Homework 5

4.1 Copper vacancies

$T = 1357\,K \quad Q = 0.90\ eV/atom$

Find N_v/N

$$N_v = N\exp\left(\frac{-.90\,eV/atom}{1357\,K\,(8.62\times10^{-5}\,eV/K)}\right)$$

$$\frac{N_v}{N} = 4.56\times10^{-4}$$

4.3 Ag Find Q

$T = 1037\,K \quad N_v = 3.6\times10^{23}/m^3$

$A_{Ag} = 107.9\,g/mol \quad \rho_{Ag} = 9.5\,g/cm^3 \times 10^6\,\frac{cm^3}{m^3} = 9.5\times10^6\,g/m^3$

$$N = \frac{N_A\rho}{A_{Ag}} = \frac{6.023\times10^{23}/mol\,(9.5\times10^6\,g/m^3)}{107.9\,g/mol}$$

$N = 5.3\times10^{28}$ atoms/m^3

$$N_v = N\exp\left(\frac{-Q}{kT}\right)$$

$$3.6\times10^{23}/m^3 = 5.3\times10^{28}/m^3\,\exp\left(\frac{-Q}{1037(8.62\times10^{-5})}\right)$$

$$Q = 1.06\ eV/atom$$

4.4

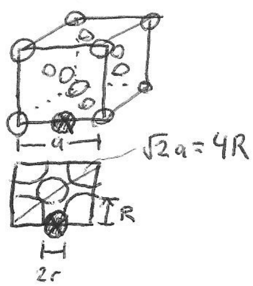
(a) Al, Pt

(b) Ag, Co, Cr, Zn, Fe

(c) H, C, O

4.5

FCC



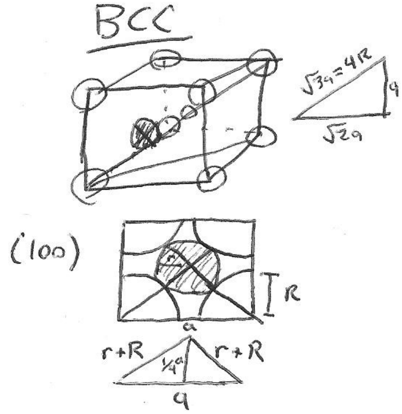
$a = 2R + 2r$

$\sqrt{2}a = 4R$

$$\frac{4R}{\sqrt{2}} = 2R + 2r$$

$$r = 0.414R$$

BCC



$$\left(\tfrac{1}{4}a\right)^2 + \left(\tfrac{a}{2}\right)^2 = (r+R)^2$$

$\sqrt{3}a = 4R$

$$\left(\tfrac{1}{4}\left(\tfrac{4R}{\sqrt{3}}\right)\right)^2 + \left(\tfrac{1}{2}\left(\tfrac{4R}{\sqrt{3}}\right)\right)^2 = (r+R)^2$$

$$\frac{R^2}{3} + \frac{4R^2}{3} = (r+R)^2$$

$$\sqrt{\tfrac{5}{3}}\,R = r + R$$

$$r = 0.29R$$

(4.8) $C'_{Cu} = 5 \text{ at}\%$

$C'_{Pt} = 95 \text{ at}\%$

Find C_{Cu}, C_{Pt}

$A_{Cu} = 63.55 \text{ g/mol}$

$A_{Pt} = 195.08 \text{ g/mol}$

$$C_{Cu} = \frac{C'_{Cu} A_{Cu}}{C'_{Cu} A_{Cu} + C'_{Pt} A_{Pt}} = \frac{5(63.55)}{5(63.55) + 95(195.08)} \times 100\%$$

