

I. PROBLEM SESSION 2

A. Problem 2.1

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 $d^2 = a^2/(h^2 + k^2 + l^2)$.

B. Problem 2.2

The primitive translation vectors of the hexagonal space lattice may be taken as:

$$\vec{a}_1 = a\frac{\sqrt{3}}{2}\hat{x} + \frac{a}{2}\hat{y}, \quad \vec{a}_2 = -a\frac{\sqrt{3}}{2}\hat{x} + \frac{a}{2}\hat{y}, \quad \vec{a}_3 = c\hat{z}. \quad (1)$$

-Show that the volume of this primitive cell is $\frac{\sqrt{3}}{2}a^2c$.

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

$$\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}, \quad \vec{b}_2 = -\frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}, \quad \vec{b}_3 = \frac{2\pi}{c}\hat{z}. \quad (2)$$

Such that the lattice is its own reciprocal, but with a rotation of the axes.

-Describe and sketch the first Brillouin zone (reciprocal Wigner-Seitz) of the hexagonal space lattice.

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 - develop Laue conditions and use the Ewald construction).

D. Problem 2.4

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).