

Engineering Physics: Semester I

Unit - III: Crystal Structure

States of matter and types of solids

Matter basically exists in three states- solid, liquids, gases. The other two states are plasma and liquid crystal.

Solids are of two types: Crystalline and Amorphous.

Crystal structure

Meaning of lattice and basis

Unit cell: Primitive and Non primitive unit cell and lattice parameters.

Q1. Explain the following terms i) Space lattice (ii) Unit cell. (2) (S-13)

Q2. Define i) Space lattice (W-14, W-15) (ii) Unit cell (2) (S-14, S-16, W-16, S-18)

Ans (i) Space Lattice

A regular periodic arrangement of points in a three dimensional space such that each point is having an identical surrounding is called a space lattice.

(ii) Unit cell

The smallest fundamental building block of the space lattice is called a unit cell. It has the minimum volume. The regular periodic repetition of this unit cell in a three dimensional space generates the complete space lattice. Two types of unit cell are-Primitive and Non-Primitive unit cell.

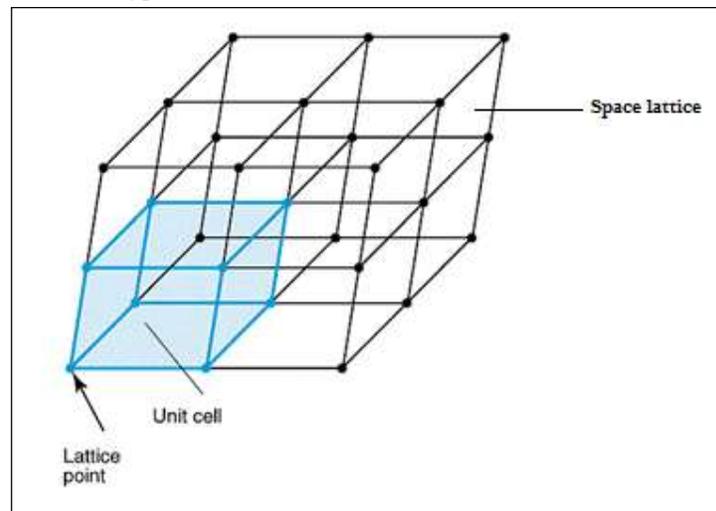


Figure1: Space lattice and Unit cell

The two types of unit cell are 1) **Primitive**- Atoms are present only at corners of unit cell.

For eg. Simple cubic cell (sc)

2) **Non-primitive**-Atoms are present at corners as well as at others places in the unit cell.

For eg. Body centered cubic (bcc) and face centered cubic (fcc).

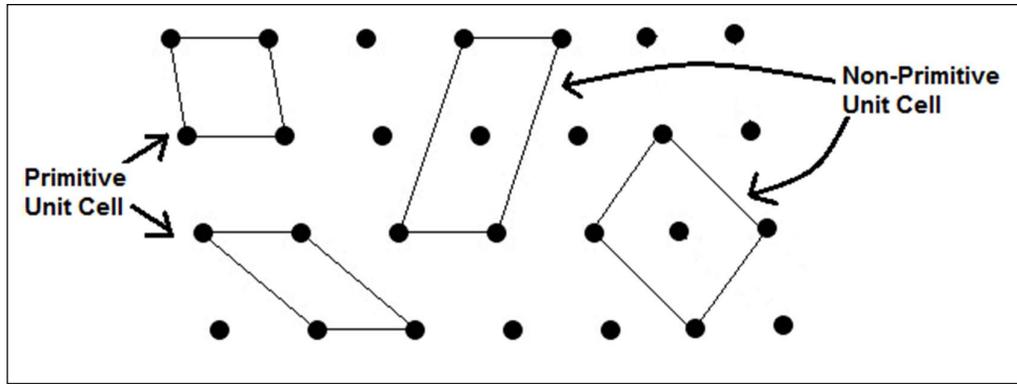


Figure2: Primitive and Non-Primitive Unit Cell.

Extra: Explain: Lattice + Basis = Crystal Structure

Ans.

Space Lattice- A regular periodic arrangement of points in a three dimensional space such that each point is having an identical surrounding as that of the other is called a space lattice.

Basis- An atom or a group of atoms identical in composition, orientation and arrangement which when arranged on the points of the space lattice in a regular periodic manner generates the complete crystal structure is called a basis.

Hence Space Lattice + Basis = Crystal Structure.

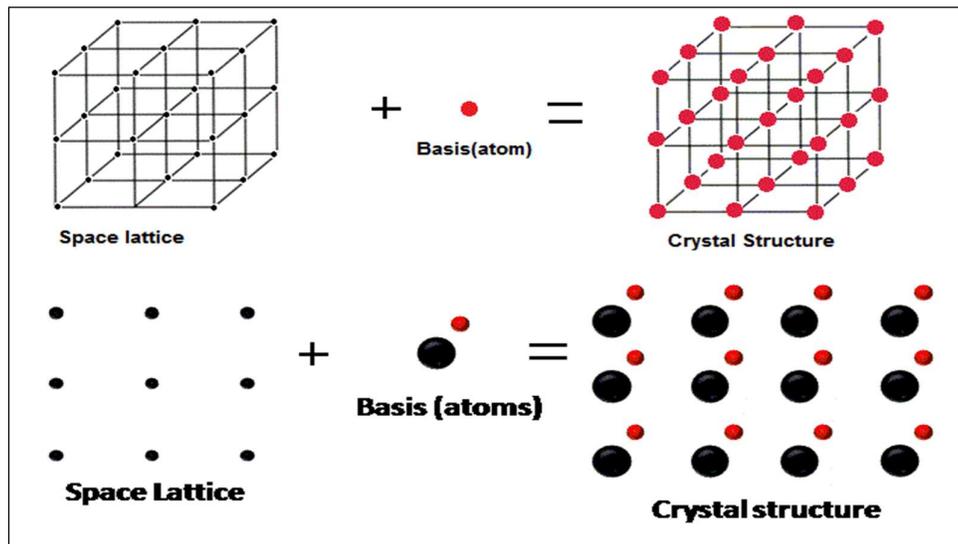


Figure3: Space Lattice + Basis = Crystal Structure.

Unit Cell Lattice parameters

As shown in figure 4, Unit cell is characterized by six lattice parameters i.e. three lattice constants along three crystallographic axes (cube edges) a , b , c and three interfacial angles α , β , γ .

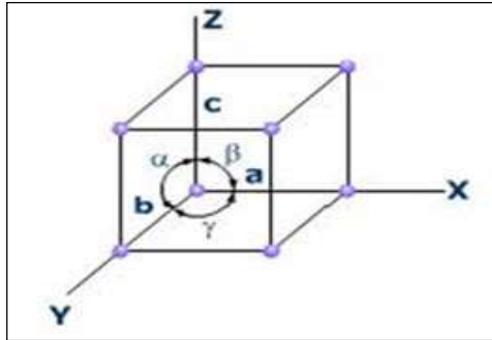


Figure4: Lattice parameters of the unit cell

Bravais' lattices and seven crystal systems

Cubic crystal structure: SC, BCC and FCC unit cells.

French Crystallographer **Bravais**, proposed that there are only 14 possible ways in which lattice points can be arranged in a regular periodic manner in three dimensional space. These 14 different arrangements are called Bravais Lattices. These Bravais lattices are grouped into seven crystal systems namely cubic, monoclinic, triclinic, orthorhombic, trigonal (rhombohedral), tetragonal and hexagonal.

For cubic system, lattice parameters are $a=b=c$ and $\alpha=\beta=\gamma=90^\circ$.

For cubic system, three types of unit cells are as shown in figure 5.

- 1) Simple cubic (sc) 2) Body centered cubic (bcc) 3) Face centered cubic (fcc).

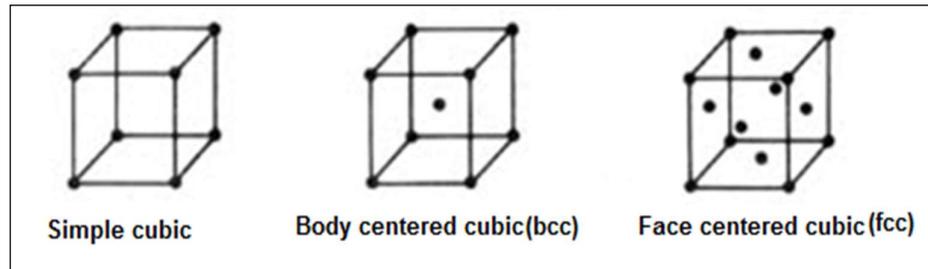


Figure 5: Cubic unit cells (sc, bcc and fcc)

Unit cell characteristics:

- i. Volume(V)
- ii. Effective number of atoms per unit cell(Z),
- iii. Atomic radius(r),
- iv. Coordination number(CN)
- v. Atomic packing fraction(APF) or packing density
- vi. Void space
- vii. Density(ρ)

(i) Volume (V) : For cubic unit cell, all sides are equal, $a=b=c$.

