Thermal Physics

Defects in a Solid

Problem 1.- A crystalline solid contains N similar, immobile, independent defects.

Each defect has 5 possible states ψ_1, ψ_2, ψ_3, ψ_4, and ψ_5 with energies $E_1 = E_2 = 0$ and $E_3 = E_4 = E_5 = \Delta$.

a) Find the partition function for the defects.

b) Find the defect contribution to the entropy of the crystal as a function of Δ and the absolute temperature τ.

c) Calculate the contribution to the internal energy due to the defects in the limit $\tau >> \Delta$. Explain your reasoning.

Solution:

a) A single defect will have the following partition function:

$$Z_1 = \sum_s e^{-E_s/\tau} = e^{-0/\tau} + e^{-0/\tau} + e^{-\Delta/\tau} + e^{-\Delta/\tau} + e^{-\Delta/\tau} = 2 + 3e^{-\Delta/\tau}$$

Since the defects are independent and we have *N* of them, the partition function for the whole ensemble is:

$$Z = (Z_1)^N \rightarrow \; Z = \left(2 + 3e^{-\Delta/\tau}\right)^N$$

b) To find the entropy we can calculate the Helmholtz's free energy first:

$$F = -\tau \log(Z) = -\tau \log\left[(2 + 3e^{-\Delta/\tau})^N\right] = -\tau N \log\left(2 + 3e^{-\Delta/\tau}\right)$$

Then, the entropy is:

$$= -\left(\frac{\partial\left(-\tau N \log\left(2 + 3e^{-\Delta/\tau}\right)\right)}{\partial\tau}\right)_V = N\log\left(2 + 3e^{-\Delta/\tau}\right) + \frac{\tau N}{2 + 3e^{-\Delta/\tau}}(3e^{-\Delta/\tau})\left(\frac{\Delta}{\tau^2}\right)$$

$$\sigma = N\left(\log\left(2 + 3e^{-\Delta/\tau}\right) + \left(\frac{\Delta}{\tau}\right)\frac{3e^{-\Delta/\tau}}{2 + 3e^{-\Delta/\tau}}\right)$$

c) To find the contribution to the internal energy, notice that at high temperature the probability of a defect being in any state is the same, so the probability of having energy Δ is 3/5 and the probability of having zero energy is 2/5, so the contribution per defect is $3/5\,\Delta$ and for N defects, it will be:

$U_{defects} = 3/5 N \Delta$