PHYS*4150: Problem Set 3

Distributed: Friday February 8, 2019
Due: Friday March 1, 2019 at 10:30am

Problem 1 (20 pts): Reciprocal lattice

a) Ashcroft & Mermin question 5.1, parts a) and b).

b) In class we showed that the reciprocal of a FCC lattice is a BCC lattice. Use the same analysis to show that the reverse is also true.

c) For a simple cubic lattice (side length a), show that the reciprocal of the reciprocal lattice is the original lattice.

Problem 2 (25 pts): Miller planes

a) Show that the reciprocal lattice vector $\mathbf{K} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is perpendicular to the Miller plane defined by h, k, l.

b) Sketch the follow Miller planes in the unit cell of a simple cubic lattice (separately):

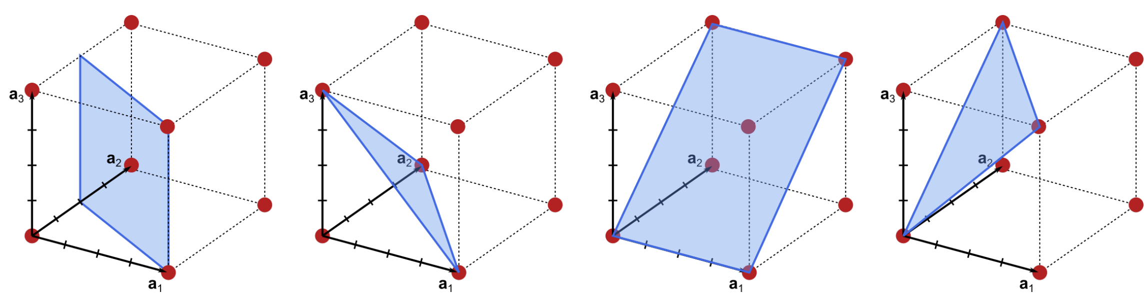
i) $(1, 3, 3)$

ii) $(2, 0, 1)$

iii) $(\bar{1}, 1, 0)$

iv) $(\bar{2}, \bar{1}, 2)$

c) Label each of the planes shown below with their Miller indices. Sketch the view of the lattice in each plane and label the dimensions appropriately. Assume the side length of the cubic cell is a.



Problem 3 (5 pts): Bragg diffraction

Prove the equivalence of the Von Laue and Bragg conditions for diffraction:

$$\begin{aligned} \text{Von Laue:} \quad & \mathbf{K} = \mathbf{k} - \mathbf{k}', \\ \text{Bragg:} \quad & 2d \sin\theta = m\lambda, \quad \text{for m=integer.} \end{aligned} \tag{1}$$

Problem 4 (15 pts): Powder diffraction

Ashcroft & Mermin question 6.1, parts a) and b). Read pages 101 to 104 and note Eq. 6.12 to aide in your understanding:

$$\mathbf{K} = 2k \sin\frac{\phi}{2}. \tag{2}$$

Problem 5 (10 pts): Atomic form factor

a) The *atomic form factor* is defined as the Fourier transform of the electronic distribution function of atom j in the lattice basis, $\rho_j(\mathbf{r})$:

$$f_j(\mathbf{K}) = \int \rho_j(\mathbf{r}) e^{\mathrm{i}\mathbf{K}\cdot\mathbf{r}}\, \mathrm{d}^3\mathbf{r}\,. \tag{3}$$

The function $\rho_j(\mathbf{r})$ is a spacial distribution and is normalized such that $\int \rho_j(\mathbf{r})\,\mathrm{d}^3\mathbf{r} = Z$, where Z is the total number of electrons in the atom/ion. If the electrons of an atom are localized at $\mathbf{r} = 0$, show that f_j simplifies to a constant equal to Z. (*Hint: in this case, the electronic distribution function is essentially a delta-function centered at each atom.*)

b) Instead, now assume $\rho_j(\mathbf{r})$ to be spherically symmetric ($\rho_j(\mathbf{r}) = \rho_j(r)$). Show that $f_j(\mathbf{K})$ is given by:

$$f_j(\mathbf{K}) = 4\pi \int r^2 \rho_j(r) \frac{\sin Kr}{Kr}\, \mathrm{d}r\,. \tag{4}$$

Recall that the dot product between two vectors can be written in the form $\mathbf{a}\cdot\mathbf{b} = ab\cos\theta$, where θ is the angle between the vectors.

In the limit $r \to 0$, the results from a) and b) are identical (you do not need to show this).

Problem 6 (20 pts): Structure factor

Potassium chloride (KCl) can be described by a simple cubic lattice with an 8-pt basis of:

$$\begin{array}{ll} \text{potassium ions at} & (0,0,0), (\tfrac{1}{2},\tfrac{1}{2},0), (\tfrac{1}{2},0,\tfrac{1}{2}), (0,\tfrac{1}{2},\tfrac{1}{2}), \\ \text{chloride ions at} & (\tfrac{1}{2},0,0), (0,\tfrac{1}{2},0), (0,0,\tfrac{1}{2}), (\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}). \end{array} \tag{5}$$

The coordinates are written in the form $(\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3})$ where $\mathbf{a_i}$ are the normal primitive cell vectors for a simple cubic cell of side length a.

a) Calculate the structure factor for KCl:

$$S_{\mathbf{K}} = \sum_j f_j e^{\mathrm{i}\mathbf{K}\cdot\mathbf{d_j}} \tag{6}$$

Assume atomic form factors of f_{K^+}, f_{Cl^-} for the potassium and chloride ions. The reciprocal lattice vectors can be written as $\mathbf{K} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ where $\mathbf{b_i}$ are the primitive lattice vectors of the reciprocal lattice. Consider the cases of $h, k, l \to$ odd/even to show that the relative intensity of diffracted spots is:

$$|S_{\mathbf{K}}|^2 = \begin{cases} 16|f_{K^+} + f_{Cl^-}|^2, & h,k,l \quad \text{all even} \\ 16|f_{K^+} - f_{Cl^-}|^2, & h,k,l \quad \text{all odd} \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

b) Sketch the planes of the reciprocal lattice corresponding to $l =$ even and $l =$ odd. Clearly indicate the scattering intensity of the reciprocal lattice points. Sketch the cubic unit cell, again indicating the scattering intensity of the points.

c) Both of the ions K^+ and Cl^- have 18 electrons (note their positions on the periodic table). Using the approximation shown in Problem 5 b), the atomic form factors of the ions can be expressed as $f_{K^+} = f_{Cl^-} = Z = 18$. How does this approximation simplify the reciprocal lattice? Sketch it, noting the type of lattice and the size of the cubic unit cell. What is the real space lattice corresponding to this new reciprocal lattice, and what is the size of the cubic unit cell?