Therefore Volume $V = a \times a \times a = a^3$ for sc, bcc and fcc unit cells.

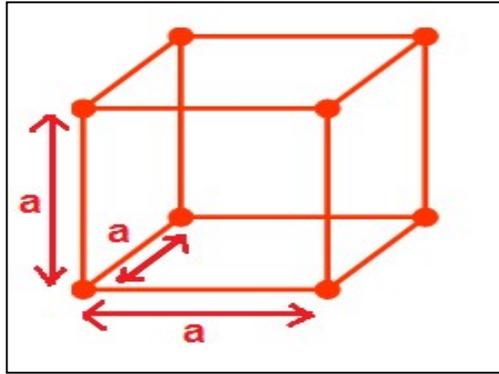


Figure6: Unit cell of side 'a'.

Q3. Define i) Packing fraction(S-14, W-15.S-16) (ii) Coordination number (W-14, W-15,S-16,S-18) (iii) Void space. (S-15.S-18) (3)

Ans.

i) **Atomic packing fraction/packing density**- It is the fraction of space occupied by all atoms in a given unit cell.

It is expressed as
$$APF = \frac{\text{Effective volume of all atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{Zv}{V} = \frac{ZX \frac{4\pi R^3}{3}}{a^3}$$

ii) **Coordination number**-Coordination number of an atom is the number of atoms which are simultaneously in contact with that atom. Coordination number of simple cubic unit cell is 6, for bcc it is 8 and for fcc unit cell its value is 12.

iii) **Void space**- It is the amount of space left unoccupied in a unit cell. It is expressed as

$$\text{Void space \%} = (1 - APF) \times 100\%$$

Q4. Find the atomic radius, packing Fraction and void space for SC cubic crystal structure. (3)

W-14

Ans.

Atomic radius(r):

Since in simple cubic unit cell, corner atoms are in contact each other as shown in figure 7.

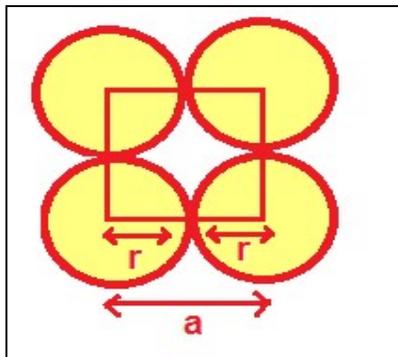


Figure 7: Calculation of atomic radius 'r' in a sc unit cell

Hence $2r = a$ and atomic radius $r = \frac{a}{2}$ ----- (1)

Atomic packing fraction/packing density (APF):

$$APF = \frac{\text{effective volume of all atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{ZXv}{V} = \frac{ZX \frac{4\pi R^3}{3}}{a^3}$$

$Z=1, r = \frac{a}{2}, \therefore a = 2r$

$$APF = \frac{1 \times \frac{4}{3} \pi r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 \text{ ----- (2)}$$

$$\text{Void space \%} = (1-APF) \times 100\% = (1-0.52) \times 100\% = 48\% \text{ ----- (3)}$$

Q5. Define atomic radius and packing fraction. Compute the atomic radius and packing fraction for BCC and FCC unit cell. (4) W-13

Q6. Obtain the following parameters for BCC and FCC cubic unit cell. i) Atomic radius (ii) Packing fraction. (4) W-16, W-17

Q7. Derive expression for atomic radius and atomic packing fraction for BCC and FCC structures and show that percentage void space is more in BCC compared to FCC structure. (6) S-17

Ans. For bcc unit cell,

Calculation of atomic radius (r) –

Atoms are in contact with each other along the body diagonal AG as shown in figure 8.

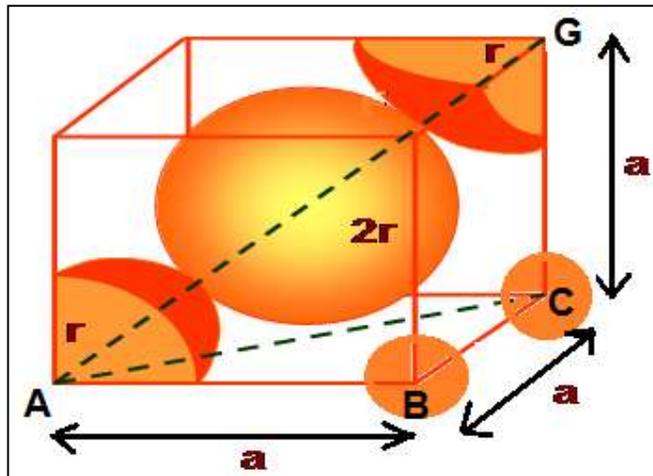


Figure8: Calculation of atomic radius (r) for bcc unit cell.

As shown in figure8, Body diagonal $AG = r + 2r + r = 4r$

In right angle triangle AGC, $AG^2 = AC^2 + CG^2 = (AB^2 + BC^2) + CG^2$

$$(4r)^2 = a^2 + a^2 + a^2$$

$$(4r)^2 = 3a^2$$

$$\text{or } 4r = \sqrt{3} a$$

$$\therefore r = \frac{\sqrt{3} a}{4} \text{ ----- (1)}$$

Calculation of atomic packing fraction (APF) –

Atomic packing fraction/packing density- It is the fraction of space occupied by all atoms in a given unit cell.

$$\text{It is expressed as } APF = \frac{\text{effective volume of all atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{Zv}{V} = \frac{Z \times \frac{4\pi R^3}{3}}{a^3}$$

$$\text{Since } Z = 2, r = \frac{\sqrt{3} a}{4}, \therefore a = \frac{4r}{\sqrt{3}}$$

$$APF = \frac{2 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} = 0.68 \text{ ----- (2)}$$

Void space % = (1-APF) X100% = (1- 0.68) X 100% = 32% ----- (3)

For fcc unit cell,

Calculation of atomic radius (r) –

Atoms are in contact with each other along the face diagonal AC as shown in figure 9.

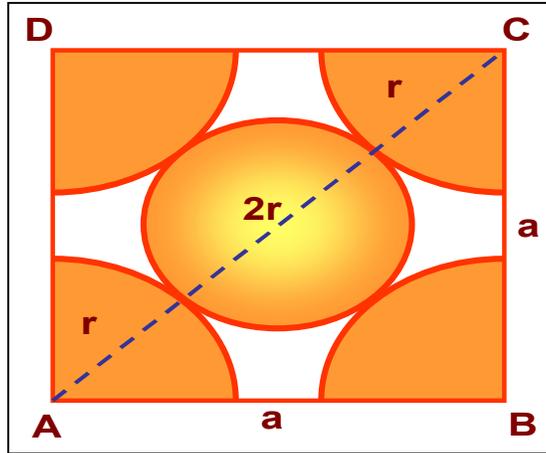


Figure8: Calculation of atomic radius (r) for fcc unit cell.

As shown in figure 9, face diagonal $AC = 4r$

In right angle triangle ABC, $AC^2 = AB^2 + BC^2$

$$(4r)^2 = a^2 + a^2$$

$$(4r)^2 = 2a^2$$

$$\therefore r = \frac{\sqrt{2}a}{4} = \frac{a}{2\sqrt{2}} \text{ ----- (4)}$$

Calculation of atomic packing fraction (APF) –

$$APF = \frac{Zv}{V} = \frac{Z \times \frac{4\pi R^3}{3}}{a^3}$$

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

$$APF = \frac{4 \times \frac{4}{3} \pi r^3}{(2\sqrt{2}r)^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ ----- (5)}$$

Void space % = (1-APF) X100% = (1- 0.74) X 100% = 26% ----- (6)

As shown above percentage void space of bcc unit cell is 32% and that of fcc unit cell is 26%, hence percentage void space is more in BCC compared to FCC structure.

Q8. Show that FCC structure is more closely packed than BCC structure. (4) S-13

Q9. Obtain the values of voids in case of FCC and BCC structures and also show that BCC has maximum voids. (4) S-14

Q10. Show that FCC structure possesses maximum packing density and minimum percentage of void space among BCC and FCC. (4) W-15

Ans. For bcc unit cell,

Calculation of atomic packing fraction (APF) –

Atomic packing fraction/packing density- It is the fraction of space occupied by all atoms in a given unit cell.

