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 fundamental difference 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 Frenkel disorder prevails.
- Give an (approximate) equation for the concentration of Frenkel defects an discuss the important terms

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2.1.3 Schottky Defects and **2.1.4. Mixed Defects**

- What, quite generally, is the *Debye length*?
- 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 ...???...eV, 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:

$$\mathbf{Na_{Na} + V_i \Leftrightarrow Na_i + V_{Na}}$$

$$\Downarrow$$

$$\frac{[\mathrm{Na_{Na}}]\cdot[\mathrm{V_i}]}{[\mathrm{Na_i}]\cdot[\mathrm{V_{Na}}]} = \text{const} = \exp\frac{G_{\text{Reaction}}}{kT}$$

$$\Downarrow$$

$$c_V(C)\cdot c_i(C) = \frac{N'}{N}\cdot\exp -\frac{H_{FP}}{kT}$$

$$\Downarrow$$

$$c_V(C) = c_i(C)$$

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

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

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