

# 0601E: Diffusion Flux, " $j$ "

## 09/20/21: Practice HW on the topic of Diffusion Flux

### 1.

What are the units for the following quantities:

- flux
- chemical potential (for a specific species)
- Diffusion coefficient
- $k_B$  the Boltzmann's constant
- $T$

### 2.

Show how the units are balanced on both sides of the equation

$$j = \frac{D}{\Omega k_B T} \frac{d\Delta\mu}{dx} \quad (1)$$

### 3.

The following equation is a phenomenological description of the coefficient of diffusion

$$D = D_o e^{-\frac{Q}{RT}} \quad (2)$$

where  $D_o$  is called the "pre-exponential",  $Q$  is called the activation energy,  $R$  is the gas constant and  $T$  is the temperature.

- Give the units for each of the above parameters.
- What is the meaning of the equation  $R = N_A k_B$ .
- If the value of  $Q$  in electron volts is equal to 5 eV, what will be its value in units that are appropriate for Eq. (2).

## 4.

Consider sintering of  $ZrO_2$  from powders into a dense body by the mechanism that we have discussed in class.

Zirconia is an ionic ceramic where zirconium ions have a charge of +4, i.e.  $Zr^{4+}$ , while oxygen ions carry a charge of -2, which satisfies the charge neutrality condition in zirconia.

It so happens that zirconium and oxygen ions diffuse at different rates such that

$$D_{Zr^{4+}} \ll D_{O^{2-}}$$

•Give physical arguments why,

(i) Why is it necessary to transport both  $Zr^{4+}$  and  $O^{2-}$  in the sintering process?

(ii) Why is it necessary to transport two oxygen ions for every one zirconium ion?

(iii) Can you give arguments that underpin the following description of the overall coefficient of diffusion

$$D_{ZrO_2} = \frac{(D_{Zr^{4+}})\left(\frac{1}{2}D_{O^{2-}}\right)}{\left(D_{Zr^{4+}}\right) + \left(\frac{1}{2}D_{O^{2-}}\right)}$$

Hint: Consider limiting cases where

$$D_{Zr^{4+}} = D_{O^{2-}}$$

$$D_{Zr^{4+}} = 2D_{O^{2-}}$$

$$D_{Zr^{4+}} \ll D_{O^{2-}} \quad \text{case (x)}$$

$$D_{Zr^{4+}} \gg D_{O^{2-}}$$

In reality case (x) is true that is the oxygen ions diffuse much faster than the zirconium ions. In this instance show that  $D_{ZrO_2} \approx D_{Zr^{4+}}$