It is expressed as $APF = \frac{\text{effective volume of all atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{Zv}{V} = \frac{ZX \frac{4\pi R^3}{3}}{a^3}$

Since $Z=2, r = \frac{\sqrt{3} a}{4}, \therefore a = \frac{4r}{\sqrt{3}}$

$$APF = \frac{2X \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} = 0.68 \text{ ----- (1)}$$

Void space % = (1-APF) X100% = (1- 0.68) X 100% = 32% ----- (2)

For fcc unit cell,

Calculation of atomic packing fraction (APF) –

$$APF = \frac{Zv}{V} = \frac{ZX \frac{4\pi R^3}{3}}{a^3}$$

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

$$APF = \frac{4X \frac{4}{3} \pi r^3}{(2\sqrt{2} r)^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ ----- (3)}$$

Void space % = (1-APF) X100% = (1- 0.74) X 100% = 26% ----- (4)

As shown above atomic packing fraction of bcc unit cell is 0.68 ie.68% and that of fcc unit cell is 0.74 ie. 74%, therefore FCC structure is more closely packed than BCC structure. Also the percentage void space of **bcc** unit cell is 32% and that of **fcc** unit cell is 26%, hence percentage void space is more in BCC compared to FCC structure.

Q11. Calculate the number of atoms per unit cell in SC and BCC lattice. Show that atomic density of BCC is double that of SC unit cell. (3) W-13

Ans.

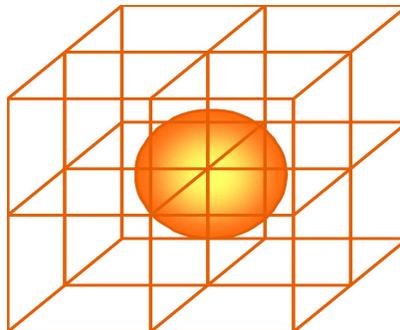


Figure10. Calculation of effective number of atoms (Z) for sc unit cell.

1) Calculation of number of atoms per unit cell in SC lattice: The effective number of atoms per unit cell(Z) is expressed as

$$Z = (\text{number of atoms per lattice point}) \times (\text{No. of lattice points per unit cell})$$

As shown in figure 10, each corner atom is in contact with corners of 8 unit cells,

$$\therefore Z = \left(\frac{1}{8}\right) \times (8) = 1.$$

Calculation of number of atoms per unit cell in bcc lattice:

For bcc unit cell, apart from corner atoms, body centered atom belongs to unit cell as whole (figure 11),

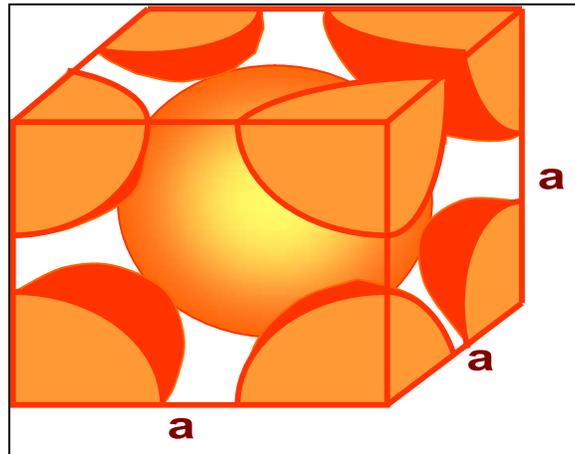


Figure11. Calculation of effective number of atoms (Z) for bcc unit cell.

$$\therefore Z = \left(\frac{1}{8}\right) \times (8) + 1(\text{body centered atom}) = 1 + 1 = 2.$$

2) Calculation of atomic density (ρ) for sc and bcc unit cell:

$$\text{Density } (\rho) = \frac{\text{effective mass of all atoms}}{\text{volume of unit cell}} = \frac{Z \times \text{mass of each atom}}{a^3} = \frac{Z \times W}{a^3} = \frac{Z \times \left(\frac{M}{N_A}\right)}{a^3}$$

where M is the molecular weight of the element
and N_A is the Avogadro's number = 6.023×10^{26} atoms/k mol

$$\text{for sc unit cell, } Z=1, \quad \therefore \text{Density } (\rho) = \frac{Z \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{1 \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{M}{N_A a^3}$$

$$\text{for bcc unit cell, } Z=2, \quad \therefore \text{Density } (\rho) = \frac{Z \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{2 \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{2M}{N_A a^3}$$

Therefore atomic density of BCC is double that of SC unit cell.

Extra: Calculation of no. of atoms of fcc unit cell and atomic density of fcc unit cell.

Ans. Calculation of number of atoms per unit cell in fcc lattice:

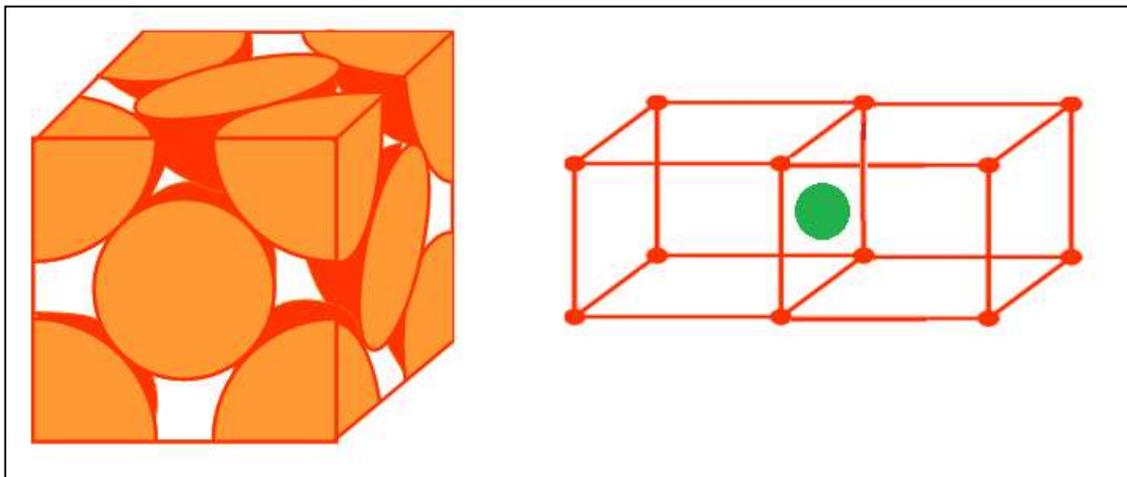


Figure12. Calculation of effective number of atoms (Z) for fcc unit cell.

As shown in figure 12, each corner atom is in contact with corners of 8 unit cells and each face centered atom is shared by two unit cells

Z = (Number of atoms per lattice point) X (No. of lattice points per unit cell) + (number of atoms per face) X (No. of faces per unit cell).

$$\therefore Z = \left(\frac{1}{8}\right) \times (8) + \left(\frac{1}{2}\right) \times 6 = 1+3 = 4.$$

2) Calculation of atomic density (ρ) for fcc unit cell:

$$\text{Density } (\rho) = \frac{\text{effective mass of all atoms}}{\text{volume of unit cell}} = \frac{Z \times \text{mass of each atom}}{a^3} = \frac{Z \times W}{a^3} = \frac{Z \times \left(\frac{M}{N_A}\right)}{a^3}$$

where M is the molecular weight of the element
and N_A is the Avogadro's number = 6.023×10^{26} atoms/k mol

for fcc unit cell, $Z=4$, \therefore Density (ρ) = $\frac{Z \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{4 \times \left(\frac{M}{N_A}\right)}{a^3} = \frac{4M}{N_A a^3}$

Q12. Show that the FCC structure possesses maximum percentage of packing density among SC, BCC and FCC. (5)

S-15

Q13. Show that FCC structure has maximum packing density among all cubic unit cell.(4) (S-16,S-18)

Ans. **Atomic packing fraction/packing density-** It is the fraction of space occupied by all atoms in a given unit cell.

It is expressed as $APF = \frac{\text{effective volume of all atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{Zv}{V} = \frac{Z \times \frac{4\pi R^3}{3}}{a^3}$

For sc unit cell, $Z=1$, $r = \frac{a}{2}$, $\therefore a = 2r$

$$APF = \frac{1 \times \frac{4}{3} \pi r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 \text{ --- (1)}$$

and Void space % = $(1-APF) \times 100\% = (1-0.52) \times 100\% = 48\% \text{ ----- (2)}$

For bcc unit cell, Since $Z=2$, $r = \frac{\sqrt{3}a}{4}$, $\therefore a = \frac{4r}{\sqrt{3}}$

$$APF = \frac{2 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} = 0.68 \text{ --- (3)}$$

Void space % = $(1-APF) \times 100\% = (1-0.68) \times 100\% = 32\% \text{ ----- (4)}$

For fcc unit cell, Since $Z=4$, $r = \frac{a}{2\sqrt{2}}$, $\therefore a = 2\sqrt{2}r$

$$APF = \frac{4 \times \frac{4}{3} \pi r^3}{(2\sqrt{2}r)^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ --- (5)}$$

Void space % = $(1-APF) \times 100\% = (1-0.74) \times 100\% = 26\% \text{ ----- (6)}$

Therefore the packing density of fcc (74%) is maximum compared to that of sc (52%) and bcc (68%) unit cells. The void space % of fcc (26%) is found to be least compared to that of sc (48%) and bcc (32%) unit cells.

