Homework 4.0

Carefully review chapter 4 lecture slides and, if time allows, read textbook sections (Askeland chapter 4; some sections, such as 4.5, can be neglected) and give an honor statement confirming the reading

Homework 4.1

Calculate the equilibrium fraction of atom sites that are vacant for lead (Pb) at its melting temperature of 327°C (600 K). Assume vacancy formation energy is 0.55 eV/atom

Leadbetter, A. J. et al., The Philosophical Magazine: A Journal of Theoretical Experimental and Applied Physics, 13(122), 371–377. https://doi.org/10.1080/14786436608212615

Convert vacancy formation energy from eV/atom to J/mol

$$Q_V = 0.55\ \frac{\text{eV}}{\text{atom}} = 0.55\frac{\text{eV}}{\text{atom}} \times ?\frac{\text{J}}{\text{eV}} \times ?\ \frac{\text{atom}}{\text{mol}} = 53000\frac{\text{J}}{\text{mol}}$$

Equilibrium concentration of vacancy in lead at 327^{o}C:

$$X_V = \exp\left(-\frac{Q_D}{RT}\right) = \exp\left[-\frac{??}{?? \times ??}\right] = \mathbf{2.44 \times 10^{-5}}$$

Homework 4.2

Cu and Ni form substitutional solid solution with face centered cubic (FCC) crystal structure, meaning Cu and Ni would randomly occupy the lattice sites. For a 60 wt% Cu-40 wt.% Ni alloy, what is the fraction of atom sites that are occupied by Ni?

Define:

n_{Cu}	Number of Cu atoms in the Cu-Ni substitutional solid solution, in mole
n_{Ni}	Number of Ni atoms in the Cu-Ni substitutional solid solution, in mole
m_{Cu}	Total mass of Cu in the Cu-Ni substitutional solid solution
m_{Ni}	Total mass of Ni in the Cu-Ni substitutional solid solution
A_{Cu}	Atomic mass of Cu, which is 63.50 g/mol
A_{Ni}	Atomic mass of Ni, which is 58.69 g/mol

As a first approximation, **neglect vacancy**

Site fraction for Ni: $$X_{Ni} = \frac{n_{Ni}}{n_{Cu}+n_{Ni}} = \frac{\frac{m_{Ni}}{A_{Ni}}}{\frac{m_{Cu}}{A_{Cu}}+\frac{m_{Ni}}{A_{Ni}}} = \frac{1}{\frac{A_{Ni}}{A_{Cu}}\cdot\frac{m_{Cu}}{m_{Ni}}+1} = \frac{1}{\frac{?}{?}\cdot\frac{?}{?}+1} = \mathbf{41.9\ atom}\ \%$$

Similarly, site fraction for Cu: $$X_{Cu} = \frac{?}{?+?} = \frac{\frac{m_{Cu}}{A_{Cu}}}{\frac{m_{Cu}}{A_{Cu}}+\frac{m_{Ni}}{A_{Ni}}} = \frac{1}{1+\frac{A_{Cu}}{A_{Ni}}\cdot\frac{m_{Ni}}{m_{Cu}}} = \frac{1}{1+\frac{?}{?}\cdot\frac{?}{?}} = \mathbf{58.1\ atom\%}$$

Or simply, $X_{Cu} = ? - X_{Ni}$

Homework 4.3

Niobium (Nb) and tungsten (W) form a substitutional solid solution with body centered cubic (BCC) crystal structure, meaning Nb and W would randomly occupy the lattice sites. Knowing a particular Nb-W alloy has a lattice constant of 0.32554 nm, and its density is 11.95 g/cm^3, please estimate **atomic percentage** of Nb and W in the Nb-W alloy. Then, convert from atomic percentage to **weight percentage**.

Hints:

Please refer to Chapter 3 class example about

- BCC structure to get the number of atoms within a unit cell
- How density is calculated based on structure and the type of atoms within it

Also need atomic mass A for both Nb and W

Knowing density for Nb-W substitutional solid solution:

$$\rho_{Nb-W} = \frac{M_{unit\ cell}}{V_{unit\ cell}} = \frac{M_{unit\ cell}}{a^3} = \frac{M_{unit\ cell}}{(0.32554\ nm)^3} = 11.95\ \frac{g}{cm^3}$$

Homework 4.3 (2)

Mass for a BCC structured unit cell in Nb-W substitutional solid solution:

$$M_{unit\ cell} = ? \times (??)^3 = 4.12\ \times 10^{-22}\ \text{g}$$

From periodic table:

Atomic mass for Nb $A_{Nb} =$?? g/mol, and mass for one Nb atom is $\frac{A_{Nb}}{N_A}$

