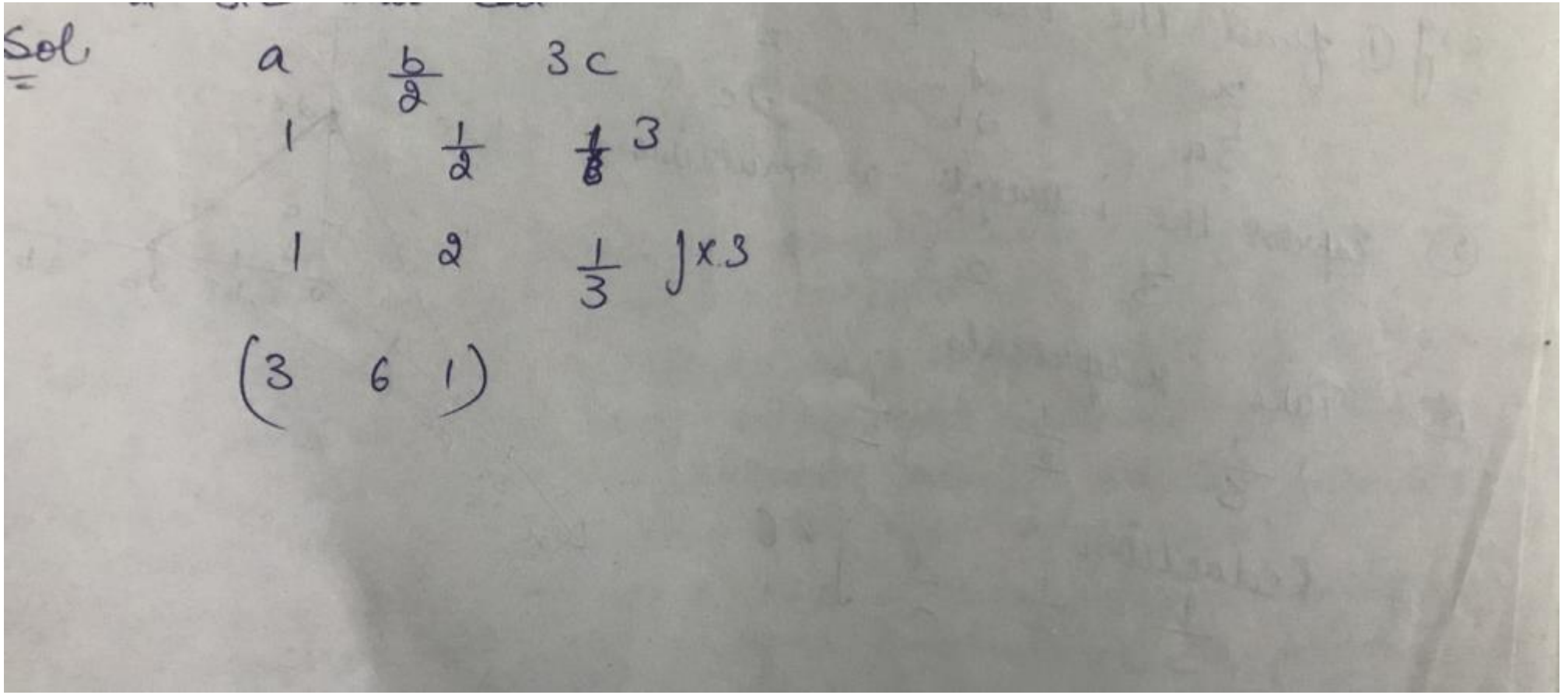
