Introduction to materials Science & Engineering Sol^n.

(MINOR-2)

(Q1)(a) Let there be N atoms and n vacancies. Introduction of vacancies in the crystal increases both the enthalpy and the entropy of the crystal. Let the increase in enthalpy due to n vacancies be ΔH and the increase in entropy be ΔS. Thus the change in free energy of the crystal due to n vacancies is given by

$$\Delta G = \Delta H - T\Delta S. \quad 1$$

Now if ΔH_f is the enthalpy increase due to a single vacancy and if the number of vacancies is small in comparison to the number of atoms, i.e.

$$n << N \quad 1$$

then there will not be much interaction between them and

$$\Delta H = n\,\Delta H_f. \quad 1$$

Total no. of sites $= n + N$.

Out of these, n are vacant.

Thus number of microstates, i.e. no. of ways of selecting n vacant sites out of $n+N$ sites is

$$W = {}^{N+n}C_n = \frac{(n+N)!}{n!\,N!} \quad 1$$

The configurational entropy of the system is given by the Boltzmann's formula

$$\Delta S = S_{real} - S_{ideal}$$

$$= k\ln W - k\cancel{\ln 1}^{\,0} \quad 1$$

$$= k\ln\frac{(n+N)!}{n!\,N!}$$

$$= k\left[\ln(n+N)! - \ln n! - \ln N!\right]$$

Using Stirlings approximation we have

$$\ln N! = N\ln N - N. \quad 1$$

$$\therefore \Delta S = k\left[(n+N)\ln(n+N) - \cancel{(n+N)} - n\ln n + \cancel{n} - N\ln N + \cancel{N}\right]$$

$$= k\left[(n+n)\ln(n+N) - n\ln n - N\ln N\right]$$

We thus have

$$\Delta G = \Delta H - T\Delta S$$
$$= n\Delta H_f - Tk\left[(n+N)\ln(n+n) - n\ln n - N\ln N\right]$$ 1

For equilibrium ΔG should be -ve and a ~~m~~ minimum

$$\frac{\partial \Delta G}{\partial n} = 0$$ 1

$$\Rightarrow 0 = \Delta H_f - kT\left[\ln(n+N) + \cancel{\frac{n+N}{n+N}\cdot 1} - \ln n - \cancel{\frac{n}{n}} - 0\right]$$ 1

$$\Rightarrow kT\ln\left(\frac{n+N}{n}\right) = \Delta H_f$$

$$\Rightarrow kT\ln\left(\frac{N}{n}\right) \approx \Delta H_f \quad \text{as } n \ll N$$ 1

$$\Rightarrow \frac{n}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$

If N is no. of atoms and n the no. of vacancies then $W = {}^{N+n}C_n$ and the solution is as above.

Instead, if N is no. of sites and n is the number of vacancies then, $\left[N = N_a + n \text{ where } N_a \text{ is atoms and } \frac{\partial N}{\partial n} = \cancel{\frac{\partial N_a}{\partial n}}^{0} + \frac{\partial n}{\partial n} = 1\right]$