$C_{Cu} = 1.68\%$

$C_{Pt} = 100\% - C_{Cu} = 98.32\%$

(4.10) $33\text{g Cu} \quad 47\text{g Zn}$

Find C'_{Cu}, C'_{Zn}

$$C_{Cu} = \frac{33\text{g}}{33+47} = 41.25\%$$

$C_{Zn} = 100\% - C_{Cu} = 58.75\%$

$A_{Cu} = 63.55 \text{ g/mol} \quad A_{Zn} = 65.41 \text{ g/mol}$

$$C'_{Cu} = \frac{C_{Cu} A_{Zn}}{C_{Cu} A_{Zn} + C_{Zn} A_{Cu}} \times 100\%$$

$$C'_{Cu} = \frac{41.25(65.41)}{41.25(65.41) + 58.75(63.55)} \times 100$$

$C'_{Cu} = 41.95\%$

$C'_{Zn} = 100 - C'_{Cu} = 58.05\%$

(4.12) $C_{Pb} = 5.5\%$

$C_{Sn} = 94.5\%$

Find C'_{Pb}, C'_{Sn}

$A_{Pb} = 207.2 \text{ g/mol}$

$A_{Sn} = 118.71 \text{ g/mol}$

$$C'_{Pb} = \frac{C_{Pb} A_{Sn}}{C_{Pb} A_{Sn} + C_{Sn} A_{Pb}} \times 100$$

$$C'_{Pb} = \frac{5.5(118.71) \times 100}{5.5(118.71) + 94.5(207.2)} = 3.23\%$$

$C'_{Pb} = 3.23\%$

$C'_{Sn} = 96.77\%$

4.15 4 pts

$$\text{concentration (Si)} = C''_{Si} = \frac{C_{Si}}{\frac{C_{Si}}{\rho_{Si}} + \frac{C_{Fe}}{\rho_{Fe}}} \cdot 10^3 \quad \left[\frac{kg}{m^3}\right] \qquad (4.9)$$

$$= \frac{0.25}{\frac{0.25}{2.33\,g/cm^3} + \frac{99.75}{7.87\,g/cm^3}} \cdot 10^3 = 19.6\ kg/m^3$$

4.17 6 pts

$$V_c = a^3 \quad \therefore \quad \rho_{ave} = \frac{n A_{ave}}{a^3 N_A} \qquad a = \left(\frac{n A_{ave}}{\rho_{ave} N_A}\right)^{1/3}$$

$$A_{ave} = \frac{100}{\frac{C_1}{A_1} + \frac{C_2}{A_2}} \qquad (4.11a)$$

with C_1, C_2 = wt% of (1,2)
A_1, A_2 = atomic mass of (1,2)

$$\rho_{ave} = \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} \qquad (4.10a)$$

$$a = \left(\frac{4 \frac{100}{\left(\frac{80\,wt\%}{107.9\,g/mol} + \frac{20\,wt\%}{106.4\,g/mol}\right)}}{\left(\frac{100}{\frac{80\,wt\%}{10.49\,g/cm^3} + \frac{20\,wt\%}{12.02\,g/cm^3}}\right) 6.023 \times 10^{23}\,mol^{-1}} \right)^{1/3} = 4.050 \times 10^{-8}\,cm = 0.4050\,nm$$

1.23 4 pts

$N_1 = (\text{atom fraction of } 1) \cdot N_T = C_1' N_T = \frac{c_1' N_A \rho_{ave}}{A_{ave}}$ with $100 - c_2' = C_1'$

$C_1' + C_2' = 100$

$$\rho_{ave} = \frac{C_1' A_1 + C_2' A_2}{\frac{C_1' A_1}{\rho_1} + \frac{C_2' A_2}{\rho_2}} \quad (4.10b)$$

$$A_{ave} = \frac{C_1' A_1 + C_2' A_2}{100} \quad (4.11b)$$

$$\therefore \quad N_1 = \frac{C_1'}{100} N_A \left(\frac{C_1' A_1 + C_2' A_2}{\frac{C_1' A_1}{\rho_1} + \frac{C_2' A_2}{\rho_2}} \right) \left(\frac{100}{C_1' A_1 + C_2' A_2} \right)$$

$$= C_1' N_A \left(\frac{1}{\frac{C_1' A_1 \rho_2 + C_2' A_2 \rho_1}{\rho_1 \rho_2}} \right)$$

$$= \frac{C_1' N_A \rho_1 \rho_2}{C_1' A_1 \rho_2 + (100 - C_1') A_2 \rho_1}$$ with $C_2' = 100 - C_1'$

$$= \frac{C_1' N_A \rho_1 \rho_2}{C_1' A_1 \rho_2 + 100 A_2 \rho_1 - C_1' A_2 \rho_1}$$

$$C_1' A_1 \rho_2 + 100 A_2 \rho_1 - C_1' A_2 \rho_1 = \frac{C_1' N_A \rho_1 \rho_2}{N_1}$$