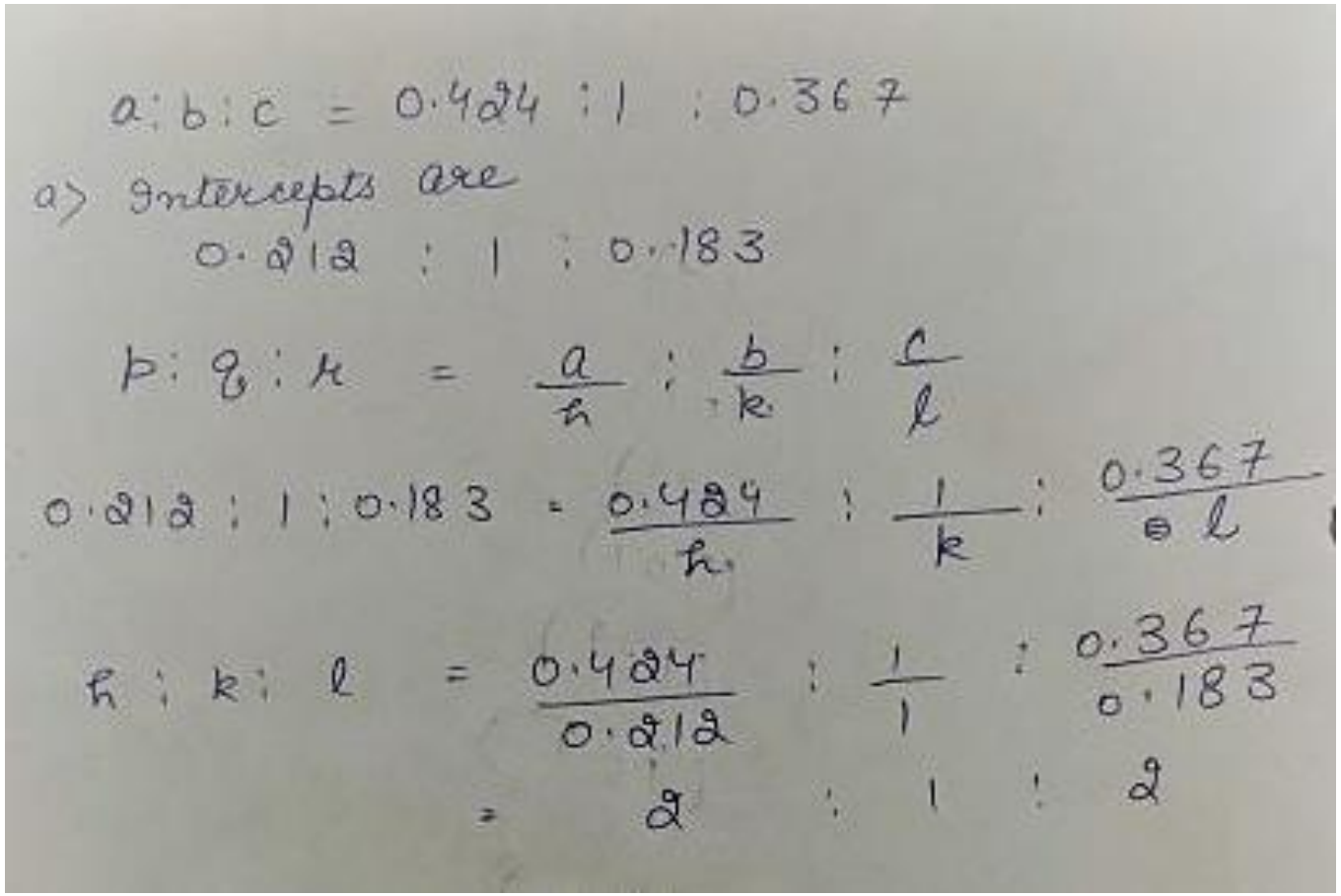
UNIT-I

