I. PROBLEM SESSION 2

A. Problem 2.1

Write down the primitive translation vectors of the simple cubic lattice. The reciprocal lattice is defined as the set of all wave vectors $\vec{K}$ that yields plane waves with the periodicity of the given Bravais lattice(i.e $e^{i\vec{K}(\vec{r}+\vec{R})} = e^{i\vec{K}\vec{r}}$, where $\vec{r}$ is an arbitrary vector and $\vec{R}$ is a lattice vector). Find the reciprocal lattice vectors of the cubic cell and check that the definition holds.

A symmetric set of primitive vectors for the FCC primitive cell is

$$\vec{a_1} = \frac{a}{2}(\hat{y}+\hat{z}), \;\; \vec{a_2} = \frac{a}{2}(\hat{z}+\hat{x}), \;\; \hat{a_3} = \frac{a}{2}(\hat{x}+\hat{y}). \tag{1}$$

-Show that the primitive translation vectors of the reciprocal lattice is:

$$\vec{b_1} = \frac{2\pi}{a}(\hat{y}+\hat{z}-\hat{x}), \;\; \vec{b_2} = \frac{2\pi}{a}(\hat{z}+\hat{x}-\hat{y}), \;\; \hat{b_3} = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}). \tag{2}$$

-What Bravais lattice does this vectors describe?
-Describe and sketch the first Brilloin zone (reciprocal Wigner-Seitz) of this real space FCC lattice.

B. Problem 2.2

Consider the plane hkl 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 $d_{hkl} = \frac{2\pi}{|\vec{G}|}$. (c) Show that for a simple cubic lattice that $d^2 = a^2/(h^2+k^2+l^2)$.

C. Problem 2.3

Show that the maxima of diffraction signals obtained from a crystal correspond to reciprocal lattice points and map hkl-families of planes in the real space. (Tip: Consider an incoming plane wave and treat lattice points as scattering centra for outgoing circular waves. Find criteria for constructive intderference for this wave, you might want to develop the Laue conditions and apply the Ewald construction).

D. Problem 2.4

(Optional, but might be useful before doing the last exercise) Structure factor of diamond: If the cell of the diamond lattice is taken as the conventional cube (see chap1 Kittel), then the basis consist of eight atoms.
-Find the structure factor S in this basis.
-Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where the indices are even and n is any integer, or else all indices are odd (Fig. 18 Kittel).

E. Problem 2.5

A reflection from the (111) planes of a cubic crystal was observed at an angle $\theta = 11.2°$ using Cu Kα radiation ($\lambda = 1.5418$Å). What is the length of the side of the unit cell? Most accurate d-spacings are those calculated from high-angle peaks, why? Consider specifically copper appearing in BCC form having aunit length of 3.613Å. What is the Bragg angle for the (100) reflection with Cuα radiation ($\lambda = 1.5418$Å)? List and provide clarifications on factors limiting the number of reciprocal lattice points observed in diffraction experiments.