

FYS2160 Termodynamikk og statistisk fysikk

Oblig 3

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Denne obligen inneholder 3 sider.

Exercise 1

- a) In a crystal with N atoms and n vacancies, there are in total $N + n$ spots where the atoms can take place. The multiplicity is therefore

$$\Omega(N, n) = \binom{N+n}{n} = \frac{(N+n)!}{n!N!} \quad (1)$$

- b) The entropy can then be written using the Boltzmann formula:

$$\begin{aligned} S &= k \ln \Omega \\ &= k \ln \binom{N+n}{n} \\ &= k \ln \left(\frac{(n+N)!}{n!N!} \right) \\ &= k [\ln((N+n)!) - \ln(n!) - \ln(N!)] \end{aligned} \quad (2)$$

- c) Using Stirling's approximation:

$$\ln(x!) \approx \ln \sqrt{2\pi x} + x \ln x - x \approx x \ln x - x, \quad (3)$$

where in the last transition the assumption of large x were made (OK since we are assuming $N \gg 1$), we can rewrite eq. (2):

$$\begin{aligned} S &\approx k [(N+n) \ln(N+n) - (N+n) - n \ln n + n - N \ln N + N] \\ &= k [(N+n) \ln(N+n) - n \ln n - N \ln N] \\ &= k \left[(N+n) \ln \left(N \left(1 + \frac{n}{N} \right) \right) - n \ln n - N \ln N \right] \\ &= k \left[(N+n) \left(\ln N + \ln \left(1 + \frac{n}{N} \right) \right) - n \ln n - N \ln N \right] \end{aligned} \quad (4)$$

Using Taylor expansion we get, for small x :

$$\ln(1+x) = x + O(x^2)$$

Using this under the assumption $n \ll N$, we can simplify eq. (4) to

$$S \approx kn \left[\ln \left(\frac{N}{n} \right) + \frac{n}{N} + 1 \right] \quad (5)$$

d) From the definition of temperature, we have that

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U} \right)_{N,V} \quad (6)$$

when the number of particles N and the volume V is held constant. To free atoms in the crystal so that there are n vacancies, requires energy equal to

$$U = n\Delta\epsilon \Rightarrow n = \frac{U}{\Delta\epsilon}$$

Plugging this back into eq. (5) and using eq. (6), we get

$$\begin{aligned} \frac{1}{T} &= \frac{\partial}{\partial U} \left(k \frac{U}{\Delta\epsilon} \left(\ln \left(\frac{N\Delta\epsilon}{U} \right) + \frac{U}{N\Delta\epsilon} + 1 \right) \right) \\ &= \frac{k}{\Delta\epsilon} \left(\ln \frac{N}{n} + \frac{2n}{N} \right) \\ \Rightarrow T &= \frac{\Delta\epsilon}{k} \left(\ln \frac{N}{n} + \frac{2n}{N} \right)^{-1} \end{aligned}$$

e) From the previous task, we have

$$T = \frac{\Delta\epsilon}{k} \left(\ln \frac{N}{n} + \frac{2n}{N} \right)^{-1}$$

In the limit when $N \gg n$ (i.e. small temperatures), $\ln \frac{N}{n} \gg \frac{2n}{N}$. In this limit, the temperature is

$$\begin{aligned} T &\approx \frac{\Delta\epsilon}{k} \left(\ln \frac{N}{n} \right)^{-1} \\ \Rightarrow n &\approx N e^{-\Delta\epsilon/(kT)} \end{aligned} \quad (7)$$

f) From eq. (7), it is evident that in the limit when $T \rightarrow 0$, $n \rightarrow 0$ which was the behaviour we wanted.

g) Assuming $\Delta\epsilon = 1$ eV, the concentration of vacancies n/N is plotted in figure 1

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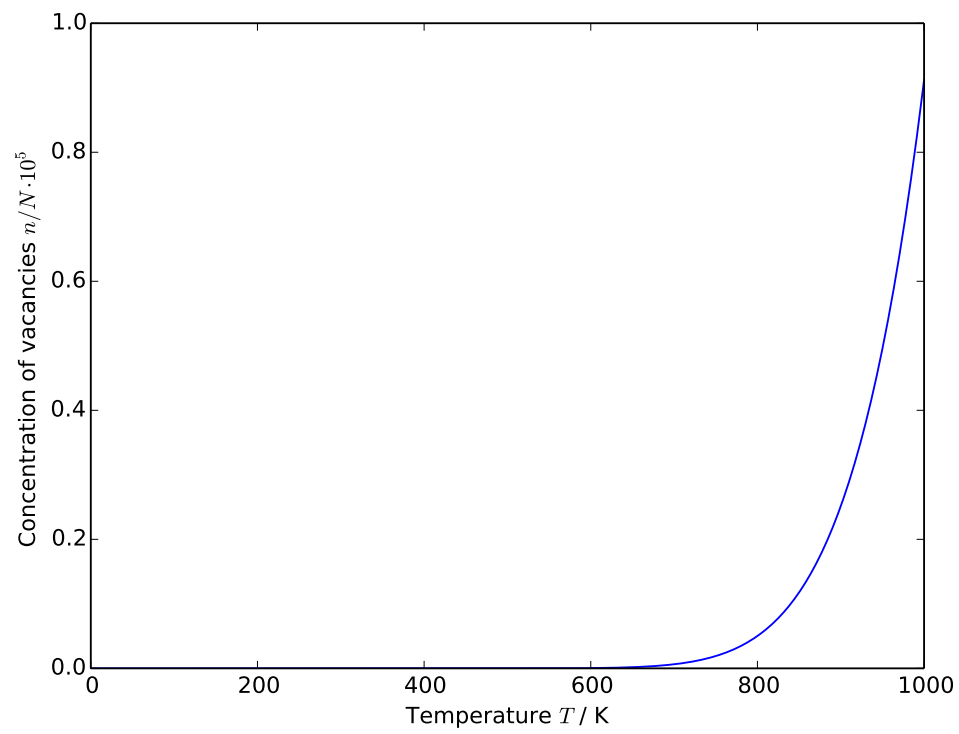


Figure 1: Concentration of vacancies n/N in the crystal as a function of temperature.