Numerical Problems

Q Obtain M.I of a plane which intercepts at $a, \frac{b}{2}, 3c$ in a S.C unit cell.


Sol
a
b/2
3c
1
1/2
1/3
3
1
2
1/3
×3
(3 6 1)

- A certain orthorhombic crystal has axial unit a:b:c or 0.424: 1: 0.367. Find the Miller indices of crystal faces whose intercepts are 0.212: 1: 0.183


a : b : c = 0.424 : 1 : 0.367
a) Intercepts are
0.212 : 1 : 0.183
h : k : l = a/h : b/k : c/l
0.212 : 1 : 0.183 = 0.424/h : 1/k : 0.367/l
h : k : l = 0.424/0.212 : 1/1 : 0.367/0.183
= 2 : 1 : 2

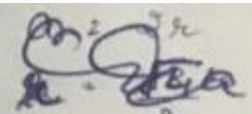
Q. Det. lattice const. for fcc lead crystal of $\lambda = 1.746\ \text{Å}$. Also find spacing of i) (111) planes (ii) (200) plane & (220) plan

Sol.

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

$= 2\sqrt{2} \times 1.746 = 4.938\ \text{Å}$

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



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

i) $d_{111} = \frac{4.938}{\sqrt{1+1+1}} = 2.851\ \text{Å}$

ii) $d_{200} = \frac{4.938}{\sqrt{4+0+0}} = 2.469\ \text{Å}$

(iii) $d_{220} = \frac{4.938}{\sqrt{4+4+0}} = 1.746\ \text{Å}$

Q A crystal with primitives 1.2 Å, 1.8 Å, 2 Å has a plane (231) which cuts an intercept 1.2 Å along x-axis. Calculate intercept along y & z-axis.

Sol

$a = 1.2\,A^\circ$

$b = 1.8\,A^\circ$

$c = 2\,A^\circ$

$(\underset{h}{2}\ \underset{k}{3}\ \underset{l}{1})$

Intercept along x-axis $= 1.2\,A^\circ$

$pa = 1.2$

$p = \frac{1.2}{a} = \frac{1.2}{1.2} = 1$

L.C.M, $D = hp = 2 \times 1 = 2$

$D = qk \Rightarrow q = \frac{D}{k} = \frac{2}{3}$

$D = rl \Rightarrow r = \frac{D}{l} = \frac{2}{1}$

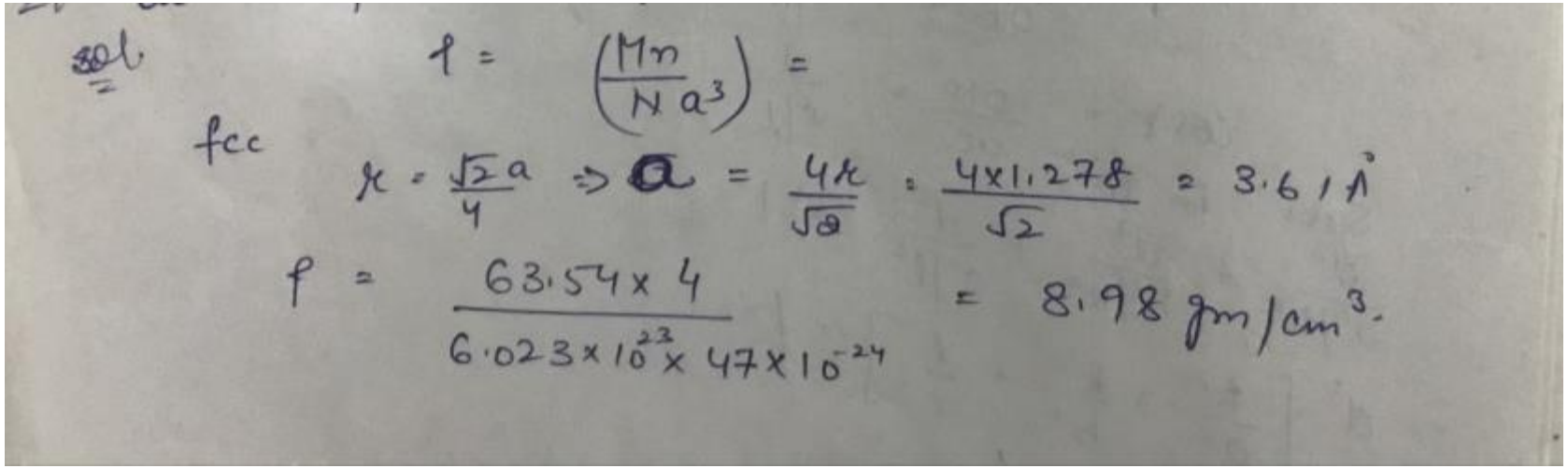
Y-intercept

$qb = \frac{2}{3} \times 1.8 = 1.2\,A^\circ$

Z-intercept

$rc = 2 \times 2 = 4\,A^\circ$

Cu has fcc structure and r = 1.278Å. Calculate density, given that atomic weight of Cu is 63.54.


