Que:9

Compute the planar density for the BCC (100), (111) and (110) planes in terms of atomic radius r.

THE PLANAR DENSITY $\rho_P = \frac{N_e}{A}$, WHERE N_e IS THE NO. OF EFFECTIVE ATOMS IN THE PLANE AND A IS THE AREA OF THE PLANE.

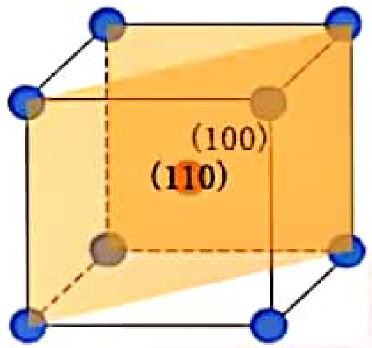
(100)

$$N_e = \frac{1}{4} \times 4 = 1$$

$$Area\ of\ the\ plane = a^2$$

$$\rho_P = \frac{1}{a^2} = \frac{1}{(\frac{4r}{\sqrt{3}})^2}$$

$$= \frac{3}{16r^2}$$



(110)

$$N_e = \frac{1}{4} \times 4 + 1 = 2$$

$$Area\ of\ the\ plane = \sqrt{2}a^2$$

$$\rho_P = \frac{2}{\sqrt{2}a^2} = \frac{2}{\sqrt{2}(\frac{4r}{\sqrt{3}})^2}$$

$$= \frac{3}{8\sqrt{2}r^2}$$

(111) plane

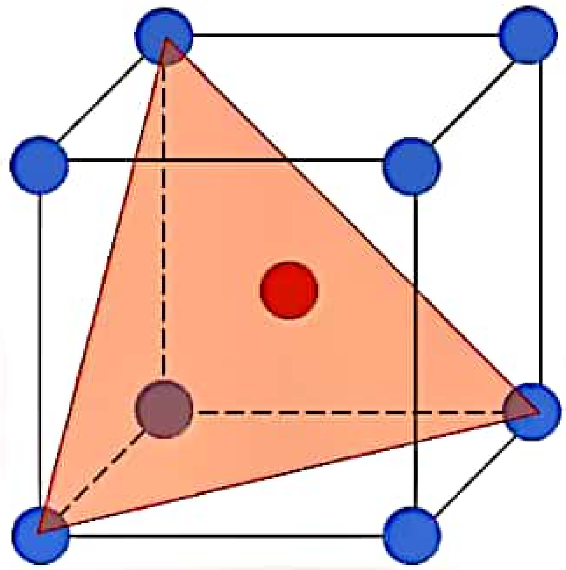
$$N_e = \frac{1}{6} \times 3 = \frac{1}{2}$$

$$Area\ of\ the\ plane = \frac{\sqrt{3}(\sqrt{2}a)^2}{4}$$

$$= \frac{\sqrt{3}}{2}a^2$$

$$\rho_P = \frac{\frac{1}{2}}{\frac{\sqrt{3}}{2}a^2} = \frac{1}{\sqrt{3}(\frac{4r}{\sqrt{3}})^2}$$

$$= \frac{\sqrt{3}}{16r^2}$$



Que:10

Calculate the planar density for (110) plane of BCC iron lattice in atoms per square millimeter. The lattice constant of iron is 0.287 nm.

Que:11

From an X - Ray powder diffraction of a pure element, peaks at the following 2θ values in degrees were obtained 38.7, 45.4, 65.7, 78.8, 83.0, 99.6, 112.5, 117.0, 138.1, and 164.2. Copper $K\alpha$ radiation was used. Find the lattice parameter and the crystal structure.

2θ	θ	sin θ	$sin^2θ$	$A = sin^2θ/sin^2θ_1$	A*2	A*3
38.7	19.35	0.331	0. 110	0. 996	2	3
45.4	22.7	0.386	0. 149	1. 355	2. 709	4. 064=˜4
65.7	32.85	0.542	0. 294	2. 671	5. 341	8. 012=˜8
78.8	39.4	0.635	0. 403	3. 666	7. 331	10. 997=˜11
83	41.5	0.663	0. 440	3. 996	7. 992	11. 988=˜12
99.6	49.8	0.764	0. 584	5. 306	10. 613	15. 919=˜16
112.5	56.25	0.832	0. 692	6. 293	12. 586	18. 879=˜19
117	58.5	0.853	0. 728	6. 615	13. 229	19. 844=˜20
138.1	69.05	0.934	0. 872	7. 931	15. 861	23. 792=˜24
164.2	82.1	0.991	0. 982	8. 928	17. 856	26. 784=˜27

From the above calculations we found that the crystal structure is FCC.

