

SMA One class of defects in a crystal are *vacancies* — *i.e.* atomic sites at which no atom is located. Vacancies are rare because the unsatisfied chemical bonds cost energy. To estimate how many vacancies occur in thermal equilibrium we will assume that either an atom or a vacancy can sit on each site of a cubic lattice with lattice constant a . We will also assume that the energy cost per vacancy is \mathcal{E} .

- a) Each atom or vacancy occupies volume a^3 . What is the change in volume of an N -atom crystal when n vacancies are incorporated?
- b) What is the difference in entropy between a crystal with N atoms and no vacancies and one with N atoms and n vacancies? (You may use Stirling's approximation in the form $\ln n! = n \ln n - n$ and the assumption $n/N \ll 1$ to simplify your answer.)
- c) Applying a pressure P to the crystal is likely to reduce the number of vacancies. By computing a suitable partition function or otherwise, find an expression for the fraction n/N of vacancies as a function of \mathcal{E} , a , P and the temperature T .
- d) If the perfect crystal has atomic density 10^{28} m^{-3} , how much pressure has to be applied to halve the number of vacancies at $T = 1\text{K}$ and also at $T = 1000\text{K}$?