Sol
$\rho = \left(\frac{Mn}{N a^3}\right) =$
fcc
$r = \frac{\sqrt{2}a}{4} \Rightarrow a = \frac{4r}{\sqrt{2}} = \frac{4 \times 1.278}{\sqrt{2}} = 3.61 \text{ Å}$
$\rho = \frac{63.54 \times 4}{6.023 \times 10^{23} \times 47 \times 10^{-24}} = 8.98 \text{ gm/cm}^3.$

- Sodium crystallizes in a cubic lattice. The edge of the unit cell is 4.3Å. The density of sodium is 963 kg/m3 and its atomic weight is 23. What type of unit cell does sodium form?

$$\rho = \frac{Z M}{N_A a^3}$$

$$Z = \frac{\rho N_A a^3}{M}$$

$$= \frac{963 \times 6.02 \times 10^{26} \times 4.3 \times 10^{-10}}{23}$$

$$= \frac{46.09}{23}$$

$$= 2 \text{ atoms/unit cell.}$$

$\therefore$ Sodium is BCC structure.

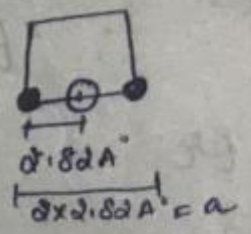
Q1- If avg. energy reqd. to produce a Sch def. is 1.97 eV in NaCl, calculate density of Sch. def. at 27°C. Given that interionic distance is 2.82 Å.

Sol. NaCl is fcc

$\therefore$ A unit cell of NaCl contains 4 molecules of NaCl.

Vol. of unit cell $= a^3 = (2 \times 2.82 \times 10^{-10})^3$

$= 1.794 \times 10^{-28}\ m^3$



Conc. of molecules, $N = \frac{4}{1.794 \times 10^{-28}} = 2.23 \times 10^{28}$

$E_s = 1.97\ eV = 1.97 \times 1.6 \times 10^{-19}\ J$

Conc. of Schottky defects, $n = N \exp\left(\frac{-E_s}{2kT}\right)$

$= 2.23 \times 10^{28} \exp\left[\frac{-1.97 \times 1.6 \times 10^{-19}}{2 \times 1.38 \times 10^{-23} \times 300}\right]$

$= 2.23 \times 10^{28} \times e^{-38}$

$= 2.23 \times 10^{28} \times 3.14 \times 10^{-17}$

$= 7 \times 10^{11}$

Q:- If the avg. energy reqd. to produce a Frenkel defect in an ionic crystal is 1.4 eV, find out the ratio of the no of Frenkel defects at 20°C & 300°C in 1 gm of crystal

Sol.

$$n = \sqrt{N N_i} \exp\left(\frac{-E_t}{2kT}\right)$$

$$n_{293} = \sqrt{N N_i} \exp\left[-\frac{1.4}{586k}\right]$$

$$n_{573} = \sqrt{N N_i} \exp\left[\frac{-1.4}{1146k}\right]$$

$$\therefore \frac{n_{293}}{n_{573}} = \exp\left[\frac{-1.4}{586k} + \frac{1.4}{1146k}\right]$$

