Assessment

Solid-state physics

UNIVERSITY of TASMANIA

Assignment 5: the reciprocal lattice and scattering

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Due: 1700, October 11, 2021

Exercise 1 *The reciprocal lattice* (11 points)

Following the normal conventions, let us denote $\mathbf{a}_i$ and $\mathbf{b}_i$ as the real-space and reciprocal space lattice vectors.

(i) A construction of lattice vectors can be achieved using the relation

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

Explicitly compute $\mathbf{a}_1 \cdot \mathbf{b}_1$, $\mathbf{a}_2 \cdot \mathbf{b}_1$, and $\mathbf{a}_3 \cdot \mathbf{b}_1$. Do these computations accord with the definition of the reciprocal lattice?

(ii) The volume of a primitive unit cell with lattice vectors $\mathbf{a}_i$ is given by $V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$. Find the volume of the corresponding primitive unit cell in reciprocal space.

(iii) Show that the general direction $[hkl]$ in a cubic crystal is normal to the planes with Miller indices (hkl).

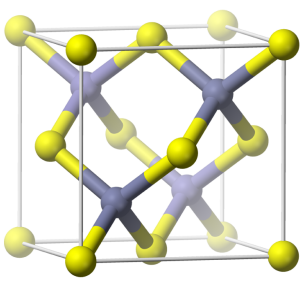
(iv) Is the above statement true for an orthorhombic crystal? Justify your response.

(v) Show that the distance between two adjacent Miller planes (hkl) of any lattice is $d = 2\pi/|\mathbf{G}_{\text{min}}|$, where $\mathbf{G}_{\text{min}}$ is the shortest reciprocal lattice vector perpendicular to these Miller planes.

(vi) Find the family of Miller planes of the BCC lattice that has the highest density of lattice points. It may of useful to think about the density of lattice points per unit area on a Miller plane which is given by $\rho = d/V$.

Exercise 2 *Lattice planes* (4 points)

In assignment four, you looked at the structure of zincblende (ZnS) (zinc atoms are yellow, sulphur atoms are grey).



(i) Draw a simplified plan view (don't worry about indicating heights) down the [001] axis, and indicate the [210] direction and the (210) family of planes

(ii) The confidence tester: explain why the family of planes above is or is not a family of lattice planes.

- If it is a family of lattice planes, do nothing and be content with your decision

- If it is not a family of lattice planes, what would be a family of lattice planes in the same direction?

Exercise 3 *Scattering* (7 points)

(i) What is the origin of the Laue condition? That is, why is the amplitude of a scattered wave zero if $\mathbf{k}' - \mathbf{k} \neq \mathbf{G}$?

(ii) Consider a two-dimensional crystal with a rectangular lattice and lattice vectors $\mathbf{a}_1 = (0.468, 0)\,\text{nm}$ and $\mathbf{a}_2 = (0, 0.342)\,\text{nm}$ (so that $\mathbf{a}_1$ points along x-axis and $\mathbf{a}_2$ points along y-axis).

(a) Sketch the reciprocal lattice of this crystal

(b) Consider an X-ray diffraction experiment performed on this crystal using monochromatic X-rays with wavelength 0.166 nm. Assuming elastic scattering, find the magnitude of the wave vectors of the incident and reflected X-rays

(c) On your sketch of the reciprocal lattice, draw the "scattering triangle" corresponding to the diffraction from (210) planes. Explicitly, use the Laue condition $\Delta\mathbf{k} = \mathbf{G}$ for constructive interference of diffracted X-rays

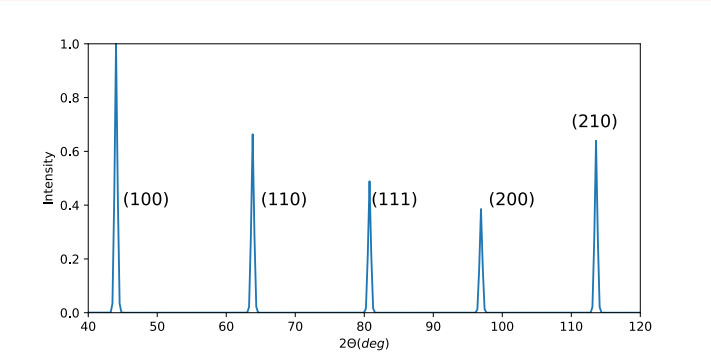
Exercise 4 *Diffraction and structure* (9 points)

(i) Compute the structure factor S of the BCC lattice.

(ii) Which diffraction peaks are missing?

(iii) How does this structure factor change if the atoms in the centre of the conventional unit cell have a different form factor from the atoms at the corner of the conventional unit cell?

(iv) A student carried out X-ray powder diffraction on chromium (Cr) which is known to have a BCC structure, and the first five diffraction peaks are given below. Delightfully, the student took the liberty of assigning Miller indices to the peaks. Were the peaks assigned correctly? Fix any mistakes and explain your reasoning.



(v) The X-ray diffraction was carried out using Cu K_α radiation ($\lambda = 1.5406\,\text{Å}$). Use this information to calculate the lattice constant a of the chromium BCC unit cell.