

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I

Due on Wed., Sept. 27.

Problem set #3

1. Consider an orthorhombic C lattice whose conventional unit cell has a size $a \times b \times c$. Determine the reciprocal lattice by giving the fundamental translation vectors \vec{b}_1 , \vec{b}_2 , and \vec{b}_3 , and specifying the Bravais lattice type.
2. In the book (and in the lecture), the Van der Waals attraction is calculated for two harmonic oscillators of same mass m and same spring constant K . Generalize that result to the case where the spring constants of the two oscillators are different and given by K_1 and K_2 . (The mass is still assumed to be the same.)
3. Assume that the interaction between two ions of charge q_i and q_j is given by

$$U_{ij} = \frac{q_i q_j}{r} + \frac{e^2}{a} \left(\frac{a}{r} \right)^{12} \quad (1)$$

To see how good (or bad) is the above form of interaction, determine the values of a for NaF and RbCl using the nearest neighbor separations in table 7 of the Kittel book on page 66. Then calculate the lattice energy compared to free ions per NaF or RbCl. (Note $e^2/1\text{\AA} = 14.39\text{eV}$.) Compare your result with the data in the table 7.

The values for γ_6 and γ_{12} are given by

lattice:	FCC	SC	BCC	diamond
γ_6 :	14.5	8.40	12.2	5.12
γ_{12} :	12.1	6.20	9.1	4.04

4. Problem 7 on page 86 in Kittel book.
5. (Due on Wed. Oct. 4)

A simplified interaction between two ions of charge q_i and q_j is given by

$$U_{ij} = \frac{q_i q_j}{r} + f \frac{e^2}{a} \left[\left(\frac{a}{r} \right)^{11} - \left(\frac{a}{r} \right)^6 \right] \quad (2)$$

which include both the Coulomb and a modified Van der Waals interaction (the exponent 12 is changed to 11). Let the charges of the two kinds of ions are given by ne and $-ne$. Here we treat n as a continuous parameter. Depending on different values of f and n , the two kinds of ions may form several kinds of crystals, which include CsCl, NaCl, and the cubic ZnS structures. In this project, we like to calculate the phase diagram of the system. Determine for what ranges of f and n that the ions form the CsCl, NaCl, or the cubic ZnS structures. Present your result in a 2D phase diagram in f - n plane. (You might need to write a small program to calculate $\gamma_{11} = \sum_j' 1/p_{ij}^{11}$. Note that γ_{11} is slightly larger than γ_{12} .)