

1. Determine the volume of an FCC unit cell in terms of the atomic radius R (2 marks)

In the FCC unit cell illustrated, the atoms touch one another across a face-diagonal, the length of which is $4R$. Because the unit cell is a cube, its volume is a^3 , where a is the cell edge length. From the right triangle on the face,

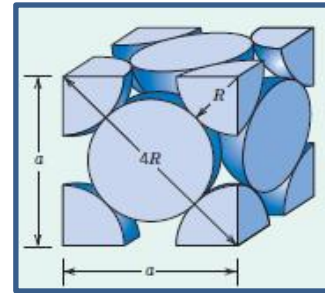
$$a^2 + a^2 = (4R)^2$$

Or, Solving for a ,

$$a = 2R\sqrt{2}$$

The FCC unit cell Volume V_c may be computed from

$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$



2. Explain why materials that are covalently bonded are less dense than those that are ionically or metallically bonded. (2 marks)

Covalently bonded materials are less dense than metallic or ionically bonded ones because covalent bonds are directional in nature whereas metallic and ionic are not; when bonds are directional, the atoms cannot pack together in a dense manner, yielding a lower mass density than solids with non-directional bonds.

3. Explain why aluminium used in long distance transmission lines cannot be strengthened by solid solution (2 marks)

For long distance transmission lines, aluminium is chosen. As a large cross section would reduce the I^2R loss, thick cables are preferred. Solid solution strengthening of aluminium wires used for transmission of electrical power is not recommended because of **Electrical conductivity of the alloy is much lower than that of the pure metal.**

4. Determine the interplanar spacing when a beam of X-ray of wavelength 1.54 \AA is directed towards the crystal at angle 30° to the atomic plane. (2 marks)

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

$$2d \sin 30 = 1.54 * 1$$

$$d = 1.54 \text{ \AA}$$

5. Define (i) space lattice (ii) basis (2 marks)

Space lattice: A lattice is a regular and periodic arrangement of points in three dimensions

Basis: To construct a crystal structure, some basic arrangement is to be fixed at each and every lattice point. This basic arrangement is said to be a basis.

6. Calculate the Bragg angle if (111) planes of a cube ($a = 3.57 \text{ \AA}$) crystal are exposed to X-rays (wavelength = 1.54 \AA) (3 marks)

$$2d \sin \theta = n\lambda \text{ and } d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d = 2.06 \text{ \AA} \text{ and } \theta = 7^\circ 32'$$

7. For a certain BCC crystal, the (110) plane has a separation of 1.181 Å. These planes are indicated with X-ray of wavelength 1.540 Å. Show that the maximum order of the Bragg's reflection that can be observed is $n = 1$. (3 marks)

Solution

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

$$\therefore n = \frac{2d \sin \theta}{\lambda}$$

$$= \frac{2 \times 1.181 \sin 90^\circ}{1.540} = 1.53$$

$d = 1.181 \text{ Å}$
 $\lambda = 1.540 \text{ Å}$

Since the value of 'n' can be integer only, and hence the highest possible value of n in this case is 1.

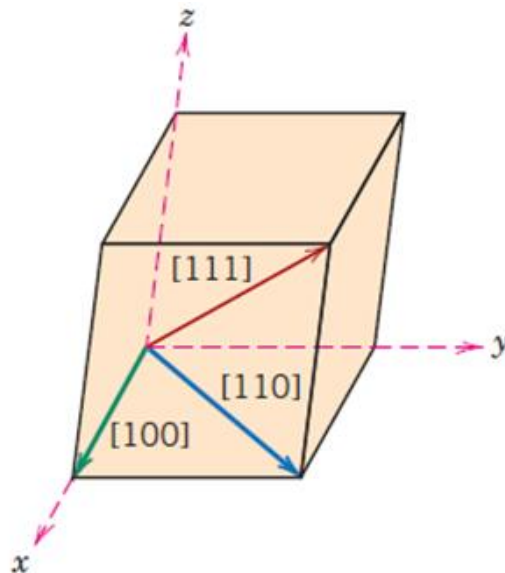
8. Copper has a 0.128 nm atomic radius, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Calculate the theoretical density of the copper (3 marks)

$$\rho_{\text{Cu}} = \frac{nA_{\text{Cu}}}{V_C N_A} = \frac{nA_{\text{Cu}}}{(16R^3\sqrt{2})N_A}$$