Atomic mass for W $A_W =$?? g/mol, and mass for one W atom is $\frac{A_W}{N_A}$

For the BCC unit cell of the Nb-W substitutional solid solution, suppose atomic fraction of Nb is X_{Nb}

$$M_{unit\ cell} = 2\left[X_{Nb}\frac{A_{Nb}}{N_A} + (1 - X_{Nb})\frac{A_W}{N_A}\right]$$

$$\frac{M_{unit\ cell} \cdot N_A}{2} = ??$$

$$\frac{M_{unit\ cell} \cdot N_A}{2} - ? = X_{Nb} \cdot ?$$

$$X_{Nb} = \frac{\frac{M_{unit\ cell} \cdot N_A}{2} - A_W}{A_{Nb} - A_W} = \frac{\frac{? \times ?}{?} - ??}{?? - ??} = 0.657 = \mathbf{65.7\ atom\%}$$

$$X_W = ? - X_{Nb} = \mathbf{34.3\ atom\%}$$

Homework 4.3 (3)

Converting from atomic fraction to mass fraction:

Define:

m_{Cu}	Total mass of Nb in the Nb-W substitutional solid solution
m_W	Total mass of W in the Nb-W substitutional solid solution
n	Total number of atoms in the Nb-W substitutional solid solution

Nb mass fraction

$$w_{Nb} = \frac{m_{Nb}}{m_{Nb} + m_W} = \frac{n \cdot X_{Nb} \cdot A_{Nb}}{n \cdot (X_{Nb} \cdot A_{Nb} + X_W \cdot A_W)} = \frac{? \cdot ?}{? \cdot ? + ? \cdot ?} = 0.492 = \mathbf{49.2\ wt}\%$$

$$w_W = ?\ - w_{Nb} = \cdots = \mathbf{0.508 = 50.8\ wt}\%$$

Homework 4.3 (4)

Alternatively, mass fraction could be directly calculated:

Suppose mass fraction of Nb is w_{Nb} mass fraction of W is $w_W = 1 - w_{Nb}$

Number of Nb atoms in a unit cell

$$n_{Nb} = \frac{M_{unit\ cell} \cdot w_{Nb}}{\frac{A_{Nb}}{N_A}}$$

Number of W atoms in a unit cell

$$n_W = \frac{M_{unit\ cell} \cdot w_W}{\frac{A_W}{N_A}} = \frac{M_{unit\ cell}(1 - w_{Nb})}{\frac{A_W}{N_A}}$$

Total number of atoms within a unit cell

$$n_{unit\ cell} = n_{Nb} + n_W = \frac{M_{unit\ cell} \cdot w_{Nb}}{\frac{A_{Nb}}{N_A}} + \frac{M_{unit\ cell}(1 - w_{Nb})}{\frac{A_W}{N_A}} = M_{unit\ cell} \cdot N_A \left(\frac{w_{Nb}}{A_{Nb}} + \frac{1}{A_W} - \frac{w_{Nb}}{A_W} \right) \equiv 2$$

$$\frac{w_{Nb}}{A_{Nb}} + \frac{1}{A_W} - \frac{w_{Nb}}{A_W} = \frac{2}{M_{unit\ cell} \cdot N_A} \qquad \frac{w_{Nb}}{A_{Nb}} - \frac{w_{Nb}}{A_W} = \frac{2}{M_{unit\ cell} \cdot N_A} - \frac{1}{A_W}$$

$$w_{Nb} = \frac{\frac{2}{M_{unit\ cell} \cdot N_A} - \frac{1}{A_W}}{\frac{1}{A_{Nb}} - \frac{1}{A_W}} = \frac{\frac{2}{? \times ?} - \frac{1}{?}}{\frac{1}{??} - \frac{1}{??}} = 0.492 = \mathbf{49.2\ wt.}\ \%$$

Homework 4.4

Given the following chemical reaction:

$2NaCl + 2H_2O = 2NaOH + Cl_2 + H_2$

Knowing that the atomic mass values

Na 22.99 g/mol

Cl 35.45 g/mol

H 1.00 g/mol

O 16.00 g/mol

- To produce **one mole** of NaOH, at least how many grams of NaCl would be needed?
- How many moles of chlorine gas (Cl_2) will be produced, under ideal condition?
- How many liters of hydrogen gas (H_2) will be produced, under standard condition?

	$2NaCl$	+	$2H_2O$	=	$2NaOH$	+	Cl_2	+	H_2
List the molar ratio of all reactants & products in the reaction	2		2		2		1		1
If **one mole of NaOH** as product, list the moles for other species	**1 mol**		1 mol		**1 mol**		**0.5 mol**		**0.5 mol**

Homework 4.4 (2)

From before, to produce 1 mol of NaOH needs, at least 1 mole of NaCl as one reactant (apart from 1 mole of H_2O)

Formula Mass for NaCl: ? g/mol (for Na) + ?? g/mol (for Cl) = ?? g/mol

Therefore, mass for one mole of NaCl consumed: ? g/mol · ?? mole = **58.44 g**

The amount of Cl_2 produced will be **0.5 mol**

The amount of H_2 produced will also be 0.5 mol

Understand standard condition (1 atm, 25^{o}C) 0.5 mol H_2 will take volume of ?? L/mol · 0.5 mol = **11.2 L**