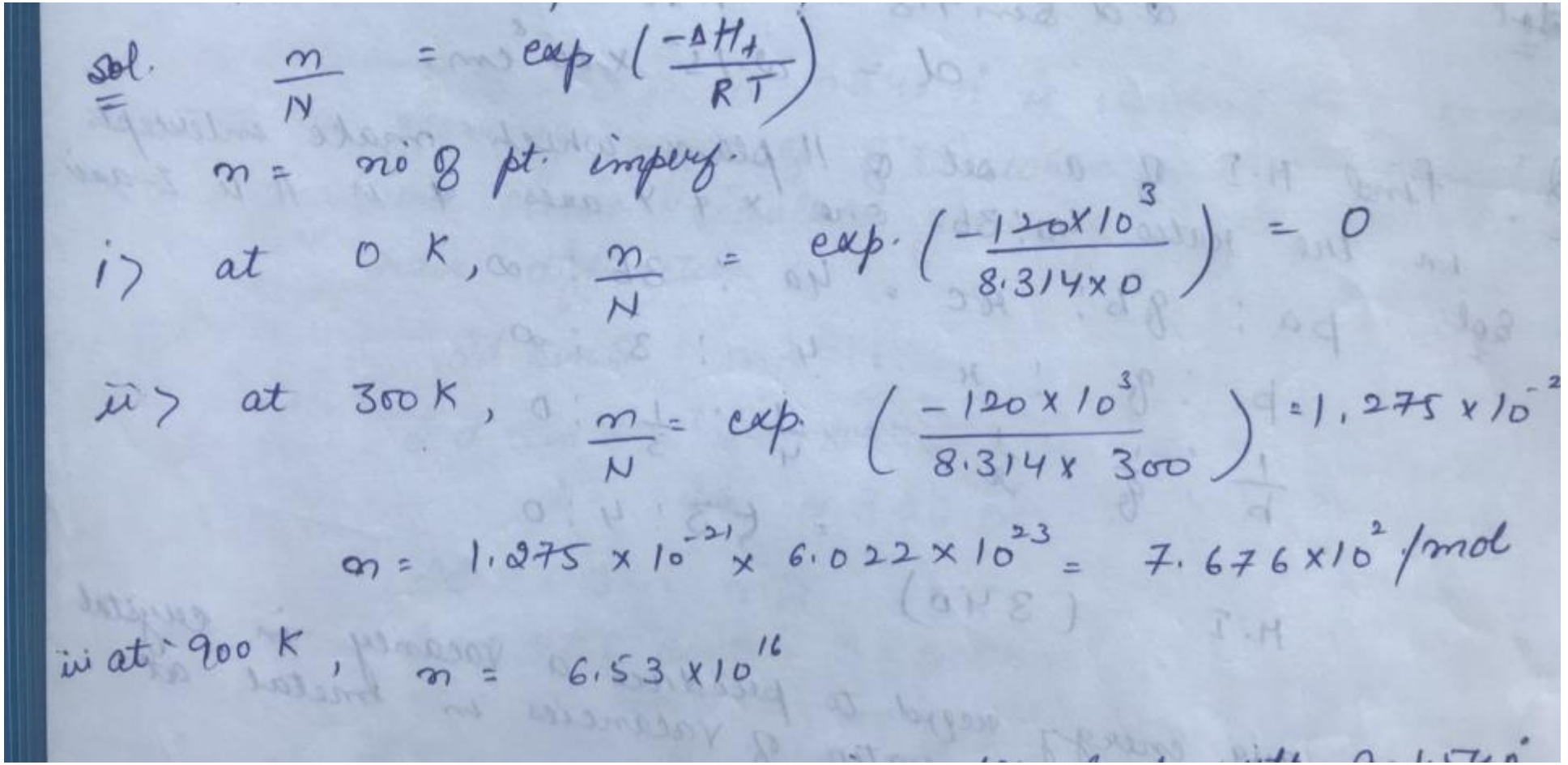
$$= \exp\left[\frac{-1.4}{k}\left\{\frac{1}{586} - \frac{1}{1146}\right\}\right] = e^{-13.47}$$

$$\frac{n_{293}}{n_{573}} = 1.4 \times 10^{-6}$$

Pb exhibits fcc structure, each side of unit cell is 4.95 Å. Calculate radius of Pb atom.