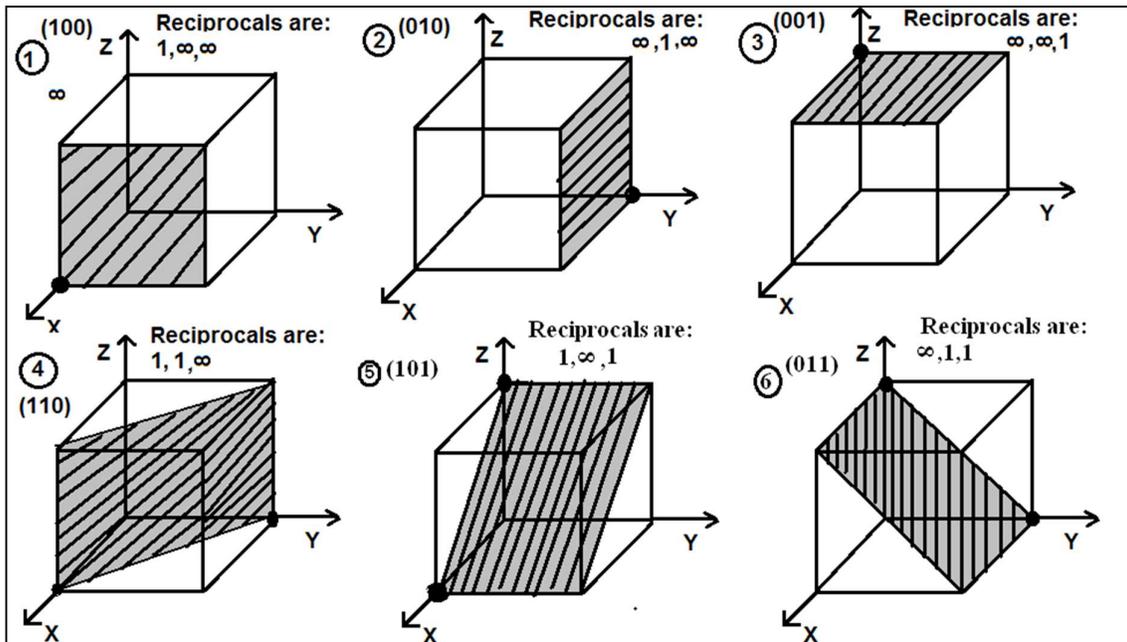
Crystal planes and Miller indices,

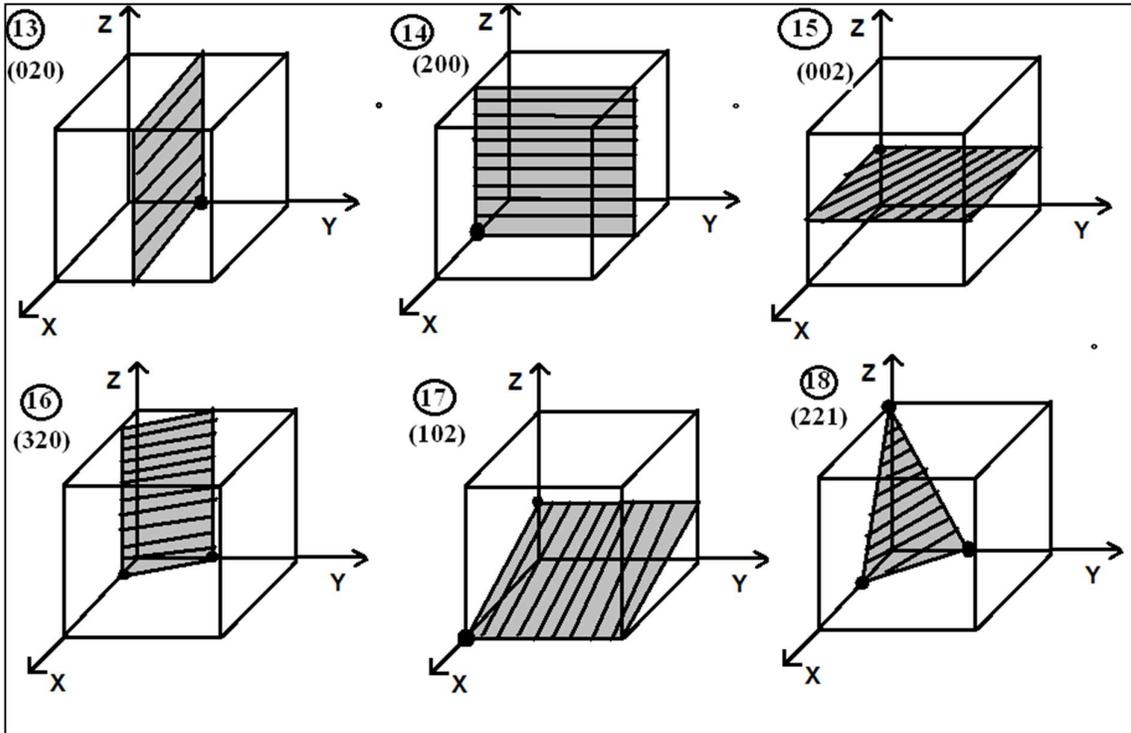
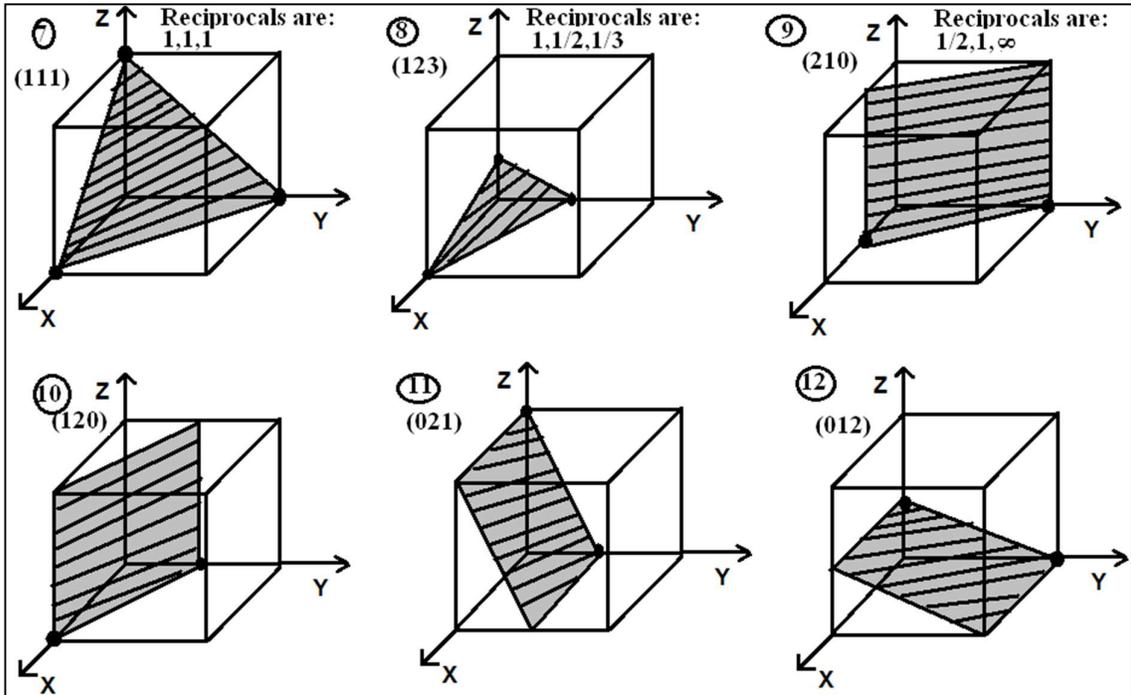
- Q14. Define (i) Miller Indices of the plane. (1)S-14, W-16
- Q15. What are Miller indices? Draw planes (2 1 0) and (0 1 0) for simple cubic structure. (3) W-15
- Q16. What are Miller indices? Draw the planes (02 0), (2 1 0). (3) S-15
- Q17. Draw the crystal planes in cubic crystal for given miller indices.
 i) (2 2 1) ii) (0 0 1) iii) (3 2 0) (3) W-16
- Q18. What are Miller indices? Draw the crystal planes in simple cubic structure having miller indices i) (102) (ii) (010). (3) S-17
- Q19. Draw following planes in a cubic unit cell.(112),(010) and (120) (3) W-2017
- Q 20. What are Miller indices? Draw planes (10 0) and (11 1) for simple cubic structure. (3) S-18