- For $\theta = 19.35$,

$$(hkl)=(111)$$

We know

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

Assuming n=1 and λ=1.54 Å (for Cu K_α radiation)

$$2 \times d \sin 19.35 = 1.54$$

$$d = 2.32 \text{ Å}$$

The lattice parameter 'a' can be calculated using the equation

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

$$2.32 = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}}$$

$$a = 4.026\text{Å}$$

Que:12

A BCC crystal is used to measure the wavelength of some X - rays. The Bragg angle for reflection from (110) plane is 20.2° . What is the wavelength? The lattice parameter of the crystal is 3.15 Å.

✓ Bragg's law is given as:

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

✓ Interplanar distance "d" is

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

✓ a= 3.15 Å, h=1, k=1, l=0 for (110)

$$d = \frac{3.15}{\sqrt{1^2 + 1^2 + 0^2}}$$

$$= 2.227\ \text{Å}$$

✓ Taking θ=20.2°, n=1, from Bragg's law

$$2 \times 2.227 \times \sin 20.2 = \lambda$$

$$\lambda = 1.5236\ \text{Å}$$

Que:13

Determine the Miller indices of cubic crystal plane that intersects the position coordinates (1, 1/4, 0), (1, 1, 1/2), and (3/4, 1, 1/4).

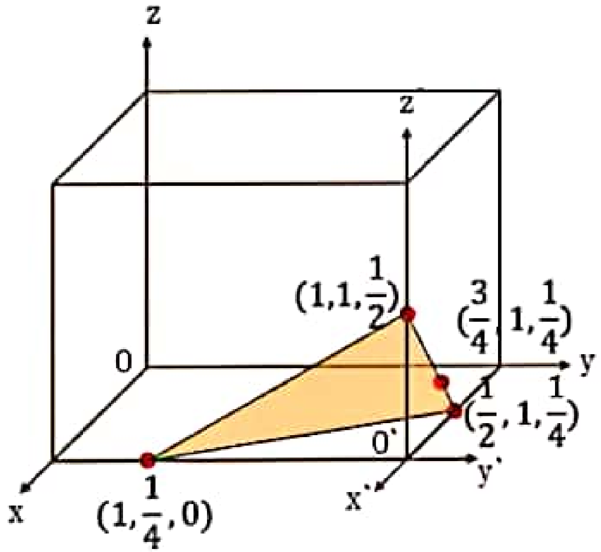
The given position coordinate are (1, 1/4, 0), (1, 1, 1/2), and (3/4, 1, 1/4).

THE INTERCEPTS ON THE X, Y AND Z AXIS ARE RESPECTIVELY $\frac{-1}{2}, \frac{-3}{4}, \frac{1}{2}$

TAKING THE RECIPROCALS $-2, \frac{-4}{3}, 2$

THE MILLER INDICES WILL BE

$$(\bar{6}, \bar{4}, 6)$$



Que:14

NaCl has the FCC lattice with $a = 5.63$ Å. What is the spacing of {100} plane?

- ✓ The formula for interplanar spacing is

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

- ✓ a= 5.63 Å, h=1, k=0, l=0.
- ✓ Substituting values in above formula

$$d = \frac{5.63}{\sqrt{1^2 + 0^2 + 0^2}}$$

= 5.63 Å

Que:15

Gold has atomic weight 197 and the density 19.3 gm/cc. What is the spacing between atoms in solid gold?

