MAT E 201: Solution to Assignment #4

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Assign. #4 | MAT E 201 | Dr. S. Djokić

Q1 Cr, BCC structure $\Rightarrow$ 2 at/u.c.

$a_0 = 28844\ \mathring{A}$, $n_v = 4.78 \cdot 10^7$ vac/cm^3

a) $n_v = n \exp\left(-\frac{Q_v}{RT}\right)$, $Q_v = -RT \ln \frac{n_v}{n}$

n - number of atoms per cm^3

$$n = \frac{2 \text{ atoms}}{(2.8844 \cdot 10^{-8} \text{cm})^3} = 8.3342 \cdot 10^{22} \text{ Cr atoms/cm}^3$$

$$Q_v = -8.314 \frac{J}{mol \cdot K} \cdot 298\,K \ln \frac{4.78 \cdot 10^7}{8.3342 \cdot 10^{22}}$$

$$Q_v = 86\,907.8 \text{ J/mol} \approx 87 \text{ kJ/mol}$$

b) Fraction $= \frac{n_v}{n} = 10^{-3} = \exp\left(-\frac{Q_v}{RT}\right)$, $Q_v = 85000$ J/mol

$$\ln 10^{-3} = -\frac{Q_v}{RT} \Rightarrow T = -\frac{Q_v}{\ln(10^{-3}) R} = \frac{-85000}{\ln(10^{-3}) \cdot 8.314}$$

$T = 1480\,K$, $t = T - 273 = 1480 - 273 = 1207\,^\circ C$

Q2 HCP Ti $A_r(Ti) = 47.9$ g/mol

$a_o = 2.9503\,\text{Å}$ $c_o = 4.6831\,\text{Å}$ $\rho = 4.502\ g/cm^3$

Number of atoms per u.c. (x)

$$x = \frac{\rho V_{uc} N_A}{A_r(Ti)}, \quad V_{uc} = ?$$

HCP structure $\Rightarrow V_{uc} = 0.866\, a_o^2 c_o$

$$V_{uc} = 0.866\,(2.9503 \cdot 10^{-8})^2 \cdot (4.6831 \cdot 10^{-8})$$

$$V_{uc} = 3.53007 \cdot 10^{-23}\ cm^3$$

$$x = \frac{4.502\ g/cm^3 \cdot 3.53007 \cdot 10^{-23}\ cm^3 \cdot 6.023 \cdot 10^{23}\ at/mol}{47.9\ g/mol}$$

$x = 1.998$

HCP structure $\Rightarrow$ Ideally 2 at/u.c.

a) $$\text{Fraction} = \frac{2 - 1.998}{2} = 1 \cdot 10^{-3}$$

b) Number of vacancies per cm^3

$$n = \frac{N_{at/u.c.} \cdot \text{Fraction}}{V_{uc}} = \frac{2 \cdot 1 \cdot 10^{-3}}{3.53007 \cdot 10^{-23}\ cm^3}$$

$$n = 5.6656 \cdot 10^{19}\ \frac{vac}{cm^3}$$

Q3 $Rate = C_0 \exp(-Q/RT)$

$Rate_1 = 8 \cdot 10^8$ jumps/s; $Rate_2 = 9 \cdot 10^{13}$ jumps/s

$t_1 = 575°C$ $Q = 300$ kJ/mol , $t_2 = ?$

$T_1 = 575 + 273 = 848K$, $R = 8.314$ J/mol K

$$\frac{Rate_1}{Rate_2} = \frac{C_0 \exp(-Q/RT_1)}{C_0 \exp(-Q/RT_2)} \Rightarrow$$

$$T_2 = \frac{1}{\frac{1}{T_1} + \frac{R}{Q} \ln \frac{Rate_1}{Rate_2}} = \frac{1}{\frac{1}{848} + \frac{8.314}{300 \cdot 10^3} \ln \frac{8 \cdot 10^8}{9 \cdot 10^{13}}}$$

$T_2 = 1166.97$ K $\Rightarrow t = 1166.97 - 273 = 893.97°C$

Q 4

$T = 900 + 273 = 1173K$, $F = \frac{n_v}{n_0} = 3.85 \cdot 10^{-2}$

$$n_v = n_0 \exp\left(-\frac{Q}{RT}\right)$$

$$\ln \frac{n_v}{n_0} = \ln F = -\frac{Q}{RT}$$

$$Q = -RT \ln F = -8.315 \frac{J}{mol K} \cdot 1173K \cdot \ln 3.85 \cdot 10^{-2}$$

$$Q = 31768.08 \frac{J}{mol}$$

Q5 $\Delta X = 0.5\,mm = 5\cdot 10^{-2}\,cm$ Si wafer, $a_0 = 5.407\,\mathring{A}$

$$\frac{\Delta c}{\Delta X} = \frac{C_{in} - C_{fin}}{\Delta X} = -0.0175\ at\%\ As/cm$$

Bottom surface 1 As atom per 10^7 Si atoms

$$C_{in} = \frac{1\ As\ atom}{10^7\ Si\ atoms}\cdot 100\% = 10^{-5}\ at\%$$

Top surface $C_{fin} = C_{in} - \frac{\Delta c}{\Delta X}\cdot \Delta X$

$$C_{fin} = 10^{-5} + 0.0175\cdot 5\cdot 10^{-2} = 8.85\cdot 10^{-4}\ at\%$$

$$C_{fin} = \frac{N}{10^7\ Si\ atoms}\cdot 100\% = 8.85\cdot 10^{-4}\ at\%$$

$\Rightarrow$ $N = 88.5$ As atoms per 10^7 Si atoms

Concentration gradient in $\left[\frac{As\ atoms}{cm^3\cdot cm}\right]$

Si - Diamond cubic structure $\Rightarrow$ 8 at/u.c.

$$V = a_0^3 = 1.5808\cdot 10^{-22}\,cm^3$$

$$V = \frac{10^7 at\cdot 1.5808\cdot 10^{-22}\,cm^3}{8\,at} = 1.976\cdot 10^{-16}\,cm^3$$

$$C_{in} = \frac{1\ As\ at.}{1.976\cdot 10^{-16}} = 5.06\cdot 10^{15}\ As\ at./cm^3$$

$$C_{fin} = \frac{88.5\ As\ at.}{1.976\cdot 10^{-16}} = 4.479\cdot 10^{7}\ As\ at./cm^3$$

$$\frac{\Delta c}{\Delta X} = \frac{C_{in} - C_{fin}}{\Delta X} = -1.012\cdot 10^{17}\ \frac{As\ at.}{cm^3}$$