4.23

Continued

$$A_1\rho_2 + \frac{100 A_2 \rho_1}{C_1'} - A_2\rho_1 = \frac{N_A \rho_1 \rho_2}{N_1}$$

$$\frac{100 A_2 \rho_1}{C_1'} = \frac{N_A \rho_1\rho_2 - N_1 A_1 \rho_2 + N_1 A_2 \rho_1}{N_1}$$

$$C_1' = \frac{100 N_1 A_2 \rho_1}{N_A \rho_1\rho_2 - N_1 A_1 \rho_2 + N_1 A_2 \rho_1}$$

Substitute C_1' into
$$C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \cdot 100$$
$$= \frac{C_1' A_1}{C_1' A_1 + (100 - C_1') A_2}$$

$$C_1 = \frac{\dfrac{100 N_1 A_1 \cancel{A_2} \rho_1}{N_A \rho_1\rho_2 - N_1 A_1 \rho_2 + N_1 A_2 \rho_1}}{\dfrac{\cancel{100} N_1 A_1 \cancel{A_2} \rho_1 - \cancel{100} N_1 A_2^{2} \rho_1}{N_A \rho_1\rho_2 - N_1 A_1 \rho_2 + N_1 A_2 \rho_1} + \cancel{100 A_2}} \cdot 100 = \frac{N_1 A_1 \rho_1}{N_1 A_1 \rho_1 - \cancel{N_1 A_2 \rho_1} + N_A \rho_1 \rho_2 - N_1 A_1 \rho_2 + \cancel{N_1 A_2 \rho_1}} \cdot 100$$

$$C_1 = \frac{100}{1 + \dfrac{N_A \cancel{\rho_1} \rho_2}{N_1 A_1 \cancel{\rho_1}} - \dfrac{\cancel{N_1 A_1} \rho_2}{\cancel{N_1 A_1} \rho_1}} = \frac{100}{1 + \dfrac{N_A \rho_2}{N_1 A_1} - \dfrac{\rho_2}{\rho_1}}$$

$\Rightarrow$ Equation 4.19 in problem 4.22

4.23

conitinued (2)

plugging into (4.19)

$$C_{Au} = \frac{100}{1 + \frac{N_A \rho_{Ag}}{N_{Au} A_{Au}} - \frac{\rho_{Ag}}{\rho_{Au}}} = \frac{100}{1 + \frac{6.02\times10^{23}\,mol^{-1}(10.49\,g/cm^3)}{(5.5\times10^{21}/cm^3)(196.97\,g/mol)} - \frac{10.49\,g/cm^3}{19.32\,g/cm^3}}$$

$$\boxed{C_{Au} = 15.9\ wt\%}$$

4.26 3pts

Edge $\vec{B} \perp$ dislocation line

Screw $\vec{B} \parallel$ disloc. line

Mixed $\vec{B}$ neither $\parallel$ nor $\perp$ to disloc line

→ $\vec{B}$ remains in the same direction as the disloc. character changes, but changes relative to the disloc. line

4.30 3 pts

a) twin boundary: an interface (grain boundary → special case) where atoms on one side are located at mirror image positions relative to atoms on the other side.

twin : ~~region~~ region between 2 twin boundaries

b) mechanical: result of applied shear forces & resulting mechanical deformation (generally in BCC & HCP metals)

annealing: result of heat treatments, twins form to releive thermal stresses (generally in FCC metals)

4.31 3 pts

. ABC ABC | BACBA ... twin

← mirror →

.. ABCA|BCBC|ABC ... 2 stacking faults

FCC HCP FCC