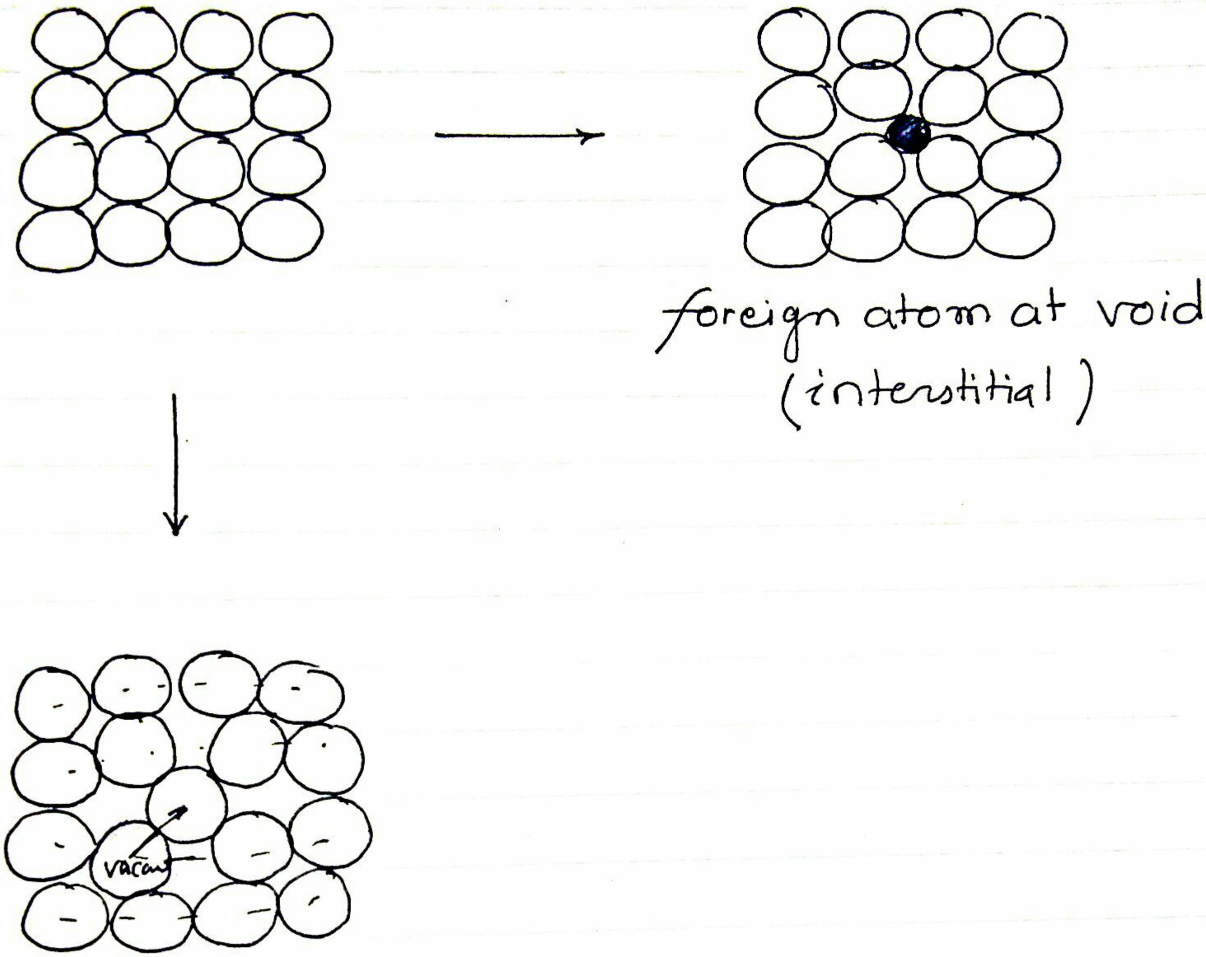
$$W = {}^{N}C_n = \frac{N!}{n!(N-n)!}$$

$$\Delta S = k\ln W = k\ln\frac{N!}{n!(N-n)!}$$
$$= k\left[\ln N! - \ln n! - \ln(N-n)!\right]$$
$$= k\left[N\ln N - \cancel{N} - n\ln n + \cancel{n} - (N-n)\ln(N-n) + \cancel{N-n}\right]$$
$$= k\left[N\ln N - n\ln n - (N-n)\ln(N-n)\right]$$

$$\Delta H_f = \cancel{k}T\cdot\frac{\partial \Delta S}{\partial n} = kT\left[\ln N + \cancel{\frac{N}{N}\cdot 1} - \ln n - \cancel{\frac{n}{n}} - \cancel{(1-1)\ln(N-n)}^{0} - \frac{N-n}{N-n}\cancel{(1-1)}^{0}\right]$$

$$\Rightarrow kT\ln\frac{N}{n} = \Delta H_f \approx \frac{n}{N} = \exp(-\Delta H_f/kT).$$

1 (b)



(self interstitial)

Name:

Minor-II

Entry No.:

Time: 1 h

Group No.:

Marks: 60

NG

Instructions:

- Please read the question paper carefully.
- Wherever needed, draw clear diagrams with appropriate labels and axes.
- For step-wise marking, you need to provide step-wise answers.

