Fys2160 – 2013 – Oblig 3

Vacancies in a crystal

(This project is inspired by an exercise developed by Terje Finstad for Fys114).

In this project we will address micro- and macro-states of vacancies in a crystal using the machinery we have developed for the microcanonical ensemble.

In crystalline matter the atoms are organized into a regular pattern – a crystal lattice as shown in the figure. When the temperature is zero and the system is in perfect equilibrium all the atoms are in their minimum energy configurations and the lattice is perfectly ordered. However, at finite temperatures the lattice will no longer be perfectly ordered, because thermal fluctuations will introduce imperfections in the lattice. The atoms will oscillate around their average positions (this occurs even at zero temperature), but at finite temperatures the atoms may leave their lattice position and move to a different position. This may leave a vacancy – an empty space in the lattice – formed as an atom leaves its equilibrium position and migrates to the surface of the crystal. We do not here specify the migration mechanisms, but introduce an energy cost $\Delta\epsilon$ assiciated with the formation of a vacancy: We assume that the energy of the system increases by $\Delta\epsilon$ when an atom is moved from an interior position to the surface, forming a vacancy in the process.

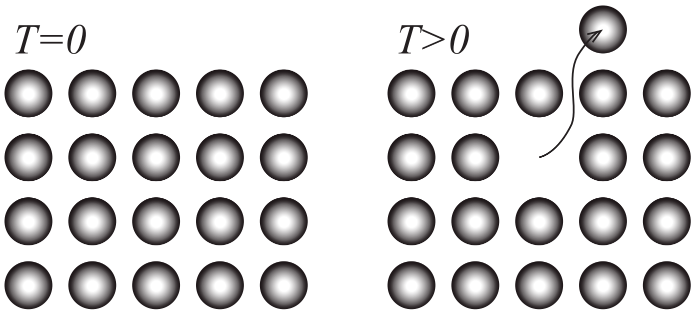

Figure 0.2: Illustration of a crystal with a vacancy.

(a) Find the multiplicity of a crystal with N atoms and n vacancies.

(b) Find the entropy $S = S(n, N, V)$.

(c) Find an approximation for the entropy without any factorials when $n \ll N$ and $N \gg 1$.

(d) What is the temperature of the crystal when it contains n vacancies.

(e) Find an expression for the number of vacancies as a function of T. Discuss if this is a fluctuating value in this system.

(f) How many vacancies are there in the limit when $T = 0$?

(g) If we assume that $\Delta\epsilon = 1\text{eV}$. Plot the concentration of vacancies as a function of T.

(h) Assume that $n \ll N$. Find an expression for the heat capacity as a function of temperature. Plot the heat capacity as a function of temperature from $T = 0$ to $T = 1000$ for this system. Comment.

(i) (Discussion question for class discussion): A real crystal will have several contributions to its entropy. Vacacies are one possibility. Interstitial atoms – atoms that occupy places in between the regular lattice spaces – are another. In addition we must include the base vibrations of the crystal. Discuss the contributions of the various effects to the entropy and to the heat capacity of a crystal.

Micro- and Macrostates of a polymer

(Exercise 3.34)

End of Oblig 3