POSTAL Book Package 2023

Mechanical Engineering

Conventional Practice Sets

Material Science

Contents

MADE EASY Publications

1 CHAPTER
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:

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

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

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

Therefore, $\rho_{Al} = \dfrac{4 \times 26.98}{66.3314 \times 10^{-24} \times 6.02 \times 10^{23}} = 2.703$ 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.

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

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

Number of atoms per unit cell in BCC structure = 2

For an area of 12.96×10^{-20} m^2, 2 atoms gets affected (destroyed).

For an area of 10^{-9} m^2, 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 = 1.5432×10^{10} atoms

Q.3 What is a slip system? What is its significance?

Solution:

The combination of a slip plane and its directions of slip is known as a **slip system**. The slipping of one plane of atoms over an adjacent plane (slip planes) under shear stress causes plastic deformation. The significance of slip system is that metals with slip systems of 5 or above are ductile, whereas those with the slip systems below 5 are not. In body-centered cubic crystals, there are 48 possible slip systems. Therefore metals with BCC structures generally have good strength and moderate ductility. In FCC crystals, there are 12 slip systems. These metals generally have moderate strength and good ductility. The Hexagonal close packed crystal has 3 slip systems and so it has a low probability of slip. Therefore, metals with HCP structure are generally brittle at room temperature.

Q.4 In an orthogonal crystal structure with lattice parameters $a \neq b \neq c$, draw the direction $[2\,\bar{1}\,2]$.

Solution:

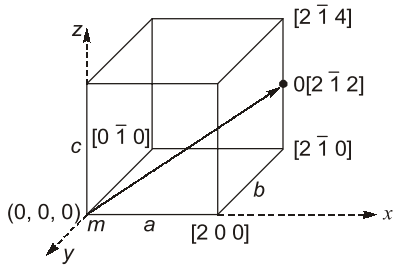
Orthogonal Crystal Structure ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$)

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.

Q.5 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

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

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

Q.6 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, $V_C = (a)^3 = (0.29 \times 10^{-7})^3\ \text{cm}^3$

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

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

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

Crystal structure of the atoms is BCC.

Q.7 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

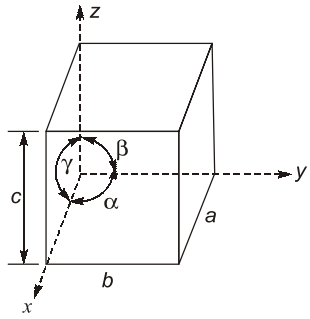
Atomic mass unit = 1.66 x 10^{-27} kg

Lattice parameter = 5.431 x 10^{-10} 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 = Lattice parameters

α, β, γ = 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.

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

$$= 8 \times \frac{1}{8} = 1 \text{ atoms}$$

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.

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

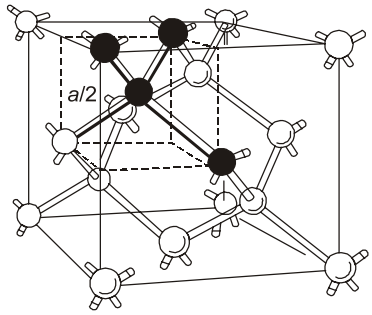
$$= 8 \times \frac{1}{8} + 1 = 2 \text{ atoms}$$

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.

$$\text{Number of atoms} = \text{Number of corner atoms } (N_C) \times \frac{1}{8} + \text{Number of face centered atom} \times \frac{1}{2}$$

$$= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4 \text{ atoms}$$

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.

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

= 1 + 3 + 4 = 8

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

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

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

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

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

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

% APF $= 34.00\%$

$$\text{Density} = \frac{N_{av} \times \text{Atomic weight}}{\text{Avagadro number} \times \text{Volume of unit}} = \frac{8\times(2\times\text{atomic number})}{6.023\times 10^{23}\times(5.431\times 10^{-10})^3}$$

$$= \frac{8\times 2\times 14\times 10^{-3}}{9.64833\times 10^{-5}} = 2321.645 \text{kg/ m}^3$$

Practice Questions : Level-II

Q.8 Prove that the packing fraction for F.C.C. structure is 0.74. Draw the phase diagram of Pb-Sn alloy and from this diagram draw cooling curve for eutectic alloy. How many atoms per mm^2 are there on the (100) planes of lead (Pb) radius 0.1750 nm? What is deformation by twinning?

