* Problems [11 Oct]

1. Calculate the no. of atoms per unit cell of a metal with lattice parameter 2.9 Å, given molecular weight 55.85 kg/m3, density is 7870 kg/m3 and Avagadro number is 6.023×10^{26} kmol^{-1}.

Sol Given data,

Lattice parameter $a = 2.9 Å = 2.9 \times 10^{-10}$ m

Molecular weight $M = 55.85$ kg/m3

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

we have, $a = \left[\frac{nM}{\rho \cdot N_A}\right]^{1/3} \Rightarrow n = \frac{\rho \cdot N_A a^3}{M}$

so, $n = \frac{7870 \times 6.023 \times 10^{26} \times (2.9)^3 \times 10^{-30}}{55.85} = 2.06 = 2$

2. Chromium has BCC structure, its atomic radius is 0.1249 nm. Calculate the free volume per unit cell.

Sol Given,

Atomic radius = 0.1249 nm

Free volume per unit cell = ?

Free volume per unit cell of BCC = $(0.32 \times a^3)$

So, a = ?

Relation between r and a in BCC is, $r = \sqrt{3}a/4$

So, $a = 4r/\sqrt{3} = \frac{4 \times 0.1249 \times 10^{-9}}{\sqrt{3}} = 0.1444 \times 10^{-19}$

∴ free volume per unit cell = $0.32 \times a^3$ = 0.32×0.240

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3. Copper has FCC structure and the atomic radius is 1.278 Å, calculate the density of copper crystal. Given atomic weight of copper is 63.5.

Sol Given,

Atomic radius $r = 1.278$ Å

Atomic weight $M = 63.5$

for FCC, relation between r and a is $r = a/2\sqrt{2}$

$\Rightarrow a = 2\sqrt{2} \times r = 3.614$ Å

Avagadro number $N_A = 6.023 \times 10^{23}\ mol^{-1}$

we have, $a = \left[\frac{nM}{\rho N_A}\right]^{1/3} \Rightarrow \rho = \frac{nM}{N_A a^3} = 8.92\ gm/cm^3$

4. Show that in a simple cubic lattice the seperation between successive lattice planes (100), (110), (111) are in the ratio 1 : 0.71 : 0.58.

Sol Given,

Lattice planes are (100), (110), (111)

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

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

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

$d_{(111)} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$

Thus $d_{(100)} : d_{(110)} : d_{(111)} \Rightarrow 1 : 1/\sqrt{2} : 1/\sqrt{3}$

$\Rightarrow 1 : 0.707 : 0.58$

5. find the miller indices of a set of parallel planes which makes intercepts in the ratio 3a : 4b on the x and y axes and are parallel to z axis. a, b, c being primitive vectors.

Sol Given,

intercepts 3a : 4b, if plane ∥ parallel to an axis then intercept is infinity ∞.

Therefore $p : q : r = 3a : 4b : \infty$

$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{r} = \frac{1}{3} : \frac{1}{4} : 0 = 4 : 3 : 0$

∴ miller indices are (4, 3, 0)

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6. In a triclinic crystal, a lattice plane makes intercepts of lengths a, 2b and -3c/2. Find the miller indices. [12Oct]

Sol Given,

intercepts a, 2b, -3c/2

Therefore $p : q : r = 1 : \frac{1}{2} : \frac{-2}{3} \quad 1 : 2 : \frac{-3}{2}$

$h : k : l = 1 : \frac{1}{2} : \frac{-2}{3} = 6 : 3 : -4$

∴ miller indices are $(6, 3, \bar{4})$

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7. Determine the spacing between i) (100) planes ii) 110 planes and iii) 111 planes in an NaCl crystal having the lattice constan a = 5.64 Å.

Sol Given,

Miller indices (100), (110), (111)

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

$$d_{100} = \frac{5.64}{\sqrt{1^2 + 0^2 + 0^2}} = 5.64 \text{ Å}$$

$$d_{110} = \frac{5.64}{\sqrt{1^2 + 1^2 + 0^2}} = 3.988 \text{ Å}$$

$$d_{111} = \frac{5.64}{\sqrt{1^2+1^2+1^2}} = 3.256\ \text{Å}$$

8. The distance between (110) planes in BCC is 0.203 nm. Calculate the size of unit cell. and radius of atom.

Sol Given,

Miller indices (110), $d = 0.203$ nm

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

$a = 0.203\sqrt{1^2+0^2+0}$

$\therefore a = 0.287$ nm

radius of atom in BCC, $r = \sqrt{3}\,a/4$

$= \sqrt{3} \times 0.287 / 4$

$=$

size of unit cell $= a^3 = (0.287)^3 =$

9. A copper has FCC structure with atomic radius 0.1279 nm, calculate the inter planar spacing for (111) and (321) planes.

Sol Given,

Atomic radius $= 0.1279$ nm

Relation b/w r and a for FCC $\Rightarrow r = a/2\sqrt{2}$

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

$a = 0.361\text{nm} = 0.361 \times 10^{-9}\text{m} = 3.61\ \text{Å}$

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

$d_{111} = \frac{0.361}{\sqrt{1^2+1^2+1^2}} = 0.2086$ nm

$d_{321} = \frac{0.361}{\sqrt{3^2+2^2+1^2}} = 0.0965$ nm

10. Potassium chloride is a FCC crystal having a density of 1980 kg/m^3. If its molecular weight is 74.6, calculate (i) the distance from one atom to the next atom of the same kind and (ii) the distance between adjacent atoms.

Sol: Given,

Density = 1980 kg/m3

M = 74.6

Avagadro Number $N_A = 6.023 \times 10^{23}$ mol^{-1}

In FCC, n = 4

we have $a = \left[\frac{nM}{\rho N_A}\right]^{1/3} = \left[\frac{4 \times 74.6}{1980 \times 6.023 \times 10^{24}}\right]^{1/3} = 6.3$ Å

(i) distance b/w atoms of same kind in KCl = a = 6.3Å

(ii) distance b/w adjacent atoms = a/2 = 3.15 Å