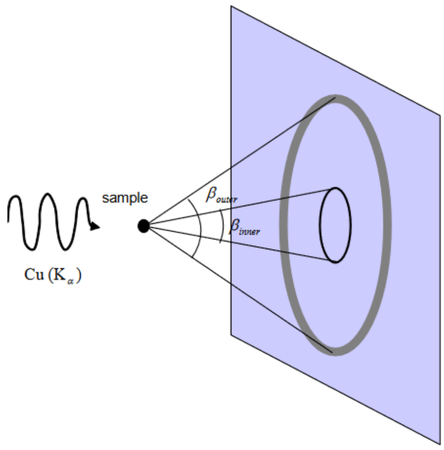
Exercise 5.1 (X-ray diffraction of LCs)

In a diffraction experiment, Cu (K_α) radiation with a wavelength of 1.54 Å is scattered by a liquid crystalline sample. Two reflexes are observed, an outer blurred halo with a cone angle β_{outer}= 40° and an inner sharp reflection at a cone angle of about β_{inner} = 6°.



a) What kind of liquid crystalline phase could give rise to this diffraction pattern?

b) Calculate the structural parameters of this phase.

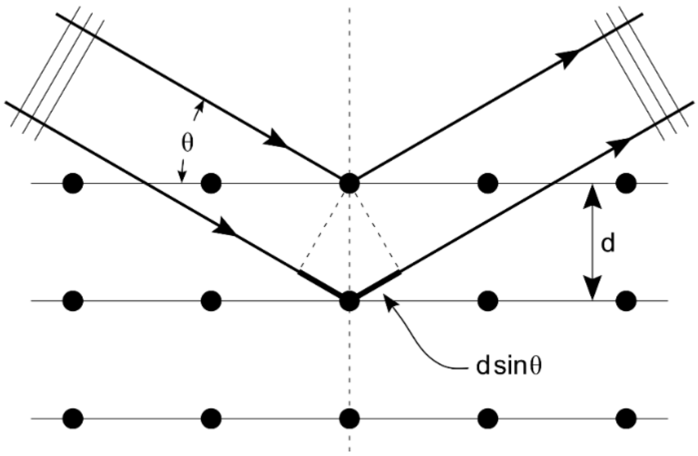
Exercise 5.1. Solution

In X-ray diffraction crystallography experiment the incoming X-ray radiation is scattered by crystal sample and creates specific scattering pattern depending on the structure of crystal lattice.

For the set of parallel planes, constructive interference between reflected rays occurs when the optical path difference $2d\sin\theta_m$ is equal to the integer number of wavelengths (the Bragg's law for the crystal lattice):

$$2d\ \sin\theta_m = m\lambda$$

Where λ is the wavelength, d is the separation of planes, θ_m angle of m-th order diffraction, m is the diffraction order (m is integer).



For a set of equidistant planes, the scattering intensity is zero everywhere except for angles where Bragg's law is satisfied. If the sample is a powder sample that composed of many microdomains with random orientation, Bragg's law will be satisfied for many of the randomly oriented domains, and the pattern will be averaged into a ring around the incident beam (see the picture in the exercise).

Often the higher order diffraction peaks are weak and we can neglect them in this exercise.

The inner cone that we observe in this experiment corresponds to a larger lattice distance than the outer cone. Also it is sharp, therefore corresponding to a well-ordered periodic structure. The outer cone therefore corresponds to smaller lattice distance and the fact that it is blurred indicates a non-perfect periodicity. Looking at the structure of liquid crystals with smectic phases, we indeed do find two such lattice distances. The first one corresponds to planes where molecules are arranged with their molecular axis perpendicular (or slightly tilted) with respect to the plane. This gives rise to the sharp inner cone in the X-ray diffraction pattern. The second lattice distance stems from the interplanar distances between molecules, which do not form a perfectly periodic lattice. In the X-ray diffraction pattern this corresponds to the outer blurred cone.

B) According to Bragg's law, we can calculate the lattice distances. However, it is important to note the relation between the given angles β and the scattering angles θ. The angle β is the full angle of the cone, so the angle from the incident beam axis will be $\beta/2$. At the same time, the scattering angle θ in Bragg's law corresponds to the angle incident to the plane (see figure above). Therefore, we have $\theta = \beta/4$.

For the outer cone:

$$d = \lambda/2\sin\theta_{outer} \approx 4.43\ A$$

For the inner cone:

$$d = \lambda/2\sin\theta_{inner} \approx 29.4\ A$$

Thus, we can assume, that the sample is a powder sample of smectic liquid crystal with average distance between molecules in a layer of 4.4 Å , and distance between equidistant planes of 29.4 Å .