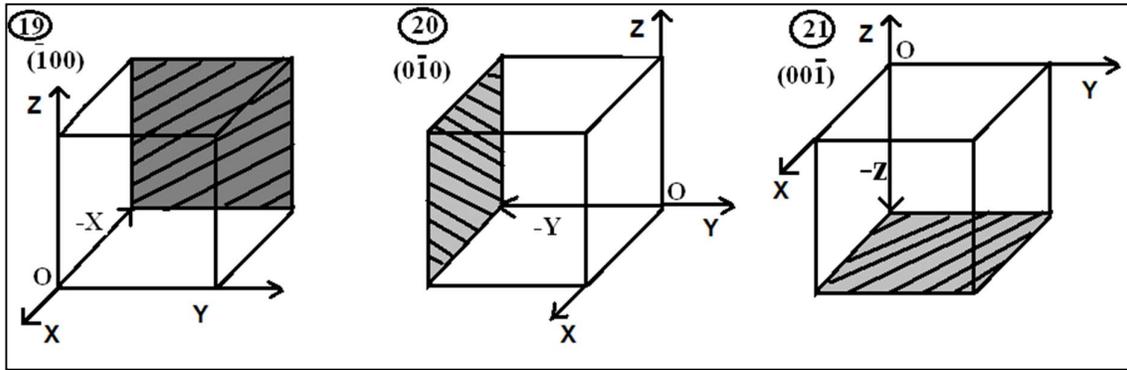
Ans.

Miller indices are the reciprocals of the intercepts made by plane on the crystallographic axes, when reduced to the smallest integers.

To draw various planes in a simple cubic structure:







Extra: How to find miller indices of a given plane?

Let a plane have intercepts $a, 2a, 3a$ on X, Y, Z axes respectively.

Step1: Take intercepts in terms of their axial lengths - 1, 2, 3.

Step2: Take reciprocals of these intercepts – $1, \frac{1}{2}, \frac{1}{3}$

Step 3: Multiply each reciprocal by LCM: $1 \times 6, \frac{1}{2} \times 6 = 3, \frac{1}{3} \times 6 = 2$

Step 4: Write the resulting three integers in a parenthesis without commas: (6 3 2)

Miller indices of given plane are (6 3 2).

Inter-planar distance between adjacent planes.

Q21. Obtain the relation between interplanar distance ‘d’ and Miller indices of the plane for a cubic crystal. (3) S-13

Q22. What are Miller indices? Obtain the relation between interplanar distance ‘d’ and Miller indices of the planes for a cubic crystal. (3) W-13

Q23. Derive the relation between interplanar distance ‘d’ and Miller indices of the planes for a cubic crystal. (4) S-14,W-14

Q24. Obtain an expression for interplanar spacing between two adjacent planes of Miller Indices (hkl) in a cubic crystal. (3)

S-15

Q25. Derive the relation between lattice constant and interplanar spacing in cubic unit cell.

(4) S-16,S-18

Q 26. Derive the relationship between interplaner distance ,lattice constant and Miller indices of the planes for a cubic cell. (4) W-17

Ans.

Miller indices are the reciprocals of the intercepts made by plane on the crystallographic axes, when reduced to smallest integers.

Interplanar spacing/distance is the distance between successive members of series of parallel planes.

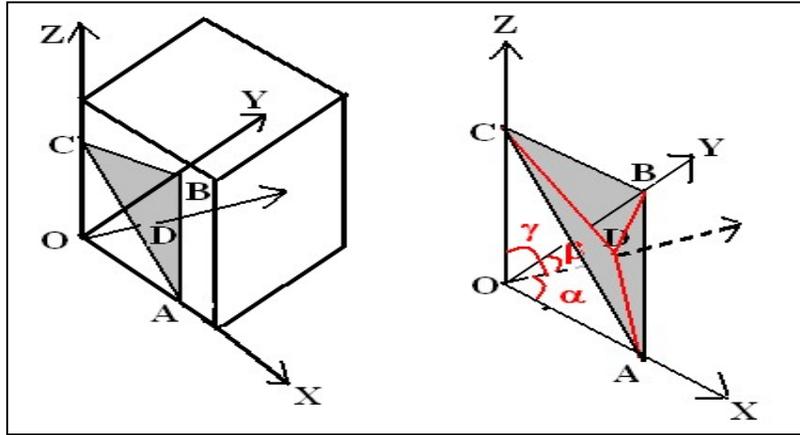


Figure 14: Relation between interplanar spacing 'd', lattice constant 'a' and miller indices h, k, l.

Consider a cubic crystal of side 'a' as shown in figure 14. Let the plane ABC be one of the planes with intercepts $OA = \frac{a}{h}$, $OB = \frac{a}{k}$ and $OC = \frac{a}{l}$ on X, Y, Z axes respectively. Let the next plane of set parallel to ABC pass through origin of the coordinates 'O'. Draw a perpendicular from O to the plane ABC. Let it be OD.

$OD = d_{hkl} =$ interplanar spacing. Let the direction cosines of OD be $\cos \alpha$, $\cos \beta$ and $\cos \gamma$. From the figure 14, $\cos \alpha = \frac{OD}{OA} = \frac{d}{\frac{a}{h}} = \frac{dh}{a}$.

Similarly $\cos \beta = \frac{dk}{a}$ and $\cos \gamma = \frac{dl}{a}$. Since

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$$

$$\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

$$\therefore \frac{d^2}{a^2} (h^2 + k^2 + l^2) = 1$$

$$\text{Or } d^2 = \frac{a^2}{(h^2 + k^2 + l^2)}$$

$$\therefore d = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

Bragg's law of X-ray diffraction

- Q27. Explain and deduce Bragg's law for X-ray diffraction. (4) S-13
 Q28. State and derive Bragg's law of X-ray diffraction. State any one of its application. (4) W-13
 Q29. Derive Bragg's law of X-ray diffraction. (3) W-15
 Q30. State and derive Bragg's law of X-ray diffraction. (4) W-16
 Q31. Derive Bragg's law for diffraction of X-ray from crystal planes. (3) S-16
 Q32. State and derive Bragg's law of X-ray diffraction. (4) S-17
 Q 33. Explain and Deduce Bragg's law of X-ray diffraction. (3) W-17

Ans.

Statement of Bragg's Law: W.H. Bragg and W.L. Bragg derived a simple relationship between wavelength of incident X-rays (λ), angular positions of scattered X-ray beam (θ) and interplanar spacing (d) between the planes in a crystal. It is given by equation

$$n \lambda = 2d \sin \theta.$$

Where 'n' is the order of reflection. This relationship is known as Bragg's law.

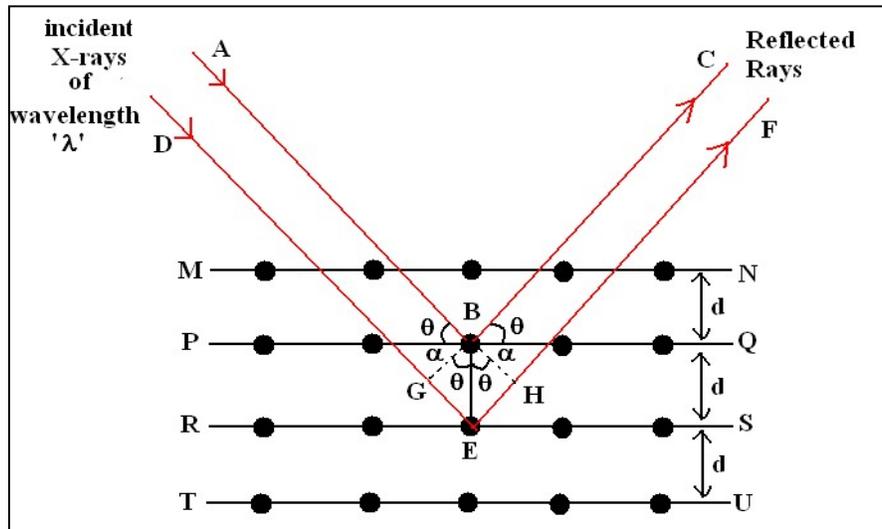


Figure15: Derivation of Bragg's Law

Consider a set of atomic planes with interplanar spacing 'd' as shown in figure 15. Let AB and DE be the parallel monochromatic beam of incident X-rays of wavelength ' λ '. The rays are scattered by atoms at position B and D and are reflected along BC and EF respectively. From the geometry of the figure, the path difference between the reflected rays $\Delta = GE + EH$.

$$\text{Since } \angle ABG = 90^\circ = \theta + \alpha \text{ ----- (1)}$$

$$\text{Also } \angle PBE = 90^\circ = \alpha + \angle GBE \text{ ----- (2)}$$

\therefore From eqns. (1) and (2) we get

$$\theta + \alpha = \alpha + \angle GBE$$

$$\text{or } \angle GBE = \theta.$$

From triangle GBE, $\frac{GE}{BE} = \sin \theta$. Or $GE = BE \sin \theta = d \sin \theta$.

