Assessment

Solid-state physics

Assignment 6: the reciprocal lattice, scattering, and semiconductors

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Due: 1700, October 16, 2023

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).

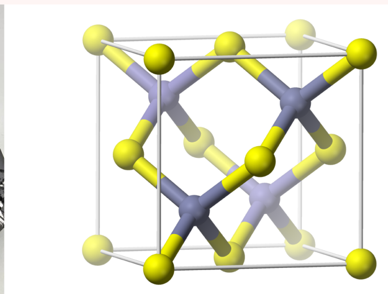
(iv) Is the above statement true for an orthorhombic crystal? Justify your response.

(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 five, 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 $\mathbf{a}_1 = (0.468, 0)$ nm and $\mathbf{a}_2 = (0, 0.342)$ 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

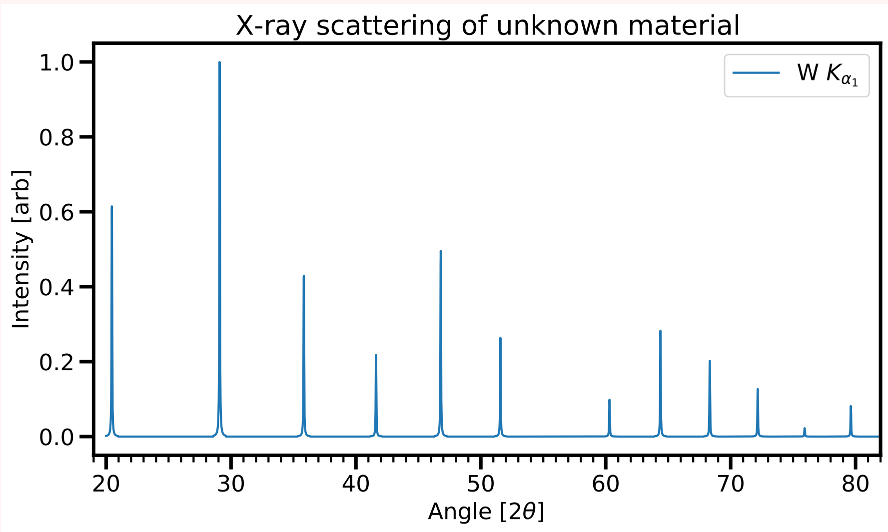
(c) On your sketch of the reciprocal lattice, draw the "scattering triangle" corresponding to the diffraction from (210) planes. Explicitly, use the Laue condition $\Delta\mathbf{k} = \mathbf{G}$ for constructive interference of diffracted X-rays

Exercise 4 *Structure determination* (15 points)

A diffraction experiment with an unknown crystalline powder sample was performed using an X-ray tube with a tungsten anode. Tungsten has K_α emission lines $K_{\alpha_1} = 59318.8\,\text{eV}$ and $K_{\alpha_2} = 57981.9\,\text{eV}$, and the ratio of intensities of the emissions lines is $\alpha_2/\alpha_1 \approx 0.115$.

(i) Explain how X-rays are produced from X-rays tubes, and describe how one would go about performing a powder diffraction experiment.

(ii) Shown below is a plot of the diffraction data measured from the experiment using the K_{α_1} emission line:



(a) Following the recipe discussed in class, produce a table with columns: diffraction angle, plane separation, ratio of the square of first plane separation to plane separation (d_a^2/d^2), $N = h^2 + k^2 + l^2$, hkl, and a (assuming some kind of cubic lattice).

(b) Use the table above to determine the lattice structure of the crystal

(iii) The basis of the lattice is given by $X = [0,0,0]$ and $Y = [1/2, 1/2, \beta], [1/2, 1/2, (1-\beta)], [1/2, \beta, 1/2], [1/2, (1-\beta), 1/2], [\beta, 1/2, 1/2]$, and $[(1-\beta), 1/2, 1/2]$ where X and Y are different atomic species, and $\beta \approx 0.2$.

   (a) Draw the unit cell for the crystal using your lattice and the basis specified above.

   (b) Explain how the intensity of the peaks could be used to determine β, and obtain an expression for the ratio of the first two diffraction peaks. Note: You do not need to solve this equation for β, just arrive at something that could be used to calculate β.

(iv) Imagine the experiment was altered such that both K_{α_1} and K_{α_2} emission lines were present. How would this alter the data as recorded above? Would you expect that one could still uniquely determine the crystal structure of the sample?

(v) Now imagine that the experiment were altered such that only K_{α_1} radiation were used, but a monocrystalline sample were used. What would be the difference in the recorded diffraction pattern?

(vi) Unfortunately, the beautiful single crystal was dropped before it could be used, resulting in a sample that is neither amorphous nor monocrystalline, rather something between the two. How would this alter the appearance of the diffraction pattern?

Note that for this question, the code as used in a *content unpacking* session can be found here, and a file containing the data used to produce the above plot is available here.

Exercise 5 *The nearly-free electron model* (12 points)

Consider an electron in a weak periodic potential in one dimension $V(X) = V(x+a)$. It is natural to write the potential as

$$V(x) = \sum_G e^{iGx} V_G$$

where the sum is over the reciprocal lattice $G = 2\pi n/a$ and $V_G* = V_{-G}$ assures the potential $V(x)$ is real.

(i) Explain why for k near to a Brillouin zone boundary (such as k near π/a) the electron wavefunction should be taken to be

$$\psi = Ae^{ikx} + Be^{i(k+G)x}$$

where G is a reciprocal lattice vector such that $|k|$ is close to $|k+G|$.

(ii) We have seen that with the above wavefunction, the energy (that is, the eigenvalues) at this wavevector are given by

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_G|$$

where G is chosen such that $|k| = |k+G|$.

   (a) Give a qualitative explanation of why these two states are separated in energy by $2|V_G|$

   (b) Provide a sketch or plot of the energy as a function of k in both the extended and reduced zone schemes. Note that one need not compute E for all k, emphasis should be on the general features of the energy spectrum.

(iii) Let us look at the case where k is not at the Brillouin zone boundary, but rather close to the boundary. Following the same method as used to achieve the above result, show that at the point $k = n\pi/a + \delta k$ the energy to second order in δk is given by

$$E_{\pm} = \frac{\hbar^2 (n\pi/a)^2}{2m} + V_0 \pm \left|V_{2n\pi/a}\right| + \frac{\hbar^2 (\delta k)^2}{2m} \left(1 \pm \frac{\hbar^2 (n\pi/a)^2}{m \left|V_{2n\pi/a}\right|}\right)$$

(iv) Calculate the effective mass of an electron at this wavevector

Exercise 6 *Semiconductors: holes* (14 points)

(i) In the context of semiconductor physics, what is meant by a hole and why is it useful?

(ii) An electron near the top of the valence band in a semiconductor has energy

$$E = -10^{-37} |k|^2$$

where E is in Joules, and k is in m^{-1}. An electron is removed from a state $k = 2 \times 10^8 \, \mathrm{m}^{-1} \hat{x}$, where $\hat{x}$ is the unit vector in the $x-$direction. For a hole, calculate (including the sign)

(a) the effective mass

(b) the energy

(c) the velocity

(d) the momentum

(iii) If there is a density $p = 10^5 \, \mathrm{m}^{-3}$ of such holes all having almost exactly this same momentum, calculate the current density and its sign.

Exercise 7 *Semiconductor devices* (10 points)

Choose a semiconductor device of interest (a few examples are provided below, but choose anything), research it, and explain what the device is and how it functions, with an emphasis on the material covered in this course.

- Zener diode
- Laser diode
- Solar cell
- Hall effect sensor