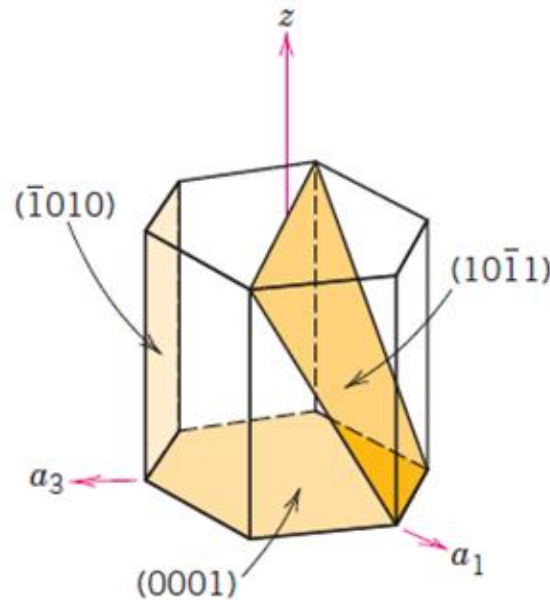
$$= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.89 \text{ g/cm}^3$$

9. Draw [100], [110], and [111] directions within a unit cell. (3 marks)



10. Draw (0001), (10 $\bar{1}$ 1), and ($\bar{1}$ 010) planes in the hexagonal crystal system (3 marks)



11. Is there any evidence of allotropy (or polymorphism) in noncrystalline materials? Is there any reason to believe that? (3 marks)

Noncrystalline materials do not display the phenomenon of allotropy; since a noncrystalline material does not have a defined crystal structure, it cannot have more than one crystal structure, which is the definition of allotropy.

12. Calculate the conductivity of copper at 26.85 °C. The collision time τ for electron scattering is 3×10^{-14} s at this temperature. (3 marks)

The number of free electrons per m³ of copper is given by

$$n = 6.023 \times 10^{23} \times 8960 / 0.06354 = 8.50 \times 10^{28} \text{ m}^{-3}$$

Electronic charge $e = 1.602 \times 10^{-19}$ C

Mass of a free electron ~ rest mass = 9.1×10^{-31} kg

$$\sigma = \frac{ne^2\tau}{m}$$

$$\sigma = 7.19 \times 10^7 \text{ ohm}^{-1} \text{ m}^{-1}$$

13. What is Bravais lattice? What is the maximum number of Bravais lattices possible? How will you account for the existence of thousands of structures from these lattices? (3 marks)

14. Explain Miller Bravais system? How is this system used to find the index of different planes? (3 marks)

15. Calculate the interplanar spacing and diffraction angle for the (220) set of planes for BCC iron. Fe has a lattice parameter of 0.2866 nm. Assume you're using monochromatic radiation with a wavelength of 0.1790 nm and a reflection order of 1. (4 marks)

- (a) The value of the interplanar spacing d_{hkl} is determined using Equation 3.10, with $a = 0.2866$ nm, and $h = 2$, $k = 2$, and $l = 0$ because we are considering the (220) planes. Therefore,

$$\begin{aligned} d_{hkl} &= \frac{a}{\sqrt{h^2 + k^2 + l^2}} \\ &= \frac{0.2866 \text{ nm}}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.1013 \text{ nm} \end{aligned}$$

- (b) The value of θ may now be computed using Equation 3.11, with $n = 1$ because this is a first-order reflection:

$$\begin{aligned} \sin \theta &= \frac{n\lambda}{2d_{hkl}} = \frac{(1)(0.1790 \text{ nm})}{(2)(0.1013 \text{ nm})} = 0.884 \\ \theta &= \sin^{-1}(0.884) = 62.13^\circ \end{aligned}$$

The diffraction angle is 2θ , or

$$2\theta = (2)(62.13^\circ) = 124.26^\circ$$

16. A diffraction pattern of a cubic crystal of lattice parameter $a = 3.16 \text{ \AA}$ is obtained with a monochromatic X-ray beam of wavelength 1.54 \AA . The first line on this pattern was observed to have $\theta = 20.3^\circ$. Obtain the interplanar spacing and Miller indices of the reflecting plane. (4 marks)

<i>Solution</i>	$2d \sin \theta = n\lambda$	$\theta = 20.3^\circ$ $\lambda = 1.54 \text{ \AA}$ $n = 1$ $a = 3.16 \text{ \AA}$
\therefore	$d = \frac{n\lambda}{2 \sin \theta}$	
	$= \frac{1 \times 1.54}{2 \times 0.3469}$	
	$= 2.22 \text{ \AA}$	

For cubic crystal, we have

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

or
$$h^2 + k^2 + l^2 = \frac{a^2}{d^2} = \frac{(3.16)^2}{(2.22)^2} = 2$$

Since $(h^2 + k^2 + l^2) = 2$ and hence the Miller indices are (110) or (101) or (011).

17. Derive the kinetic energy of free electrons as a function of their wave number. (5 marks)

The Free Electron Theory

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$