Similarly $EH = d \sin \theta$.

Hence path difference $\Delta = GE + EH = d \sin \theta + d \sin \theta = 2 d \sin \theta$.

For constructive interference between the reflected rays, path difference $\Delta = n \lambda$.

$$\therefore 2 d \sin \theta = n \lambda \text{ ----- (3)}$$

where 'n' is the order of reflection ($n=1,2,3, \dots$).

Equation 3 is known as Bragg's Law.

Application: Bragg's law is used to determine crystal structure.

Extra: Q Why is Bragg's law not useful in case of amorphous solids?

Ans. In amorphous solids, atoms are arranged randomly. The interatomic spacing 'a' is not fixed. Hence the condition of occurrence of diffraction is not satisfied ($\lambda \approx a$). Therefore, Bragg's law is not useful for crystal structure determination in case of amorphous solids.

Q Why are X-rays preferred than visible light for crystal structure determination?

Ans. The interatomic spacing in a crystal $\sim 1 \text{ \AA}$ to 2 \AA . The wavelength of X-rays is also of same order. Hence the condition of obtaining diffraction is satisfied by X-rays. The wavelength of visible rays is $\sim 4000 \text{ \AA}$ to 7500 \AA . This is very large compared to interatomic spacing. Therefore the condition of obtaining diffraction is not satisfied. Therefore X-rays are preferred than visible light for crystal structure determination.

Tetrahedral and Octahedral voids.

Extra:Q What are tetrahedral and octahedral voids?

Ans. Tetrahedral Voids

When a sphere fits over the triangular void formed by three spheres in contact with each other of the adjacent layer, the void formed is called tetrahedral Voids. When the centres of these four spheres are joined, the shape of the void is like a tetrahedron. Tetrahedral voids are shown in figure 16. These

voids are of two types- inverted and upright. In a three dimensional structure, there are 2 tetrahedral Voids per sphere.

Octahedral Voids

When a triangular void formed by three spheres in close contact in one layer comes over the top of triangular void formed by three spheres in close contact in adjacent layer, an Octahedral void is formed. When the centres of these six spheres are joined, the shape of the void is like a octahedron. Octahedral Voids are shown in figure 16. In a three dimensional structure, there is one octahedral Void per sphere. These voids are bigger in size but smaller in number compared to tetrahedral voids.

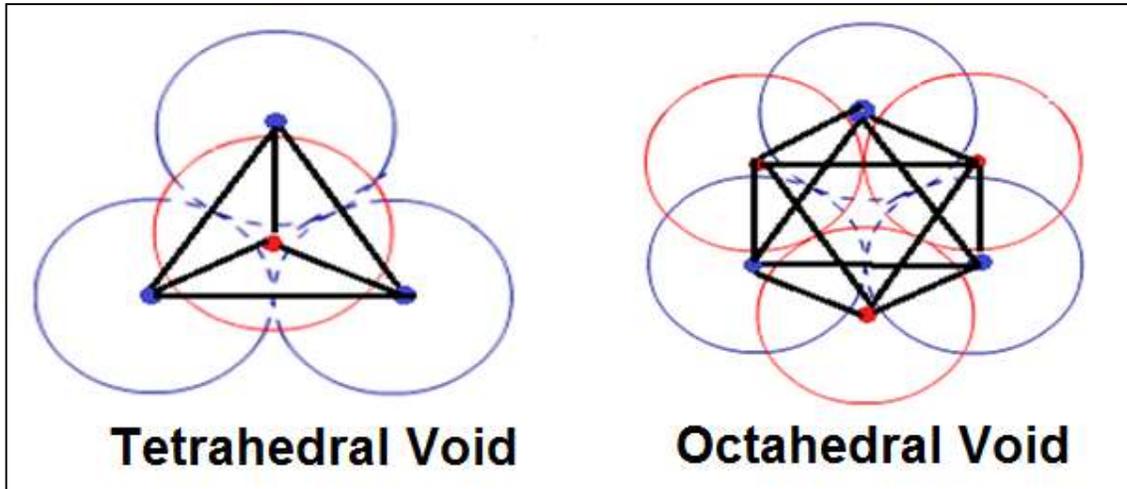


Figure16.Tetraheral and Octahedral Voids

Unit cell characteristics of sc, bcc and fcc unit cells

Unit cell	Volume (V)	Effective no. of atoms per unit cell (Z)	Atomic radius (r)	Atomic packing fraction (APF)	Void space %	Density (ρ)	Coordination number (CN)
sc	a^3	1	$\frac{a}{2}$	0.52	48%	$\frac{M}{N_A a^3}$	6
bcc	a^3	2	$\frac{\sqrt{3}}{4} a$	0.68	32%	$\frac{2M}{N_A a^3}$	8
fcc	a^3	4	$\frac{a}{2\sqrt{2}}$	0.74	26%	$\frac{4M}{N_A a^3}$	12

Numericals

Numericals based on density:

Formulae:

1) Density(ρ) = $\frac{ZM}{N_A a^3}$ where $N_A = 6.023 \times 10^{26}$ atoms /k mol=Avogadro's number.

Point to remember: For such numericals convert Å to 10^{-10} m.

1) Molybdenum has a BCC structure .Its density is $10.2 \times 10^3 \text{ kg/m}^3$.and its atomic weight is 95.94.Determine the radius of molybdenum atom. (3) S-13, S-17,W-10

Ans. Given: for bcc structure, $Z=2$

$$\text{Density } \rho = 10.2 \times 10^3 \text{ kg/m}^3$$

$$\text{Atomic weight } = M = 95.94$$

$$N_A = 6.023 \times 10^{26} \text{ atoms /k mol}$$

$$\text{Atomic radius 'r' } = ?$$

$$\text{Solution: } \rho = \frac{ZM}{N_A a^3}$$

$$10.2 \times 10^3 = \frac{2 \times 95.94}{6.023 \times 10^{26} \times a^3}$$

$$a^3 = \frac{2 \times 95.94}{6.023 \times 10^{26} \times 10.2 \times 10^3} = 3.12176 \times 10^{-29}$$

$$a = 3.218 \times 10^{-10} \text{ m} = 3.218 \text{ \AA}$$

$$\text{For bcc structure, } r = \frac{\sqrt{3}}{4} a = \frac{\sqrt{3}}{4} \times 3.218 \text{ \AA} = 1.393 \text{ \AA}$$

2) Aluminium has fcc structure. Its density is 2700 kg / m^3 . Calculate the unit cell dimension and the atomic diameter. Atomic weight of Aluminium = 26.98.

(4) S-14,W-15,W-15,W-09,W-18

Ans. Given: for fcc structure, $Z=4$

$$\text{Density } \rho = 2700 \text{ kg/m}^3$$

$$\text{Atomic weight } M = 26.98$$

$$N_A = 6.023 \times 10^{26} \text{ atoms /k mol}$$

$$\text{Unit cell dimension } a = ? \text{ and atomic diameter } = ?$$

$$\text{Solution: } \rho = \frac{ZM}{N_A a^3}$$

$$2700 = \frac{4 \times 26.98}{6.023 \times 10^{26} \times a^3}$$

$$a^3 = \frac{4 \times 26.98}{6.023 \times 10^{26} \times 2700} = 6.636 \times 10^{-29}$$

$$a = 4.049 \times 10^{-10} \text{ m} = 4.049 \text{ \AA}$$

$$\text{For fcc structure, } r = \frac{a}{2\sqrt{2}} \times 4.049 \text{ \AA} = 1.4315 \text{ \AA}$$

$$\text{Atomic diameter} = 2r = 2 \times 1.4315 \text{ \AA} = 2.863 \text{ \AA}$$

3) The density of copper is 8980 kg / m^3 and unit cell dimension is 3.61 A. Atomic weight of copper is 63.54. (i) Determine crystal structure (ii) Calculate atomic radius. (3) W-14, S-15, W-12.W-04.

