M00T.3

Solution to M00T.3 - Defects in a Crystal

a) We treat the on-site atoms and the defect atoms as two systems which can exchange energy and particle number. This leads us to write down a total partition function as the product of the partition function for each system. We also include a chemical potential in both subsystem partition functions. Then:

$$Z = (1 + z)^N (1 + ze^{\beta\epsilon})^{N_i}$$

where $z = e^{\beta\mu}$. Using the standard relation between the partition function and free energy, we find:

$$F = -kTln(Z) = -kT[Nln(1 + z) + N_i ln(1 + ze^{\beta\epsilon})]$$

So $f = F/N = -kT[ln(1 + z) + \rho\ ln(1 + ze^{\beta\epsilon})]$ We also conclude that the chemical potential must satisfy the relation:

$$N = N[\frac{z}{1+z} + \rho\ \frac{z}{e^{\beta\epsilon}+z}]$$

b) $n(T) = K/N$, where $K = N\rho\ \frac{z}{e^{\beta\epsilon}+z}$. So:

$$n(T) = \rho\ \frac{z}{e^{\beta\epsilon}+z}$$

c) We need to write out z explicitly to find its behavior at large and small temperatures. The solution to the above equation for z is:

$$z = \frac{1-\rho+\sqrt{(1-\rho)^2+4\rho\ e^{\beta\epsilon}}}{2\rho}$$

For $T \to \infty$, $z \to \rho^{-1}\left[1 + \frac{\epsilon}{T}\frac{\rho}{1+\rho} + \ldots\right]$. Then:

$$n = \frac{\rho}{1+\rho} - \frac{\epsilon}{T}\left(\frac{\rho}{1+\rho}\right)^2 + \ldots$$

For $T \to 0$, $z \to \rho^{-1/2}\ e^{2\beta\epsilon} + \ldots$ and:

$$n = \sqrt{\rho}\, e^{-2\beta\epsilon} + \ldots$$

d) $S = -kln(Z)$, so we can write it as:

$$S = -k[Nln(1+z) + N_i ln(1 + ze^{\beta\epsilon})]$$

Finally, $C = \frac{dE}{dT}$, but $E = \epsilon\ n(T)$. So:

$$C = \frac{\beta^2\epsilon}{\rho} e^{\beta\epsilon} z^{-1} n^2 [1 - \frac{e^{\beta\epsilon}}{sqrt(1-\rho)^2 + 4\rho\, e^{\beta\epsilon}}]$$