- Gold has FCC crystal structure.
- Density,

$$\rho = \frac{M}{V} = \frac{m \times N_e}{a^3}$$

M is mass of an atom, N_e is no. of effective atoms in fcc and a^3 is volume of fcc.

$$m = \frac{atomic\ weight\ (m_A)}{Avagadro's\ number\ (N_A)}$$

$$\rho = \frac{m_A \times N_e}{a^3 \times N_A}$$

$$19.3 = \frac{197 \times 4}{a^3 \times 6.022 \times 10^{23}}$$

$$a = (6.78 \times 10^{-23})^{\frac{1}{3}}$$

$$a = 4.077\ \text{Å}$$

Que:16

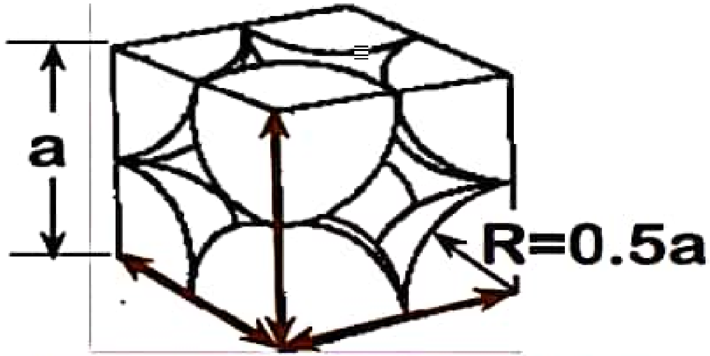
Compare packing fraction for SC and FCC lattice.

Atomic Packing Factor (APF)

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

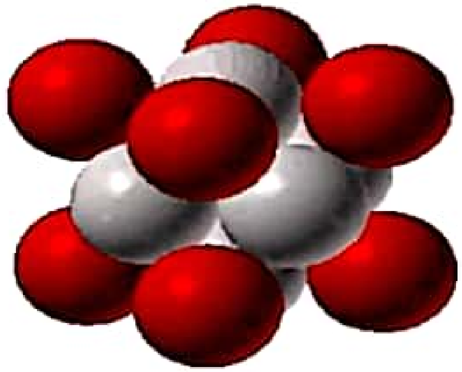
1 atom/unit cell

$$APF = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{1}\ \overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi(0.5a)^3}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

Face Centered Cubic (FCC)

- Close packed directions are face diagonals.

-Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.



- Coordination # = 12

Close-packed directions:

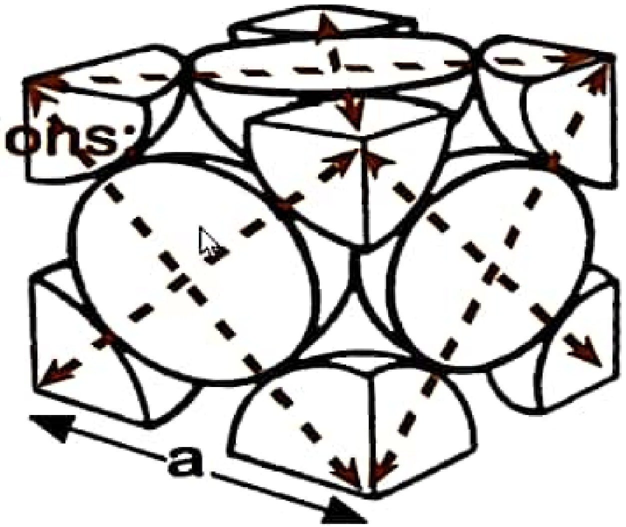
length = 4R

$= \sqrt{2}\, a$

Unit cell contains:

6 x 1/2 + 8 x 1/8

=4 atoms/unit ce



$$\text{APF} = \frac{\overbrace{4}^{\frac{\text{atoms}}{\text{unit cell}}}\ \overbrace{\frac{4}{3}\pi(\sqrt{2}a/4)^3}^{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}}$$

- APF for a FCC = 0.74

Que:17

In powder diffraction pattern for lead with radiation of λ = 1.54 Å the (220) Bragg reflection angle is θ = 32°. What is the radius of atom?

- Lead has FCC structure. We know

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

$$2\times\frac{a}{\sqrt{2^2+2^2+0^2}}\sin 32^\circ = 1.54$$

$$a = 4.11\ \text{Å}$$

Now, for FCC,

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

$$r =\ 1.45\ \text{Å}$$