11.4
Oxygen Potentials

How can we predict the partial pressure of oxygen around a hot pellet?

- **Use thermodynamics -- see chapter 5**
- **At equil. all chemical potentials are equal**

$$\frac{1}{2}\mu_{O_2}(g) = \mu_O(g)$$

$$\mu_O(g) = \mu_O \text{ (solution)}$$

$$\mu_{O_2}(g) = G^{\circ}_{O_2} + RT \ln(\Pi_{O_2})$$

Gibbs Free Energy of Pure O_2 gas at Temp. T ***Partial Pressure of O_2*** ***(Figure 11.6)***

$= \overline{\Delta G_{O_2}}$ = **partial molar free energy of oxygen in the solid per mole of O_2**

$\overline{\Delta G_{O_2}} = 2\mu_O$ **(solution) -** $G^{\circ}_{O_2}$ **@ 1 atm.**

= a way of expressing equilibrium partial pressure over the material

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11.4.1 , 11.4.2 show ways to measure $\overline{\Delta G_{O_2}}$

11.4.3 Measured Oxygen Potentials

$$\overline{\Delta G_{O_2}} = \overline{\Delta H_{O_2}} - \overline{\Delta S_{O_2}} \left(\frac{T}{1000} \right)$$

partial molal (Enthalpy/entropy) of oxygen in solid oxide

11.4.4 UO_2

Can get oxygen partial pressure over hyperstoichiometric UO_2 from figure 11.10

A.) Knowing $\overline{\Delta H_{O_2}}$, $\overline{\Delta S_{O_2}}$, ***T*** **==>** $\overline{\Delta G_{O_2}}$

B.) Knowing $\overline{\Delta G_{O_2}}$ **==>** Π_{O_2}

Can get oxygen partial pressure over hypostoichiometric UO_2 from figure 11.11

<1300°C can get Π_{O_2} over U(l) + $UO_{2.00}$

>1300°C can have some UO_{2-x} by converting some U^{+4} --> U^{+2}

Note - the higher the temperature, the lower $-\overline{\Delta G_{O_2}}$, the higher Π_{O_2}

i.e., $\Pi_{O_2} = \exp(\overline{\Delta G_{O_2}}/RT)$

as x--> 0, Π_{O_2} increases