



POSTAL BOOK PACKAGE 2025

MECHANICAL ENGINEERING

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CONVENTIONAL Practice Sets

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Basic Crystallography

Practice Questions : Level-I

- Q.1** Aluminium has an FCC crystal structure. Its atomic weight equals 26.98 amu. The approximate atom radius equals 1.431 Å (Å = 10⁻¹⁰ m). Determine the weight density of aluminum.

Solution:

$$\rho = \frac{(\text{number of atoms/ unit cell}) \times (\text{atomic weight/ } A_0)}{\text{volume of unit cell}}$$

$$\rho_{\text{Al}} = \frac{(4 \text{ atoms})(26.98 \text{ amu/ } 6.02 \times 10^{23} \text{ amu/ g})}{a^3}$$

From table,

$$a_{\text{fcc}}^3 = 66.314 \times 10^{-24} \text{ cm}^3 \quad [\because \text{For FCC } \sqrt{2} a = 4r]$$

Therefore,

$$\rho_{\text{Al}} = \frac{4 \times 26.98}{66.3314 \times 10^{-24} \times 6.02 \times 10^{23}} = 2.703 \text{ g/cm}^3$$

- Q.2** In a body centered cubic crystal of lattice parameter 3.6 Å, a positive edge dislocation of 1 mm long climbs up by 1 μm. How many vacancies are created?

Solution:

When a dislocation of 1 mm long climbs up by 1 μm.

$$\text{Area affected} = 1 \times 10^{-3} \times 1 \times 10^{-6} = 10^{-9} \text{ m}^2$$

$$\text{Area of unit cell, } a^2 = (3.6 \times 10^{-10})^2 = 12.96 \times 10^{-20} \text{ m}^2$$

Number of atoms per unit cell in BCC structure = 2

For an area of 12.96 × 10⁻²⁰ m², 2 atoms gets affected (destroyed).

For an area of 10⁻⁹ m², the number of atoms destroyed

$$= \frac{2 \times 10^{-9}}{12.96 \times 10^{-20}} = 1.5432 \times 10^{10} \text{ atoms}$$

Number of vacancies created = 1.5432 × 10¹⁰ atoms

- Q.3** In an orthogonal crystal structure with lattice parameters $a \neq b \neq c$, draw the direction $[2 \bar{1} 2]$.

Solution:

Orthogonal Crystal Structure ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$)

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

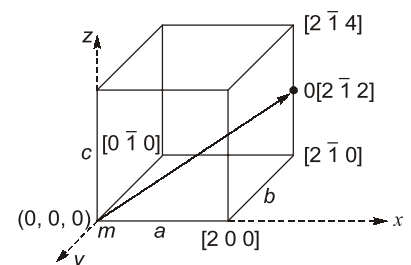
Here,

$$x = 2$$

$$y = -1$$

$$z = 2$$

Joining the point $0[2 \bar{1} 2]$ with the origin $m[0 0 0]$ gives the crystal direction.



Q4 Silver is face-centred cubic with lattice constant 4.086 Å. Calculate the planar density of atoms (a) on the (100) plane, (b) on the (111) plane and (c) the linear density of atoms along the [110] direction.

Solution:

Silver is FCC with lattice constant 4.086 Å.

$$\text{Planar density} = \frac{\text{Number of atoms}}{\text{Area of plane}}$$

(i) On the (100) Plane

$$\rho_{(100)} = \frac{2}{a^2} = \frac{2}{(4.086 \times 10^{-10})^2} = 1.1979 \times 10^{19} \text{ atoms/m}^2$$

(ii) On the (111) plane

$$\rho_{(111)} = \left(\frac{2}{\frac{\sqrt{3}}{2} a^2} \right) = \frac{4}{\sqrt{3} \times (4.086 \times 10^{-10})^2}$$

$$\rho_{pl} = 1.3832 \times 10^{19} \text{ atoms/m}^2$$

(iii) Linear density of atoms along the [110] direction

$$\rho_l = \frac{\text{Number of atoms on the direction vector}}{\text{Length of the direction vector}}$$

$$= \frac{2}{\sqrt{2}a} = \frac{2}{\sqrt{2} \times (4.086 \times 10^{-10})} = 3.4611 \times 10^9 \text{ atoms/m}$$

Q5 Calculate the number of atoms per unit cell of a metal having lattice parameter of 0.29 nm, density of 7.868 g/cc, atomic weight is 55.85 g/mol and Avogadro's number is 6.023×10^{23} . What is the crystal structure of metal?

