Practice HW2.3-Processing (Diffusion and Oxidation)

(i) Please completely understand how the chemical potential of a species in a given state is related to its standard state and the activity of the species in that state, that i

$$\mu_{A(thespecies)} = \mu_A^o + RT \ell n(a_A) \tag{i}$$

- (ii) Understand the meaning of activity and its relationship to the partial pressure for gaseous species.
- (iii) Note that the chemical potential can be used to enforce equilibrium between the two state of the same species, for example  $O_2^{gas}(gas)=O_2^{SiO_2}(dissolved\,in\,silica)$  therefore,

$$\mu_{O_2^{gas}} = \mu_{O_2^{silica}}$$

That is, the activity of  $O_2$  in the gas phase and as dissolved in silica is equal.

Note that the activity of a species in gas phase where the molecules are not interacting is equal to the partial pressure of the species.

(iv) Can you argue the form of the following equation from physical arguments

$$J_A = \frac{C_A D_A}{RT} \frac{d\mu_A}{dx} \tag{1}$$

Show that the Eq. (1) reduces to the following if the activity of the species is equal to its molar concentration,

$$J_A = D_A \frac{dC_A}{dx}$$

which is classical Fick's Law.

(v) Show that Eq. (1) reduces to the following for the growth of the silica overgrowth, h, during oxidation of silicon,

$$\frac{dh}{dt} = n_{O_2} D_{O_2} \frac{\ln(p_{O_2}^{\text{(surface)}} / p_{O_2}^{\text{(interface)}})}{h}$$
 (2)

Using the information given in the attached paper (Chemical Potential etc.) obtain a value for the parabolic rate constant at 1100  $^{\circ}$ C in units of nm $^{2}$ s $^{-1}$  and compare your result with the values given in this paper.