Exercise 2.1-8

Quick Questions to

2.1 Intrinsic Point Defects and Equilibrium

2.1.2 Frenkel Defects; 2.1.3 Schottky Defects; 2.1.4 Mixed Point Defects

- Here are some quick questions:
 - The answers are sometimes (and possibly only indirectly) contained in the links.

2.1.2 Frenkel Defects

- Why do we need "Frenkel" and "Schottky" defects besides vacancies, self-interstitials and their agglomerates?
- Draw a schematic picture of a crystal with "Frenkel" and "Schottky" defects. What kind of "conservation laws" do you have to consider, and why does that lead to a <u>fundamental difference</u> between the two defect kinds?
- What kind of charge would "the" vacancy carry in a NaCl crystal? (Consider only the realistic case).
- Give some crystals where <u>Frenkel disorder prevails</u>.
- Give an (approximate) equation for the concentration of Frenkel defects an discuss the important terms

2.1.3 Schottky Defects and 2.1.4. Mixed Defects

- What, quite generally, is the <u>Debye length</u>?
- How does the Debye length come into consideration when discussion Schottky defects (and Frenkel defects)?
- If the formation enthalpies of two defect kinds differs by roughly <u>...???...eV</u>, one defect type will be dominating and the other one can be neglected.
- Why do we usually consider either Schottky or Frenkel defects in ionic crystals but not mixed defects? For the answer check this exercise.
- Can you predict for a given ionic crystal which kind of defect type (Schottky or Frenkel) will be prevalent?
- Discuss the details in the following set of equations:

$$\begin{aligned} \text{Na}_{\text{Na}} + \text{V}_{\text{i}} &\Leftrightarrow \text{Na}_{\text{i}} + \text{V}_{\text{Na}} \\ & & \downarrow \\ & \frac{[\text{Na}_{\text{Na}}] \cdot [\text{V}_{\text{i}}]}{\text{econst}} = \text{exp} \quad \frac{G_{\text{Reaction}}}{\text{k}T} \\ & & \downarrow \\ & c_{\text{V}}(\text{C}) \cdot c_{\text{i}}(\text{C}) = \frac{N}{N} \cdot \exp{-\frac{H_{\text{FP}}}{\text{k}T}} \\ & & \downarrow \\ & c_{\text{V}}(\text{C}) = c_{\text{i}}(\text{C}) \end{aligned}$$

Derive in an equivalent way the final relation for Schottky defects:

$$c_V(A) \cdot c_V(C) = \exp{-\frac{H_S}{kT}}$$

$$c_V(A) = c_V(C)$$