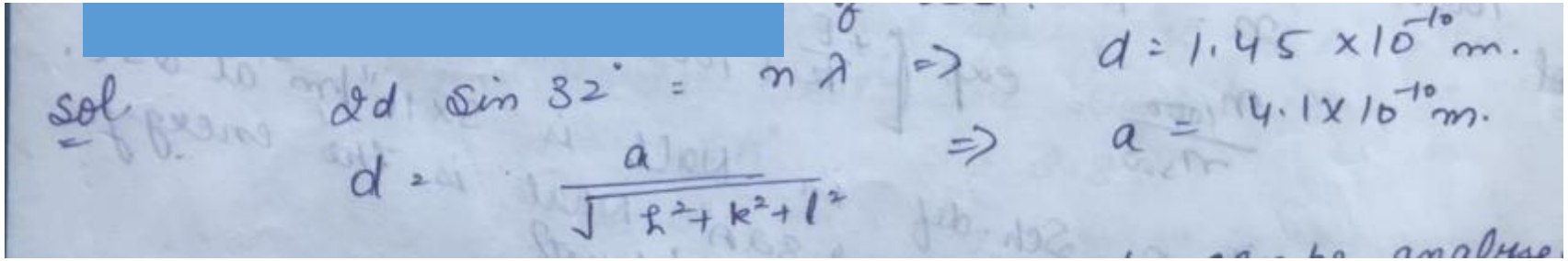
$$r = \frac{\sqrt{2}}{4} a = \frac{\sqrt{2}}{4} \text{x } 4.95 = 1.75\text{Å}$$

1. Calculate Eqlb. conc. of vacancies in Cu at 0 K, 300 K, 900 K. For Cu, enthalpy of formation of point imperfection or vacancies ΔH_f = 20 kJ/mol.

