Problem session 3

Problem 3.1
Consider a liner ionic crystal containing 2N ions of alternating charge ±q. Assume two different repulsive potentials: (a) A/R and (b) A/R^2. What would be the equilibrium separation between atoms (R_0) and total energies for crystals (a) and (b)? What would be the total energy associated with crystal (b) if it is compressed so that the separation between atoms $R = R_0/2$?

Problem 3.2
The cubic crystal is subjected to tension in [100] direction. Find the expressions in terms of elastic stiffnesses for Young's modulus and Poisson ration as defined in Fig.21 in p.87 in Kittel's book.

Problem 3.3
Show that the minimum free energy in a crystal having N sites is reached only when a certain number of defects (n) are available. Derive an expression for the concentration of vacant sites (C_V) in a crystal kept at temperature T and compressive isotropic pressure P. Explain the quantities of activation energy and activation volume. Hint: Minimize the free energy $G = U - TS + PV$, expressed as a function of the number of vacant sites. The relation $\ln X! \approx X(\ln X - 1)$, valid for large X, might be useful.

B. Problem 3.4
Suppose that the energy required to remove a silicon atom from the bulk of a silicon crystal to the surface is 4eV. Calculate the concentrations of Schottky vacancies in Si at normal conditions at 300 and 1687K. Assume that the activation volume of a silicon vacancy is roughly equal to the Si atomic volume in the crystal. How much of isotropic pressure, in terms of magnitude and sign, should be applied at 300K to lift the vacancy concentration up to that 1687K? Note, that 1687K is a melting temperature for Si at normal conditions.