}{\sqrt{(0^2+3^2+0^2)}} = 1.66\ Å$$ For fcc structure, $r = \frac{a}{2\sqrt{2}} = \frac{5Å}{2\sqrt{2}} = 1.76\ Å$	4
26	X- rays of wavelength 1.5 Å are incident on NaCl crystal having a grating spacing of 2.8 Å. What is the highest order that the crystal can diffract? **Ans. Given:** λ = 1.5 Å, d = 2.8 Å, highest order n =? **Solution**: For highest order n, θ = 90° According to Bragg's law, 2d sin θ = nλ $2 \times 2.8\ Å \times \sin 90° = n \times 1.5\ Å$ Hence $n = \frac{2 \times 2.8}{1.5} = 3.73 \approx 3$	3
27.	Show that FCC is more closely packed than BCC structure.	

Atomic packing fraction (APF): The fraction of space occupied by atoms in a unit cell is known as atomic packing fraction. It is defined as the ratio of volume occupied by the atoms in a unit cell (v) to the total volume of the unit cell (V).

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

$$= \frac{(\text{No.of atoms per unit cell})(\text{Volume of each atom})}{\text{Total Volume of unit cell}} = \frac{Zv}{V} = \frac{Z \times \frac{4}{3}\pi r^3}{a^3} \quad \text{---------- (1)}$$

BCC	FCC
For BCC, $Z = 2$ and $a = \frac{4r}{\sqrt{3}}$ Volume of spherical atom $= v = \frac{4}{3}\pi r^3$ Total Volume of unit cell, $V = a^3$ $= 64\frac{r}{3\sqrt{3}}^3$ Substituting the value of Z, v and V in equation 1, we get $\therefore APF = \frac{2 \times \frac{4}{3}\pi r^3}{64\frac{r}{3\sqrt{3}}^3} = \frac{\pi\sqrt{3}}{8}$ $\boldsymbol{APF = 0.68}$	In case of FCC cell, $Z = 4$ and $a = 2\sqrt{2}\,r$, Total Volume of unit cell = $a^3 = (2\sqrt{2}r)^3 = 16\sqrt{2}r^3$ Volume of spherical atom, $v = \frac{4}{3}\pi r^3$ Substituting the value of Z, v and Vin equation1, we get $\therefore APF = \frac{4 \times \frac{4}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}}$ $\boldsymbol{APF = 0.74}$

From above results, we conclude that APF of FCC unit cell is greater than that of BCC.