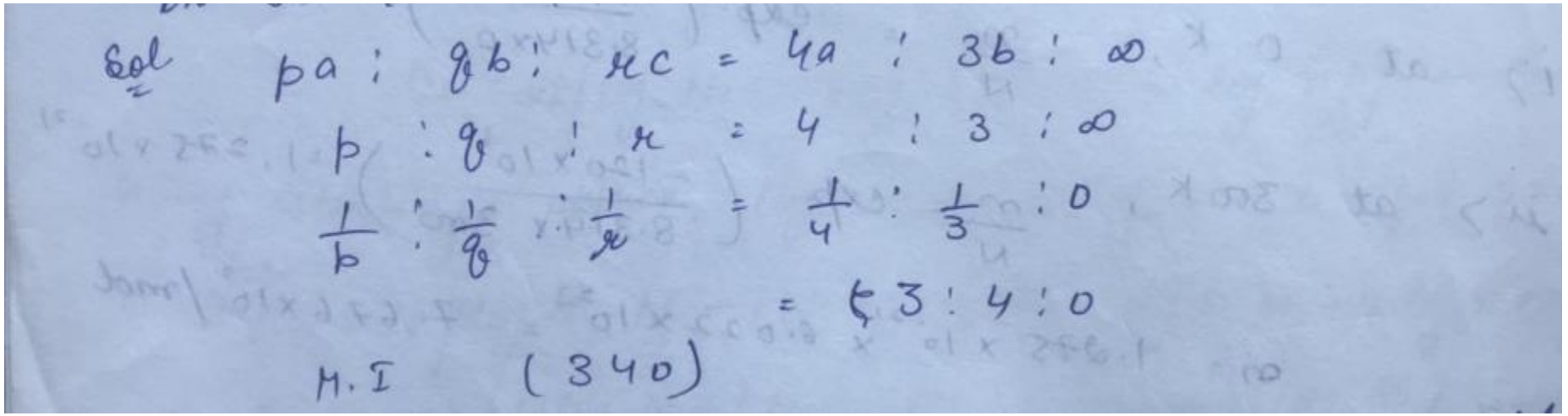

Sol. $\frac{n}{N} = \exp\left(\frac{-\Delta H_f}{RT}\right)$
n = no of pt. imperf.
i) at 0 K, $\frac{n}{N} = \exp.\left(\frac{-120\times10^3}{8.314\times0}\right) = 0$
ii) at 300 K, $\frac{n}{N} = \exp\left(\frac{-120\times10^3}{8.314\times300}\right) = 1.275\times10^{-2}$
$n = 1.275\times10^{-21}\times 6.022\times10^{23} = 7.676\times10^{2}$ /mol
iii at 900 K, $n = 6.53\times10^{16}$

Q)- A powder pattern is obtained for lead with $\lambda = 1.54 \text{ Å}$. The (220) ref. is observed at Bragg angle $\theta = 32^\circ$. What is lattice parameter of lead? assume $n = 1$.

$d = 1.45 \times 10^{-10} \text{ m}$.


sol
2d sin 32° = nλ
d = a / √(h² + k² + l²)
=>
d = 1.45 × 10⁻¹⁰ m.
=>
a = 4.1 × 10⁻¹⁰ m.

Q. Find M.I of a set of // planes which make intercepts in the ratio 4a : 3b on X & Y axes & is // to Z-axis.


Sol
pa : qb : rc = 4a : 3b : ∞
p : q : r = 4 : 3 : ∞
1/p : 1/q : 1/r = 1/4 : 1/3 : 0
= 3 : 4 : 0
M.I (340)

Q:. X-Rays of unknown wavelength give 1st order Bragg ref.,
at glancing angle $\theta = 20^\circ$ with (2 1 2) planes of Cu.
having fcc structure Find λ if lattice const. for
Cu is 3.615 Å

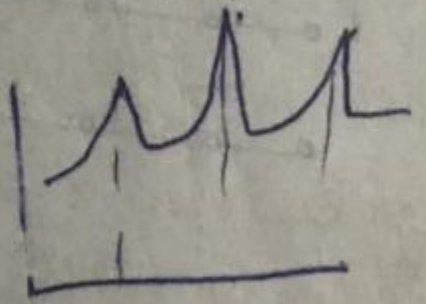
Sol.

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{3.615\,\text{Å}}{\sqrt{2^2+1^2+2^2}} = \frac{3.615}{\sqrt{9}} = 1.205\,\text{Å}$$

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

$$2 \times 1.205 \times \sin 90^\circ = 1\lambda$$

$$\lambda = 0.824\,\text{Å}$$



Ques.

If average energy required to produce a vacancy in crystal is 1 eV. Calculate the ratio of vacancies in metal at 1000K and 500K.

$$n = N \exp\left(\frac{-E_v}{kT}\right)$$

$$\frac{n_{1000}}{n_{500}} = \exp\left[\frac{+E_v}{k}\left(\frac{-1}{1000} + \frac{1}{500}\right)\right]$$

$$= \exp\left[\frac{1 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23}}\left(-0.001 + 0.002\right)\right]$$

$$= \exp\left[11.59\right]$$

$$= 1.08 \times 10^{5}$$

- Calculate the glancing angle at which the 1^{st} order and 2^{nd} order diffraction maxima will be observed when X-rays of wavelength 2Å are reflected from then cleavage of calcite with interplanar distance of 3.2Å

Sol

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

$$\sin\theta = \frac{n\lambda}{2d} = n \times \frac{2}{2 \times 3.2}$$

$$\sin\theta = 0.3125\, n$$

For 1st order $\Rightarrow$ $\sin\theta = 0.3125 \times 1$

$$\theta = 18^\circ 12'$$

For 2nd order $\Rightarrow$ $\sin\theta = 2 \times 0.3125$

$$= 0.6150$$

$$\theta = 37^\circ 58'$$

- Monochromatic X-rays of wavelength 1.5Å are incident on a crystal face having an interplanar spacing 1.5Å. Find the various orders in which Bragg's reflection takes place.