Solution:

Given data: Avogadro's number, $N_A = 6.023 \times 10^{23}$; Lattice parameter; $a = 0.29 \text{ nm} = 0.29 \times 10^{-7} \text{ cm}$
Density, $\rho = 7.868 \text{ g/cm}^3$; Atomic weight, $A = 55.85 \text{ g/mol}$

Number of atoms/unit cell = n

Volume of one unit cell, $V_C = (a)^3 = (0.29 \times 10^{-7})^3 \text{ cm}^3$

$$\rho = \left(\frac{nA}{V_C N} \right)$$

$$\Rightarrow 7.868 = \frac{n \times 55.85}{(0.29 \times 10^{-7})^3 \times 6.023 \times 10^{23}}$$

$$n = \frac{7.868 \times (0.29 \times 10^{-7})^3 \times 6.023 \times 10^{23}}{55.85} = 2.06 \approx 2$$

Crystal structure of the atoms is BCC.

Q6 Define unit cell of a space lattice. Derive the effective number of lattice points in the unit cell of cubic lattices. Calculate the packing efficiency and density of silicon which has diamond cubic structure. Use the following properties for silicon :

Atomic Number = 14

Atomic mass unit = $1.66 \times 10^{-27} \text{ kg}$

Lattice parameter = $5.431 \times 10^{-10} \text{ m}$

Assume radius of Si atom in diamond cubic structure to be $\left(\frac{\sqrt{3}}{8} \right)$ times the lattice parameter.

Solution:

Unit cell: The atomic order in crystalline solids, indicates that small group of atoms that form a repetitive pattern.

$$a, b, c = \text{Lattice parameters}$$

$$\alpha, \beta, \gamma = \text{Interfacial angles}$$

Effective number of lattice points/ atoms in the unit cell of cubic lattices.

1. **Simple cubic structure:** In simple cubic structure, with atoms located at each of the corners of a unit cell.

$$\begin{aligned} \text{Number of atoms} &= \text{Number of corner atoms } (N_C) \times \frac{1}{8} \\ &= 8 \times \frac{1}{8} = 1 \text{ atoms} \end{aligned}$$

2. **Body centered cubic structure (BCC):** In this crystal structure a cubic unit cell with atoms located at all eight corner and a single atom at the cube center.

$$\begin{aligned} \text{Number of atoms} &= \text{Number of corner atoms } (N_C) \times \frac{1}{8} + \text{Body centered atom } (N_B) \\ &= 8 \times \frac{1}{8} + 1 = 2 \text{ atoms} \end{aligned}$$

3. **Face centered cubic structures (FCC):** In face centered cubic structure a unit cell with atoms located at each of the corners and the centers of all the cube faces.

$$\begin{aligned} \text{Number of atoms} &= \text{Number of corner atoms } (N_C) \times \frac{1}{8} + \text{Number of face centered atom} \times \frac{1}{2} \\ &= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4 \text{ atoms} \end{aligned}$$

Diamond cubic structure (Si)

Si has a diamond cubic structure. In this structure 8 atoms are arranged at corners and 6 atoms are arranged at face centers and 4 atoms are arranged inside cell on 4 body diagonal.

$$\begin{aligned} \text{Average number of atoms in the diamond cubic unit cell} &= \frac{1}{8} \times 8 \text{ (Corner atoms)} \\ &+ \frac{1}{2} \times 6 \text{ (Face centered atoms)} + 1 \times 4 \text{ (Atoms inside the cell)} \\ &= 1 + 3 + 4 = 8 \end{aligned}$$