Q1	Q2	Q3	Q4	Total

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1. a) Derive an expression for equilibrium concentration of vacancy. State assumptions if any. [10]

N = Total no. of atomic sites

n = No. of vacant sites

$N-n$ = Total no. of atoms

ΔH_f = Enthalpy of formation of vacancies

ΔS = change in Entropy

$\rightarrow$

$\Delta G = \Delta H - T\Delta S$

For n no. of vacancies

$\Delta G = n\,\Delta H_f - T\Delta S_{config.}$

$\Delta S_{config} = K \ln W$

Where K = Boltzman const.

W = no. of arrangements of same Energy

$\Delta S_{config} = K \ln \frac{\lfloor N}{\lfloor N-n \, \lfloor n}$

Since $n \gg 1$, we can use Stirling's appr.

$= K\left[N\ln N - (N-n)\ln(N-n) - n\ln n\right]$

Since $n \ll N$, $N-n \approx N$

To determine min^m $\frac{\partial \Delta G}{\partial n} = 0$

$= \Delta H_f - KT\left[-\ln n \cancel{-1} + \ln(N-n) \cancel{+1}\right]$

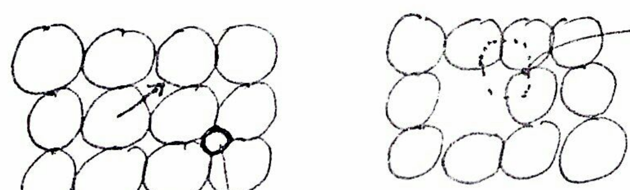
$= \Delta H_f - KT\left[\ln\left(\frac{N-n}{n}\right)\right]$

$\Delta H_f = KT \ln\left[\left(\frac{N-n}{n}\right)\right]$

$-\frac{\Delta H_f}{KT} = \ln\left[\frac{n}{N}\right]$

$\frac{n}{N} = \exp\left(-\frac{\Delta H_f}{KT}\right).$

b) Show schematically how a self-interstitial defect would be different from an interstitial defect. [5]



Impurity atom in Interstitial site

2. a) Estimate the energy per unit length of a dislocation in silver (Cubic-F). Data for silver: shear modulus = 28.8 GPa and lattice parameter = 0.409 nm. [5]

$b = \frac{1}{2}\langle 110\rangle$ (1)

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

$= \frac{\sqrt{2}}{2} \times \frac{\sqrt{2}a}{\sqrt{2}} = \frac{a}{\sqrt{2}}$ (1)

$U = \frac{1}{2} G b^2$ (1)

$= \frac{1}{2} \times 28.8 \times 10^9 \times \left(\frac{0.409}{\sqrt{2}}\right)^2 \times 10^{-18}$

$= 1.2 \times 10^{-9}$ J/m 1 (2)

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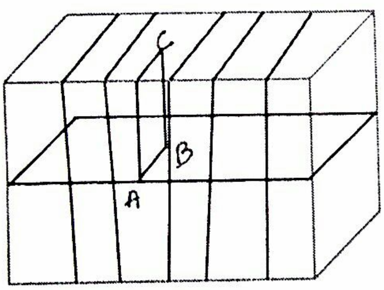
b) Determine whether the following dislocation is *edge*, *screw* or *mixed*.
Burgers vector: [100], Dislocation line vector: [111] [3]

$$\cos\theta = \frac{1.1 + 0.1 + 0.1}{\sqrt{3}\ \sqrt{1}} \quad 1$$

$$\cos\theta = \frac{1}{\sqrt{3}}$$

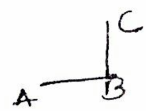
$$\theta = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.7^\circ$$, its mixed disl^n 1

c) A schematic drawing of a dislocation is shown below. Whether such configuration is possible inside the crystal or not? If yes then mark the dislocation line. [3]