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

for $n=1$, $\quad 2d \sin\theta_1 = \lambda$

$$\sin\theta_1 = \frac{\lambda}{2d}$$

$$\sin\theta_1 = \frac{1.5}{2\times 1.5} = 0.5$$

$$\theta_1 = 30^\circ$$

for $n=2$, $\quad 2d \sin\theta_2 = 2\lambda$

$$\sin\theta_2 = \frac{2\times 1.5}{2\times 1.5} = 1$$

$$\theta_2 = 90^\circ$$

for $n=3$, $\quad 2d \sin\theta_3 = 3\lambda$

$$\sin\theta_3 = \frac{3\lambda}{2d}$$

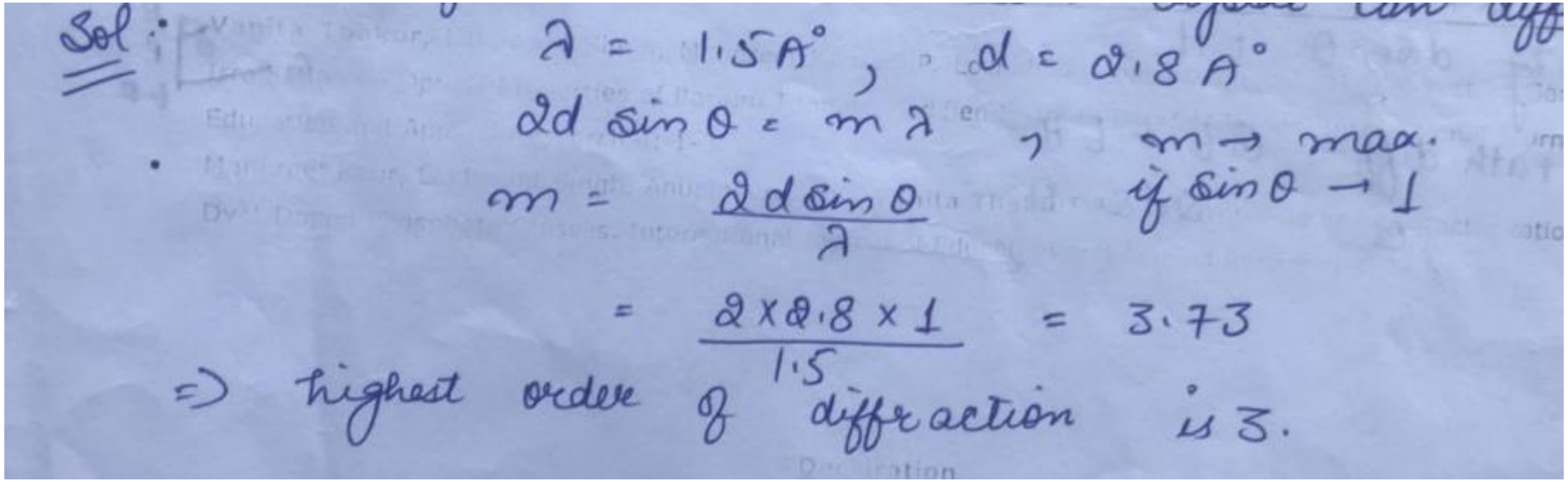
$$\sin\theta_3 = \frac{3\times 1.5}{2\times 1.5} = 1.5$$

θ_3

$\sin\theta = 1.5$ is not possible.

Hence, in this case 3rd order is not possible.

Q. X-Rays of wavelength 1.5 Å are incident on NaCl crystal having a grating spacing of 2.8 Å. What is the highest order that the crystal can diffract?


Sol:
$\lambda = 1.5 A^\circ$, $d = 2.8 A^\circ$
$2d \sin\theta = n\lambda$, $n \to$ max.
$n = \frac{2d\sin\theta}{\lambda}$ if $\sin\theta \to 1$
$= \frac{2 \times 2.8 \times 1}{1.5} = 3.73$
$\Rightarrow$ highest order of diffraction is 3.

That's all!!!