

Exercise 4.1.

For following oxides, write down the defect formation processes (Schottky, Anti-Schottky, Frenkel, Antti-Frenkel) and suitable reaction constant for each:

- Cu_2O
- Cr_2O_3
- TiO_2
- V_2O_5

Exercise 4.2.

For Cu_2O , knowing that the main type of defects are Frenkel defects and knowing values of K_S , K'_S , K'_F , find concentration of interstitial copper ions.

Exercise 4.3.

Find all defect concentrations ($[V_{Ti}^{4'}]$, $[V_O^{\bullet\bullet}]$, $[Ti_i^{4\bullet}]$, $[O_i^{''}]$) for TiO_2 . Assume that dominating type of defects are Schottky defects. K_F , K'_S , K'_F are known.

Exercise 4.4.

For given oxides, write defect formation processes (and reaction constants) assuming nonstoichiometry of compounds. For every oxide take under consideration all possible cases:

- Excess of a metal ($\text{Me}_{n+y}\text{X}_m$)
- Shortage of an oxidant ($\text{Me}_n\text{X}_{m-y}$)
- Shortage of a metal ($\text{Me}_{n-y}\text{X}_m$)
- Excess of an oxidant ($\text{Me}_n\text{X}_{m+y}$)

Oxides:

- Cr_2O_3
- ZrO_2
- Cu_2O

Exercise 4.5.

Knowing that ZnO usually has an excess of a metal, Zn_{1+y}O , find concentrations of every type of defects ($[V_O^{\bullet\bullet}]$, $[e^-]$, $[Zn_i^{2\bullet}]$, $[h^\bullet]$, $[O_i^{''}]$, $[V_{Zn}^{2'}]$) as a functions of oxygen pressure. All reaction constantans (K_1 , K_2 , K_3 , K_4 , K_F , K'_F , K_S , K'_S , K_e) are known, where:

$$K_e = [h^\bullet][e^-]$$

Exercise 4.6.

Knowing that ZrO_2 usually has shortage of oxygen: ZrO_{2-y} , find concentrations of every type of defects ($[V_O^{\bullet\bullet}]$, $[e^-]$, $[Zr_i^{4\bullet}]$, $[h^\bullet]$, $[O_O'']$, $[V_{Zr}^{4'}]$) as a functions of oxygen pressure. All reaction constantans (K_1 , K_2 , K_3 , K_4 , K_F , K_F' , K_S , K_S' , K_e) are known, where:

$$K_e = [h^\bullet][e^-]$$