yes, possible. 1.5

ABC



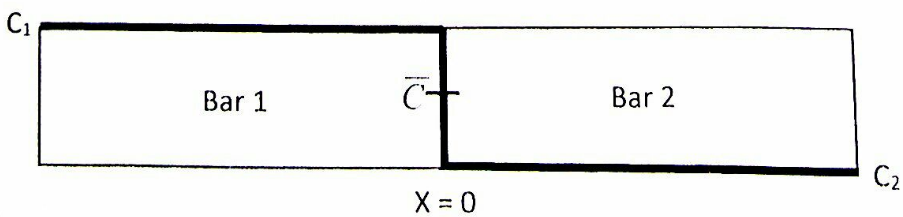
Disl^n line. 1.5

d) State whether the volume of crystal increases or decreases during dislocation a) climb-up and b) climb-down. [4]

Climb-up – Vol^m decreases 2

Climb-down – Vol^m increases 2

3. Following figure shows a diffusion couple consisting of two semi-infinite metal bars with initial solute concentration of C_1 and C_2 in bar 1 and 2, respectively. If $C_1 = 2\%$ and $C_2 = 1\%$, how much time would it take to achieve a composition of C = 1.3% at x = 5 mm in bar 2 at 950 °C. The diffusivity parameters of the solute in both bars are $D_0 = 0.25 \times 10^{-4}\ m^2.s^{-1}$ and Q = 121 KJ.mol^{-1}. The error function table is given in the next page. [15]



Name: Entry No.: Group No.:

Minor-II Time: 1 h Marks: 60

$D(950^\circ C) - ?$

$$D = D_0 \exp\left(\frac{-Q}{RT}\right). \quad -(2)$$

$$= 0.25\times10^{-4}\ \frac{m^2}{s} \cdot \exp\left(-\frac{121\times10^3}{8.314\times1223\ K}\right) \quad -(1).$$

$$= 1.692\times10^{-10}\ m^2/s \quad (1+1).$$

z	erf(z)	z	erf(z)
0.000	0.0000	0.85	0.7707
0.025	0.0282	0.90	0.7970
0.05	0.0564	0.95	0.8209
0.10	0.1125	1.0	0.8427
0.15	0.1680	1.1	0.8802
0.20	0.2227	1.2	0.9103
0.25	0.2763	1.3	0.9340
0.30	0.3268	1.4	0.9523
0.35	0.3794	1.5	0.9661
0.40	0.4284	1.6	0.9763
0.45	0.4755	1.7	0.9838
0.50	0.5205	1.8	0.9891
0.55	0.5633	1.9	0.9928
0.60	0.6039	2.0	0.9953
0.65	0.6420	2.2	0.9981
0.70	0.6778	2.4	0.9993
0.75	0.7112	2.6	0.9998
0.80	0.7421	2.8	0.9999

$$C(x,t) = A - B\ \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad -(2)$$

at $t=0$, $x<0$ $C = C_1$

$x>0$ $C = C_2$

Apply these boundary conditions. $-(1)$

$$C(x,0)_{x<0} = C_1 = A - B\ \mathrm{erf}(-\infty).$$

$$A + B = C_1 \quad -①$$

$$C(x,0)_{x>0} = C_2 = A - B\ \mathrm{erf}(\infty) \quad -(1).$$

$$C_2 = A - B \quad -②$$

from ① & ② $\quad A = C_1 + C_2/2 \quad -(1)$, $\quad B = \frac{C_1 - C_2}{2} \quad (1).$

$$C(x,t) = \frac{C_1+C_2}{2} - \frac{C_1-C_2}{2}\ \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right).$$

$$1.3 = \frac{2+1}{2} - \frac{2-1}{2}\ \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right).$$

