



Discussion on 15th March

Due on 22nd March

Exercise 1 *Laue method*

Estimate the maximal possible number of interference maxima of a Laue recording. Assume that the voltage of the X-ray tube is 60 kV and the crystal is simple cubic with a lattice constant of 0.2 nm. The X-ray tube produces a continuous spectrum of Bremsstrahlung.

Exercise 2 *Debye-Scherrer method*

Powder specimens of three different monoatomic cubic crystals are analysed with a Debye-Scherrer camera. It is known that one sample is face-centred cubic, one is body-centred cubic, and one has the diamond structure. The approximate positions of the first four diffraction rings in each case are given in table 1. The meaning of the angle ϕ is shown in figure 1. Pay attention to the definition of the angle in Bragg's law and the definition of the angle in the figure.

A	B	C
42.2°	28.8°	42.8°
49.2°	41.0°	73.2°
72.0°	50.8°	89.0°
87.3°	59.6°	115.0°

Table 1: The angles ϕ of the diffraction rings in samples A, B, and C.

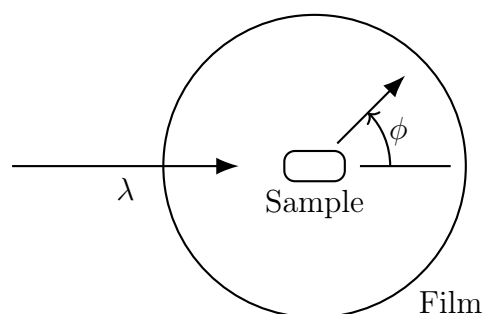


Figure 1: The working principle of a Debye-Scherrer camera.

- Identify the crystal structure of A, B, and C.
- If the wavelength of the incident X-ray beam is 1.5 \AA , what is the length of the side of the conventional cubic cell in each case?
- If the diamond structure were replaced by a zincblende structure with a cubic unit cell of the same side, at what angles would the first four rings now occur?

Exercise 3 *Screened and unscreened Coulomb potentials*

a) The screened Coulomb potential

$$V(r) = \frac{qQ}{4\pi\epsilon_r\epsilon_0 r} e^{-r/\lambda_D} \quad (1)$$

describes the Coulomb interaction in, for example, an ionic solution. Its typical reach is λ_D (the Debye screening length). In cells λ_D is very small, which is why biological systems feel essentially no Coulomb force. Calculate the differential scattering cross section

$$\frac{d\sigma}{d\omega} = \left| f(\vec{k}, \vec{k}') \right|^2,$$

where

$$f(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2} \int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} V(\vec{r}) d^3r.$$

The result should (hopefully) be:

$$\frac{d\sigma}{d\omega} = \left(\frac{2mqQ}{\hbar^2 4\pi\epsilon_r\epsilon_0} \right)^2 \frac{1}{[2k^2(1 - \cos\Theta) + \lambda_D^{-2}]^2}. \quad (2)$$

b) Derive the scattering cross section for the unscreened Coulomb potential by considering the limit $\lambda \rightarrow \infty$ (no screening). (Plug this into equation (2).) Why is it necessary to compute the case for the screened potential first? Why do we not take the unscreened Coulomb potential in equation (1)?