Ans. Given: Density $\rho = 8980 \text{ kg/m}^3$

$$\text{Atomic weight of Cu} = M = 63.54$$

$$N_A = 6.023 \times 10^{26} \text{ atoms /k mol}$$

$$\text{Unit cell dimension } a = 3.61 \text{ \AA} = 3.61 \times 10^{-10} \text{ m}$$

$$\text{Atomic radius } = ? \text{ Crystal structure } = ?$$

$$\text{Solution: } \rho = \frac{ZM}{N_A a^3}$$

$$8980 = \frac{Z \times 63.54}{6.023 \times 10^{26} \times (3.61 \times 10^{-10})^3}$$

$$Z = \frac{6.023 \times 10^{26} \times (3.61 \times 10^{-10})^3 \times 8980}{63.54} = 4$$

Since $Z=4$, Cu has fcc structure.

$$\text{For fcc structure, } r = \frac{3.61 \text{ \AA}}{2\sqrt{2}} = 1.276 \text{ \AA}$$

4) Lattice constant for BCC iron at 20°C is 2.80 Å. Density of iron is 7870 kg/m³. Determine its atomic mass and radius. (4)W-16, S-05

Ans. Given: Density $\rho = 7870 \text{ kg/m}^3$

For bcc structure, $Z=2$

$$N_A = 6.023 \times 10^{26} \text{ atoms /k mol}$$

$$\text{Lattice constant 'a' = } 2.80 \text{ \AA} = 2.80 \times 10^{-10} \text{ m}$$

Atomic radius =? Atomic weight of Iron = $M = ?$

$$\text{Solution: } \rho = \frac{ZM}{N_A a^3}$$

$$7870 = \frac{2 \times M}{6.023 \times 10^{26} \times (2.80 \times 10^{-10})^3}$$

$$M = \frac{6.023 \times 10^{26} \times (2.80 \times 10^{-10})^3 \times 7870}{2} = 56$$

$$\text{For bcc structure, } r = \frac{\sqrt{3}}{4} a = \frac{\sqrt{3}}{4} \times 2.80 \text{ \AA} = 1.212 \text{ \AA}$$

5) Silver has FCC structure and atomic radius 1.441 Å. Calculate density of silver. Atomic weight of silver is 108. (3) S-16

Ans. : Given: For fcc structure, $Z=4$

$$\text{Atomic radius} = r = 1.441 \text{ \AA}$$

$$\text{Atomic weight of Silver} = M = 108$$

$$N_A = 6.023 \times 10^{26} \text{ atoms /k mol}$$

Density $\rho = ?$

$$\text{Solution: } \rho = \frac{ZM}{N_A a^3} \text{ and For fcc structure, } r = \frac{a}{2\sqrt{2}}$$

$$\text{Hence } a = 2\sqrt{2} r = 2\sqrt{2} \times 1.441 \text{ \AA} = 4.075 \text{ \AA} = 4.075 \times 10^{-10} \text{ m}$$

$$\rho = \frac{ZM}{N_A a^3} = \frac{4 \times 108}{6.023 \times 10^{26} \times (4.075 \times 10^{-10})^3} = 10643.9 \text{ kg/m}^3$$

6) Nickel crystallizes in a FCC lattice. The edge of the unit cell is 3.52 Å. The atomic weight being 58.71 kg/k mol. Determine the density of the Nickel. (3) W-17, S-14, S-19

Ans: Given: For fcc structure, $Z=4$

$$\text{Unit cell edge} = a = 3.52 \text{ \AA} = 3.52 \times 10^{-10} \text{ m}$$

Atomic weight of Nickel =M = 58.71

$N_A = 6.023 \times 10^{26}$ atoms /k mol

Density $\rho = ?$

Solution: $\rho = \frac{ZM}{N_A a^3}$

$$\rho = \frac{ZM}{N_A a^3} = \frac{4 \times 58.71}{6.023 \times 10^{26} \times (3.52 \times 10^{-10})^3} = 8944 \text{ kg/m}^3$$

7) Sodium crystallizes in a cubic lattice. The edge of the unit cell is 4.3 Å. The density of sodium is 963 kg/m³, its atomic weight being 23. What type of unit cell does sodium form? (3)W-01

Ans. Given: Density $\rho = 963 \text{ kg/m}^3$

Atomic weight of Na=M = 23

$N_A = 6.023 \times 10^{26}$ atoms /kmol

Unit cell dimension $a = 4.3 \text{ Å} = 4.3 \times 10^{-10} \text{ m}$

Type of unit cell sodium forms =?

Solution: $\rho = \frac{ZM}{N_A a^3}$

$$963 = \frac{Z \times 23}{6.023 \times 10^{26} \times (4.3 \times 10^{-10})^3}$$

$$Z = \frac{6.023 \times 10^{26} \times (4.3 \times 10^{-10})^3 \times 963}{23} = 2$$

Since $Z=2$, Sodium has bcc structure

Numericals on Miller indices and interplanar spacing

Formula : $d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}} = \text{interplanar spacing}$

8) For an FCC cubic crystal, interplanar spacing is 2 Å of (110) plane. Calculate its atomic radius. (3) W-13

Ans. Given: $d=2\text{Å}$

For fcc structure, $r = \frac{a}{2\sqrt{2}}$

Miller indices (h k l) = (110), Atomic radius 'r'=?

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

$$d_{(110)} = 2\text{Å} = \frac{a}{\sqrt{(1^2+1^2+0^2)}} = \frac{a}{\sqrt{2}}$$

$$\therefore a = 2\sqrt{2} \text{ Å} . \text{Hence } r = \frac{a}{2\sqrt{2}} = \frac{2\sqrt{2} \text{ Å}}{2\sqrt{2}} = 1 \text{ Å}$$

9) Find the spacing of (2 1 2) and (0 3 0) planes in a FCC crystal having lattice constant 5Å and also find radius. (3) W-16

Ans. Given: $a=5\text{Å}$, find $d_{(212)}$, $d_{(030)}$ and atomic radius 'r'.

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

$$d_{(212)} = \frac{5\text{\AA}}{\sqrt{(2^2+1^2+2^2)}} = 1.66 \text{\AA}, \quad d_{(030)} = \frac{5\text{\AA}}{\sqrt{(0^2+3^2+0^2)}} = 1.66 \text{\AA}$$

For fcc structure, $r = \frac{a}{2\sqrt{2}} = \frac{5\text{\AA}}{2\sqrt{2}} = 1.76 \text{\AA}$

10) The d_{110} interplanar spacing in a BCC metal vanadium is 2.15A. Find its lattice constant a. (3) S-17

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

$$d_{(110)} = \frac{a}{\sqrt{(1^2+1^2+0^2)}} = \frac{a}{\sqrt{2}} \cdot a = d_{(110)} \times \sqrt{2} = 2.15\text{\AA} \times \sqrt{2} = 3.04 \text{\AA}.$$

11) Find the Miller indices of the atomic planes having intercepts a, 2a and ∞ on x, y and z axes respectively. Find its distance from the origin. (3)W-06

Ans. Intercepts are: a, 2a, ∞

Reciprocals of intercepts are: $\frac{1}{a}, \frac{1}{2a}, \frac{1}{\infty}$

L.C.M =2a

Multiplying by LCM, $\frac{1}{a} \times 2a = 2, \frac{1}{2a} \times 2a = 1, 0$

Miller indices are: (210)

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

$$d_{(210)} = \frac{a}{\sqrt{(2^2+1^2+0^2)}} = \frac{a}{\sqrt{5}}$$

Numericals on interplanar spacing and Bragg's law

Formulae: 1) $d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$ = interplanar spacing

2) $2d \sin\theta = n\lambda$

12) Gold with atomic radius 1.44 A and fcc structure is being used to determine wavelength of X-rays. Calculate the wavelength of X-rays if the (111) plane diffracts the beam by 32°. Assume first order diffraction. (3)S-13 , S-15

Ans. Given: atomic radius r=1.44 A

For fcc structure, $r = \frac{a}{2\sqrt{2}}$

Miller indices (h k l) = (111), $\theta = 32^\circ$, order of reflection n=1

Wavelength of X-rays = $\lambda = ?$

Solution: $r = \frac{a}{2\sqrt{2}}$

$$a = 2\sqrt{2} r = 2\sqrt{2} \times 1.44 \text{\AA} = 4.07 \text{\AA}$$

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

$$d_{(111)} = \frac{4.07\text{\AA}}{\sqrt{(1^2+1^2+1^2)}} = 2.35 \text{\AA}$$

According to Bragg's law, $2d \sin\theta = n\lambda$

$$\text{For } n = 1, 2 \times 2.35 \text{\AA} \sin 32^\circ = \lambda$$

$$\lambda = 2.498 \text{\AA}$$

13) Bragg's Spectrometer is set for the first order reflection to be received by the detector at glancing angle 10° . Calculate the angle through which the detector is rotated to receive the second order reflection for the same face of crystal. (3) W-13

