

J09T.2 - Defects in a Lattice

Problem

In a lattice of N sites, each site is occupied by an atom at zero temperature. A lattice defect occurs when an atom moves to an interstitial site. The energy cost of a defect is Δ . At finite temperature T , we expect a finite number $\langle n(T) \rangle$ of defects to exist in equilibrium. Assume that defects do not interact with each other.

- a) Write down an expression for the partition function Z .
- b) Calculate $\langle n \rangle$ and the total free energy F of the lattice from Z at temperature T .
- c) Find the entropy $S(T)$ and heat capacity C_V from F .
- d) Use a purely statistical argument to rederive the entropy S starting with the total number of configurations W_n with n defects. Using your answer for $\langle n \rangle$, show that S agrees with part c).
- e) Use physical arguments to reproduce your answer for C_V in the low T limit ($\beta\Delta \gg 1$, where $\beta = 1/k_B T$).