M00T.3—Defects in a Crystal

Problem

In a crystal lattice, a defect is created when an atom hops from a lattice site to an interstitial site. The ground state is a configuration with no defects. However, when the lattice is in *equilibrium* at a finite temperature T, defects appear spontaneously.

Consider the case where the number, N, of atoms is equal to the number of lattice sites and the number of possible interstitial sites is N_i. Consider the thermodynamic limit where $N,\ N_i \to \infty$ at constant $N_i/N = \rho$. The energy required to create a defect is ε. Denoting by K the number of defects, let $n = K/N$ be their density.

a) Find an expression for the *free energy* per particle at temperature T.

b) Calculate the density of defects, $n(T)$.

c) Sketch the curve of $n(T)$ versus T and describe the behavior of $n(T)$ as $T \to 0$.

d) Calculate the entropy S and the heat capacity C *due to the defects* at temperature T.