Relations between atomic radius (R) and lattice parameter (a)

$$R = \frac{a\sqrt{3}}{8}$$

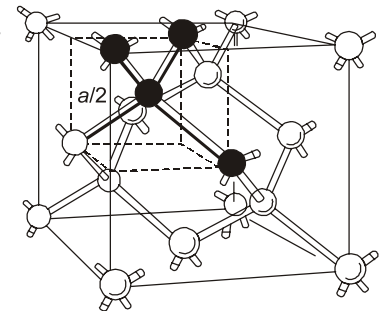
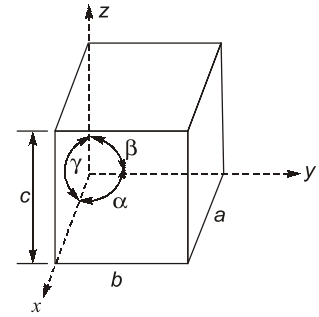
$$\text{Lattice parameter (a)} = 5.431 \times 10^{-10} \text{ m}$$

$$\text{Atomic radius (R)} = \frac{5.431 \times 10^{-10} \sqrt{3}}{8} = 1.1758 \times 10^{-10} \text{ m}$$

$$\text{Volume unit cell} = a^3 = (5.431 \times 10^{-10})^3$$

$$\text{Atomic packing factor} = \frac{N_{av} \times \frac{4}{3} \pi R^3}{a^3} = \frac{8 \times \frac{4}{3} \times \pi (1.1758 \times 10^{-10})^3}{(5.431 \times 10^{-10})^3} = 0.3400$$

$$\% \text{ APF} = 34.00\%$$



Q.11 Zinc has an HCP crystal structure and a density of 7 g/cm^3 . For zinc $\frac{c}{a}$ ratio is 1.864 and atomic weight of zinc is 65.40 g/mol . What will be the atomic radius of zinc?

Solution:

For HCP crystal structure:

Number of atoms per unit cell, $n = 6$

Density of zinc, $\rho = 7 \text{ g/cm}^3$

Atomic weight of zinc, $A = 65.40 \text{ g/mol}$

Given,

$$\frac{c}{a} = 1.864$$

Volume of unit cell,

$$V_C = \text{Base area} \times \text{height}$$

$$= 2 \times \left(\frac{1}{2}(a + 2a) \frac{\sqrt{3}}{2} a \right) \times c$$

$$= \frac{3\sqrt{3}}{2} a^2 \times 1.864a = \frac{3\sqrt{3}}{2} \times 1.864 \times (2r)^3$$

$$= 38.7425 r^3$$

We know that,

$$\text{Density, } \rho = \frac{nA}{V_C \times N_A}$$

Where, N_A is Avogadro's number = $6.023 \times 10^{23} \text{ atoms/mol}$

Now, Density,

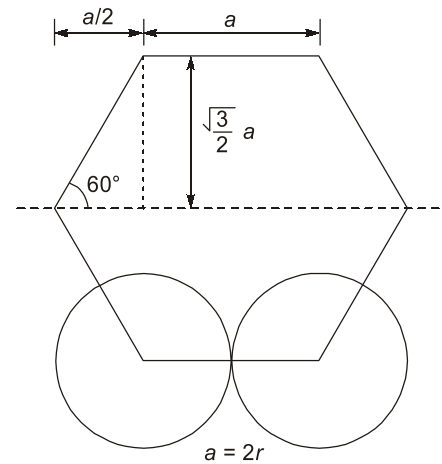
$$\rho = \frac{nA}{V_C \times N_A}$$

$$7 = \frac{6 \times 65.40}{(38.7425r^3) \times 6.023 \times 10^{23}}$$

$$r^3 = 0.2402318 \times 10^{-23} = 2.402318 \times 10^{-24} \text{ cm}^3$$

$$r = 1.3393 \times 10^{-8} \text{ cm}$$

Atomic radius of zinc, $r = 1.34 \text{ \AA}$ or 0.134 nm



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