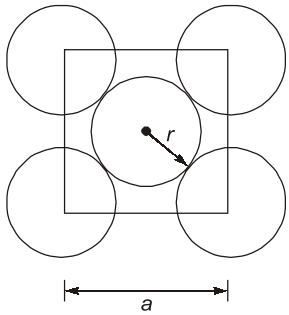
Solution:

Atomic Packing Fraction,

$$APF = \frac{N_{avg} \times V_{molecule}}{V_{unit\ cell}}$$

$N_{avg.}$ = Average number of atoms in a unit cell

$V_{molecule}$ = Volume of one atom/molecule



For FCC structure, $\left(\sqrt{2}a = 4r\right)$

$$APF = \frac{4\times\frac{4}{3}\pi r^3}{a^3} = \frac{16}{3}\frac{\pi r^3}{a^3} = \frac{16}{3}\pi\frac{\left(\frac{\sqrt{2}}{4}a\right)^3}{a^3} = 0.74$$

Assuming lead (Pb) forms FCC structure.

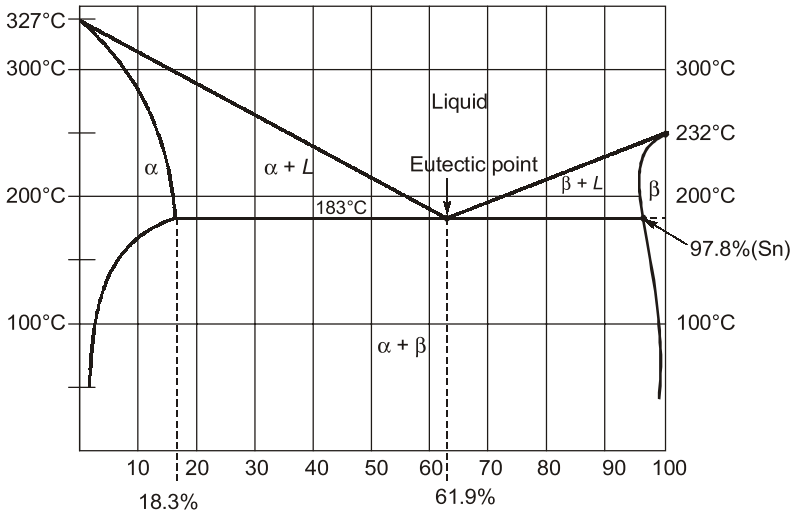
$$\text{Planar Density (100)} = \frac{\text{Number of atoms}}{\text{Area of plane}} = \frac{2}{a^2}$$

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

$$a = \frac{4r}{\sqrt{2}} = \frac{4\times 0.1750\times 10^{-9}}{\sqrt{2}}\text{m} = 0.495 \times 10^{-9} \text{ m} = 0.495 \times 10^{-6} \text{ mm}$$

$$\text{Planar density}(100) = \frac{2}{(0.495\times10^{-9}\times10^{3})^2} = 8.1624\times10^{12}\ \text{atoms/mm}^2$$

The Lead-Tin phase diagram



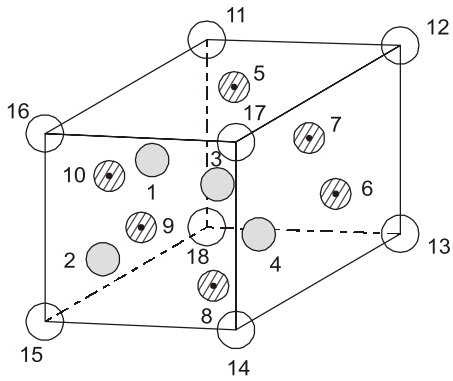
The other mechanism of plastic deformation is twinning, in which a portion of the crystal forms a mirror image of itself across the plane of twinning. Twins forms abruptly and are the cause of the cracking sound (" tin cry") that occurs when tin or zinc rod is bent at room temperature. Twinning usually occurs in HCP metals.

Q.9 **What is the packing factor of diamond? Mass of carbon is 12 amu and lattice size is 0.3569 nm. Diamond is having a cubic unit cell. What is the density of diamond?**

Solution :

The strength of covalent bonds and the arrangement by which atoms are held in structure make diamond a very hard and strong material with a high melting point.

There are four atoms (within the unit cell) marked 1–4, six atoms at the centre of six faces (marked 5–10) and eight atoms at corners (marked 11–18) (figure).



Diamond - Atomic Structure

Effective number of atoms in a diamond cubic unit cell

$$= \frac{1}{8}\times8+\frac{1}{2}\times6+4 = 8$$

$$\text{Volume of each spherical atom} = \frac{4}{3}\pi r^3$$

where r is the atomic radius of carbon atom.

Radius of atom, $r = a\sqrt{3}/8$, where a is the lattice parameter.

$$\text{volume of atoms in unit cell} = 8\times\frac{4}{3}\pi r^3 = \frac{32}{3}\pi r^3 = \frac{32}{3}\times\pi\left(\frac{a\sqrt{3}}{8}\right)^3 = \frac{32}{3}\times\frac{\pi\times3\sqrt{3}}{512}\times a^3 = 0.340\ a^3$$

$$\text{Volume of unit cell} = a^3$$

$$\text{Packing factor} = \frac{0.34a^3}{a^3} = 0.340$$