Problem session 2

A. Problem 2.1

Consider a (*hkl*) plane in a crystal lattice. (a) Prove that the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to this plane. (b) Prove that the distance between two adjacent planes of the lattice is $d_{hkl} = 2\pi / \left|\vec{G}\right|$. (c) Show that for a simple cubic lattice $d^2{}_{hkl} = a^2 / (h^2 + k^2 + l^2)$.

B. Problem 2.2

Show that maxima of diffraction signals obtained from a crystal correspond to reciprocal lattice points. (Tips: Consider an incoming plane wave and treat lattice points as scattering elements for outgoing circular waves. Find criteria for constructive interference for this wave. You may benefit from develop the Laue conditions and apply the Ewald construction). Map low index (≤2) *hkl*-families of planes in two dimensional reciprocal space of a crystal having triclinic symmetry.

C. Problem 2.3

Consider specifically the reciprocal lattice vector $\vec{G}$ corresponding to (010) family of plains. Show that x-ray waves having $\vec{k}$-vectors smaller than $1/2\vec{G}$ can not undergo diffraction at these planes. Developing Laue equation $\Delta\vec{k} = \vec{G}$ to the form of $2\vec{k} \bullet \vec{G} = \vec{G} \bullet \vec{G}$ and considering the Bragg plane may be useful. Are there any other planes available for the waves having $\vec{k}$-vectors smaller than $1/2\vec{G}$ in this particular case to undergo diffraction? Generalize to the Brillouin zone concept.

D. Problem 2.4

Using λ and ρ values taken from Table 7 in the Kittel book (p.66) and Madelung constants given in p.65 (Kittel book) calculate the cohesive energies of KCl in cubic zinc blend and rock salt structures. Compare the values and conclude.