$\boxed{\mathrm{erf}^{-1}(\mathrm{erf}(x)) = x}$

$$\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.4 \quad (2).$$

$$\frac{x}{2\sqrt{Dt}} \simeq 0.37 \quad [\text{from linear interpolation from the table}]$$

$$t = \frac{x^2}{4D(0.37)^2} = \frac{(5\times10^{-3}\ m)^2}{4\times1.697\times10^{-10}\ m^2 \times (0.37)^2}$$

$$(1+1) \quad = 269026\ s = 74.7h \approx 3\ days$$

SN-

4. Consider a hypothetical binary eutectic system of components A and B. The melting points of components A and B are 1400 K and 1200 K, respectively. The eutectic temperature is 800 K. In the α phase the maximum solid solubility of B in A is 10 wt.% and in the β phase the maximum solid solubility of A in B is 5 wt.%. The microstructure of a sample just below the eutectic temperature showed 100% lamellar structure with lamellae of α and β phases with the fraction of α phase as 0.41. The same sample on further cooling down to 700 K shows the fraction of α phase as 0.43. Further analysis revealed that at the temperature of 700 K the β phase was essentially pure B.

i) Determine the composition of the sample. [3]

$$f_\alpha = 0.41 = \frac{0.95 - x}{0.95 - 0.1} \;=\; 0.95 - x = 0.85 \times 0.41$$

$$x = 0.6$$

i.e. the eutectic composition of alloy ~ 60

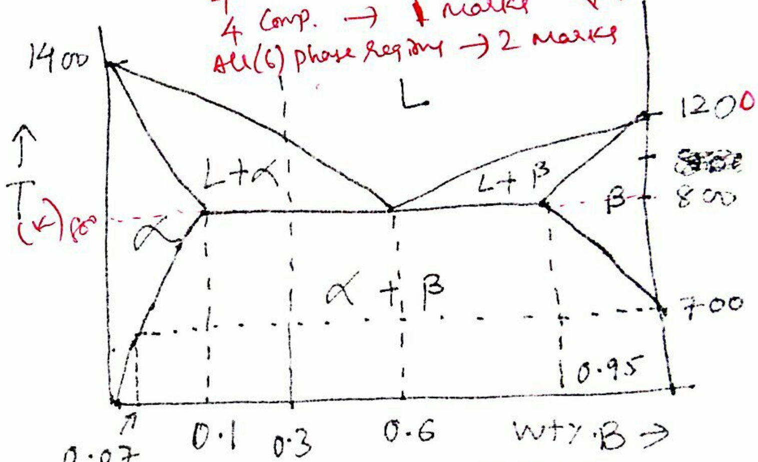
ii) Sketch and label the phase diagram completely (specify all the important temperatures and compositions). [7]

Axes Label & units → 1 Mark
4 T's → 1 marks
4 Comp. → 1 Marks
All (6) phase Regions → 2 Marks
P.D → 2 mark.

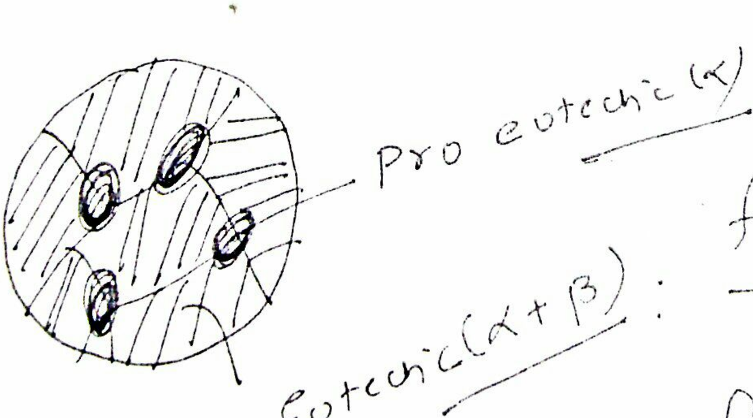
at 700K, what is the solubility of B in A ie. C_α − ??

$$f_\alpha = 0.43 = \frac{1 - 0.6}{1 - C_\alpha}$$

$$C_\alpha = 0.07$$



iii) Take a 30 wt.%B alloy and cool it from high temperature to room temperature. Sketch and label its expected microstructure at room temperature. What would be the proportion of various phases? [5]



$$f_\alpha = \frac{60 - 30}{60 - 10} \times 100 = 60\%.$$

$$f_{(\alpha+\beta)} = 1 - f_\alpha = 40\%.$$