Ans. Given: $n = 1, \theta_1 = 10^\circ$, find θ_2 for $n=2$

Solution: From Bragg's Law, $2d \sin \theta = n \lambda$

$$\text{For } n=1, 2d \sin \theta_1 = \lambda \text{ --- (1) ,}$$

$$\text{For } n=2, 2d \sin \theta_2 = 2\lambda \text{ ----- (2)}$$

$$\text{Dividing eqn.(2) by(1) we get, } \frac{2d \sin \theta_2}{2d \sin \theta_1} = \frac{2\lambda}{\lambda} \text{ or } \frac{\sin \theta_2}{\sin 10^\circ} = 2$$

$$\therefore \sin \theta_2 = 2 \times \sin 10^\circ = 2 \times 0.1736 = 0.3472$$

$$\theta_2 = \sin^{-1}(0.3472) = 20.32^\circ.$$

14) X- rays of unknown wavelength give first order Bragg reflection at glancing angle 20° with (212) planes of copper having F.C.C. structure. Find wavelength of X-rays if the lattice constant for copper is 3.615\AA . (4)S-14, S-08, S-03,S-06

Ans. Given: $a = 3.615 \text{\AA}$

Miller indices $(h k l) = (212)$, $\theta = 20^\circ$, order of reflection $n=1$

Wavelength of X-rays $= \lambda = ?$

$$\text{Solution: } d_{(hkl)} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$$

$$d_{(212)} = \frac{3.615\text{\AA}}{\sqrt{(2^2+1^2+2^2)}} = 1.205 \text{\AA}$$

According to Bragg's law, $2d \sin \theta = n\lambda$

$$\text{For } n = 1, 2 \times 1.205 \text{\AA} \sin 20^\circ = \lambda$$

$$\text{or } \lambda = 0.842 \text{\AA}$$

15) An X-ray beam of wavelength 1.5\AA is diffracted from (110) planes of Nickel crystal. The first order diffraction is obtained at an angle of 27.6 . Determine the lattice constant of the unit cell of Nickel having FCC structure. (3) W-13, W-14, W-07

Ans. Given: $\lambda = 1.5\text{\AA}$, Miller indices $(h k l) = (110)$, $\theta = 27.6^\circ$, order of reflection $n=1$.

$a = ?$

Solution : According to Bragg's law, $2d \sin \theta = n\lambda$

$$\text{For } n=1, 2d \sin 27.6^\circ = 1 \times 1.5\text{\AA}$$

$$d = \frac{1.5\text{\AA}}{2 \times \sin 27.6^\circ} = 1.619 \text{\AA}$$

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

Hence $a = d \times \sqrt{(h^2 + k^2 + l^2)} = 1.619 \text{ \AA} \times \sqrt{(1^2 + 1^2 + 0^2)} = 1.619 \text{ \AA} \times \sqrt{2} = 2.29 \text{ \AA}$.

16) An X-ray beam of wavelength 3 \AA is diffracted from (110) planes of a cubic crystal.

The first order diffraction is obtained at an angle of 40° . Determine the spacing between the (100) planes and the volume of the unit cell. 5) S-09

Ans. Given: $\lambda = 3 \text{ \AA}$, Miller indices (h k l) = (110), $\theta = 40^\circ$, order of reflection $n=1$.

$d_{(110)} = ?$ Volume of the unit cell = ?

Solution: According to Bragg's law, $2d \sin \theta = n\lambda$

For $n = 1$, $2d \sin 40^\circ = 1 \times 3 \text{ \AA}$

Hence $d = \frac{3 \text{ \AA}}{2 \sin 40^\circ} = 2.33 \text{ \AA}$

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

$$2.33 \text{ \AA} = \frac{a}{\sqrt{(1^2 + 1^2 + 0^2)}}$$

hence $a = 3.299 \text{ \AA}$

Volume of unit cell = $a^3 = (3.299 \times 10^{-10} \text{ m})^3 = 35.9 \times 10^{-30} \text{ m}^3$

and $d_{(100)} = \frac{a}{\sqrt{(1^2 + 0^2 + 0^2)}} = a = 3.299 \text{ \AA}$

17) X-rays of wavelength 1.5 \AA are incident on NaCl crystal having a grating spacing of

2.8 \AA . What is the highest order that the crystal can diffract? (2) W-12

Ans. Given: $\lambda = 1.5 \text{ \AA}$, $d = 2.8 \text{ \AA}$ highest order $n = ?$

Solution: For highest order n , $\theta = 90^\circ$.

According to Bragg's law, $2d \sin \theta = n\lambda$

$$2 \times 2.8 \text{ \AA} \sin 90^\circ = n \times 1.5 \text{ \AA}$$

$$\text{Hence } n = \frac{2 \times 2.8}{1.5} = 3.73 \approx 3$$

18) A beam of X-rays of $\lambda = 0.842 \text{ \AA}$ is incident on a crystal at a glancing angle of $8^\circ 35'$ where the first order Bragg's reflection occur? Calculate the glancing angle for second order reflection. (4) S-10, W-18

Ans. Given: $\lambda = 0.842 \text{ \AA}$, $n = 1$, $\theta_1 = 8^\circ 35'$, find θ_2 for $n=2$

Solution: Bragg's Law, $2d \sin \theta = n\lambda$

For $n=1$, $2d \sin \theta_1 = \lambda$ --- (1),

For $n=2$, $2d \sin \theta_2 = 2\lambda$ ----- (2)

Dividing eqn.(2) by(1) we get, $\frac{2d \sin \theta_2}{2d \sin \theta_1} = \frac{2\lambda}{\lambda}$ or $\frac{\sin \theta_2}{\sin 8^\circ 35'} = 2$

or $\sin \theta_2 = 2 \times \sin 8^\circ 35' = 2 \times 0.1492$

$\theta_2 = \sin^{-1}(0.2984) = 17.36^\circ$.

Problems for practice:

1) Determine the lattice constant for FCC lead crystal of radius 1.746 \AA . Also draw Planes (200) and (011) in a cubic unit cell. (4) W11

Ans. $a = 4.938 \text{ \AA}$

2) The Bragg angle corresponding to the first order reflection from the plane (1 1 1) in a crystal is 30° when X-rays of wavelength 1.75 \AA are used. Calculate interplanar spacing and lattice constant. (3) W-15, S-18

Ans. $d = 1.75 \text{ \AA}$ $a = 3.03 \text{ \AA}$

3) A beam of X-rays of $\lambda = 0.842 \text{ \AA}$ is incident on a crystal at a glancing angle of $8^\circ 35'$ when the first order Bragg's diffraction occurs. Calculate the glancing angle for 3rd order diffraction. (3) S-04

Ans. 26.59°

4) Copper has FCC structure and its atomic radius is 0.1278 nm . Calculate the interplanar spacing for (111) and (321) planes. (3) S-01

Ans. $a = 3.61 \text{ \AA}$, $d_{111} = 2.084 \text{ \AA}$, $d_{321} = 0.9648 \text{ \AA}$

5) Using the following data find the type of unit cell GaAs forms. Density of GaAs : 5.324 gm/cm^3 , atomic weight of Ga = 69.7, atomic weight of As = 74.9, lattice constant of GaAs = 5.65 \AA . (5) S-02

Ans. GaAs forms fcc structure as $Z=4$.

6) Lead is FCC crystal with atomic radius of 1.746 \AA . Find the spacing of (2 0 0) and (1 2 0) planes. (3) S-16

Ans. 2.469 \AA and 2.208 \AA

7) Lead crystallizes in FCC structure and has lattice constant of 4.95 \AA . Calculate the interplanar spacing of d_{110} , d_{111} , and d_{220} planes. (3) S-18, S-11

Ans. 3.5 \AA , 2.85 \AA , 1.745 \AA

8) An X-ray of wavelength 3 \AA is diffracted at 40° from (110) planes of a cubic crystal considering first order diffraction. Find lattice constant of the crystal structure. (3) W-17, S-12

Ans. $a = 3.299 \text{ \AA}$

9) X-rays with a wavelength of 1.54 \AA are used to calculate the spacing of (200) planes in aluminium. Bragg angle for this reflection is 22.4° . What is the size of unit cell of aluminium crystal? (3) [S 19]

Ans: $d = 2.020 \text{ \AA}$, $a = 4.040 \text{ \AA}$

