Exercise 2.2-2

Quick Questions to

2.2 Extrinsic Point Defects and Point Defect Agglomerates

2.2.1 Impurity Atoms and Point Defects; 2.2.2 Local and Global Equilibrium

Here are some quick questions:

- The *answers* are sometimes (and possibly only indirectly) contained in the links.

Let's look at combined defects - double vacancies, impurity atom - vacancy complex (and so on):

- Derive from the mass action law and write down the *essential* equations for the concentrations of
  - Divacancies (c_{2V})
  - Clusters with n vacancies (c_{nV}).
  - Impurity atom - vacancy complex (c_C; c_F = impurity atom conc.).

  Forget pre-exponential factors etc., if you don't remember, or make simple assumptions.

Now let's do something important. *You really should do this, it will teach you a lot!*

- Make *sketches* of various concentrations in an Arrhenius plot. Try to produce intellegent and neat sketches with parameters as follows:
  - The concentration of single vacancies at T_m is roughly $c_V \approx 10^{-4}$
  - Positive binding energies in all case; about **10 % - 20 %** of the vacancy formation enthalpy $H_F(V)$.
  - Always include the Arrhenius plot for the single vacany as reference.
- *First*, produce one Arrhenius diagram showing single *and* double vacancies.
- *Second*, produce an Arrhenius diagram for single vacancies, impurities, and impurity atom - vacancy complex
- *Third*, produce one Arrhenius diagram showing single *and* double vacancies *but* assume that the single vacancy concentration *cannot* decline anymore at some lower temperature.
- Discuss you curves (in particular the **2nd** and **3rd**), take into account how the temperature changes in "theory" and in "real life"

Now a few really quick ones:

- If all vacancies present at thernal equilibrium near the melting point at a concentration of $c_V \approx 10^{-4}$ end up in vacancy clusters with an average of **100** vacancies, what is the concentration of these clusters? What is their average cluster distance compared to the average vacancy distance (assume a typical lattice constant around **0.3. nm**)?
- Given a equilbrium vacancy concentration of c_V, an (substitutional) impurity concentration c_F, and some binding enthalpy and entropy H_C and S_C, the concentration c_C of vacancy - (substitutional) impurity complexes should be proportional to:**........**?
- What would you expect for the case of no binding enthalpy and entropy?