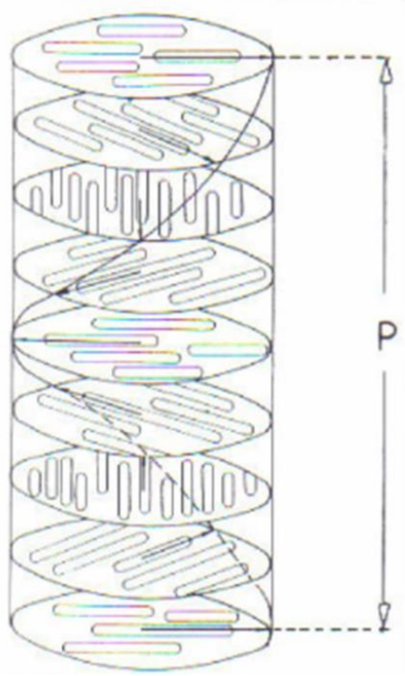
Exercise 5.2 (twisted nematic LCs)

In a twisted nematic (cholesteric) liquid crystal, polarized light passing through the crystal along the twist direction exits the crystal with a different polarization.

a) Explain the origin of this phenomenon called optical activity.

b) Given that the refractive index of right-handed circularly polarized light (n_R=1.55) and left handed circularly polarized light (n_L=1.50) are different, calculate the rotation of the incident polarization of the light beam after passing through the crystal with a thickness of 1 μm. The wavelength of the incident light is 500 nm.

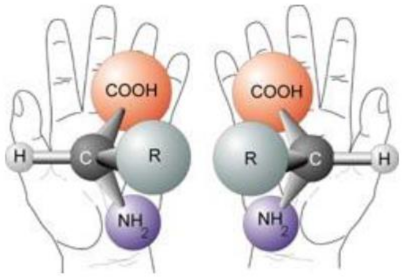
c) What would be the thickness required to turn the polarization by 90°?



Exercise 5.2 solution.

A) Optical activity in general the ability of a medium to rotate the plane of plane-polarized light. The origin of the optical activity is the different permittivity of the medium for different polarizations because of the structure.

There are two groups of optically active media. The first group exhibit the optical activity only in crystal (ordered) phase. For this group the optical activity is the property of the crystal as a whole, so the molecules themselves don't show the effect of optical activity. The second group of optically active materials exhibit intrinsic optical activity, that is a property of molecules. It means, that the second group of optically active materials shows the phenomenon in any state (gas, liquid, solid). A molecule is optically active if it is chiral - it is nonsuperimposable on its mirror image (a chiral molecule cannot be mapped onto its mirror image by rotations and translations, see the picture below).



B) If the refractive indices for right-handed and left-handed circular polarization are different, then after passing the distance d in the optically active medium the right-handed wave will have the phase:

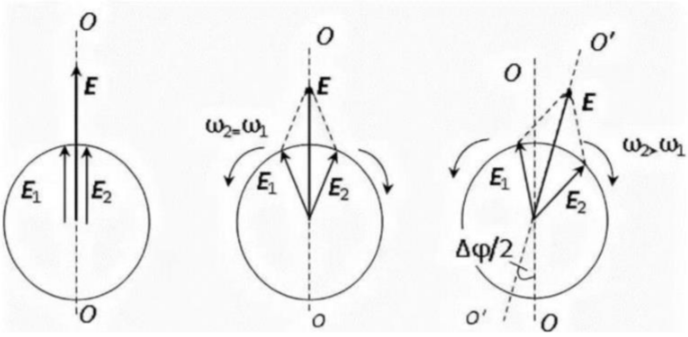
$$\varphi_R = k_R d = k_0 n_R d$$

Let's agree, that for the right-handed wave the phase will be positive (clockwise direction, $\varphi_R > 0$), and for the left-handed wave the phase is negative (counterclockwise direction, $\varphi_L < 0$)The left-handed wave will have the phase:

$$\varphi_L = -k_L d = -k_0 n_L d$$

Therefore, the angle of polarization rotation α is the average between the left- and right-handed phases:

$$\alpha = \frac{\varphi_R + \varphi_L}{2} = \frac{\pi d}{\lambda}(n_R - n_L)$$



From this expression it is clear, that if the refractive index is the same for both polarizations, the phase of each wave will increase along the propagation in the material, but it will be the same for each polarization. Therefore, the average of two phases in opposite directions (φ_R positive and φ_L negative) will be zero. So, no rotation of the polarization plane.

For the values $n_R = 1.55$, $n_L = 1.5$, $d = 1000$ nm, $\lambda = 500$ nm the angle of polarization rotation:

$$\alpha = \frac{1000\pi}{500}(1.55 - 1.5) = 2\pi \cdot 0.05 = 0.31\, rad = 18°$$

C) In order the polarization rotation angle α to be 90 degrees we need the thickness:

$$d = \frac{\lambda\alpha}{\pi(n_R - n_L)} = 5000\, nm$$