

DRP Report

Liquid Crystals and Photonic Band theory

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Abstract

1 Introduction

This semester-long Directed Research project served as an extension to the Condensed Matter Physics class I took along with this project. The coursework for this study discussed the basics of crystal structures and an introduction to the Photonic bands.

Liquid Crystal, as paradoxical as the name may sound, is a macroscopic state of matter and depends on the molecular packing of the material. These are interesting classes of materials. As the name suggests, they have some degree of crystalline order and can still exhibit their fluid capabilities.

Photonic-Bands are reminiscent of the Electronic Band theory detailed extensively in the condensed matter class, where we see the crystal scattering photon under the permittivity potential. The photonic band theory in line with the Electronic Band structure is described by the Bloch theorem.

2 Liquid Crystals

As already discussed, liquid crystal is a macroscopic state of matter; it involves a certain method of molecular packing sensitive to the environment. Liquid Crystals, due to their crystalline and, simultaneously, fluid nature, have anisotropy (directionality); Isotropy usually means that the material's properties/ structure remain the same in all directions; however, anisotropy attaches directionality to the properties of the material and its structure. For this section Linda's Fundamental of soft matter Science [3] serves as the primary source, and [2] is also a good reference.

The measure of anisotropy in a material is often described by the order parameter, which is a vector that describes the average alignment of molecules. For a perfectly aligned phase, the magnitude of the order parameter is 1, whereas for complete isotropy, the order parameter is 0.

2.1 Thermotropic Liquid Crystals

Liquid crystal packing is primarily formed by keeping the concentration constant and achieving the state at a certain temperature. The liquid crystal packing highly dependent on temperature forms the Thermotropic Liquid crystals. The other technique involves varying the concentration of the liquid crystal also known as the Lyotropic Liquid crystal. The Liquid Crystals part of this study mainly revolved around the different phases of the Thermotropic liquid crystals.

2.2 Phases of the Thermotropic Liquid Crystals

Anisotropy involves directionality to order; however, the directionality is fairly arbitrary, and a liquid crystal phase is associated with each directional anisotropy. It is important to understand that this directional packing of molecules is to minimize the energy of arrangement of these dipoles.

2.2.1 The Nematic Phase

The nematic phase is the simplest Thermotropic liquid crystal phase, where all of the molecules direct themselves along a single axis. Their translation degree of freedom is available; however, the rotational modes are frozen to minimize the energy. This packing is similar to that of shaking a matchbox, and finding all of the matches aligned straight. Apart from energy, entropy also starts taking part in the alignment of molecules as we are dealing with a macrostate[3].

The order parameter for the nematic phase is :

$$S = \frac{1}{2} \langle 3\cos^2(\theta) - 1 \rangle \quad (1)$$

where $\theta = 0$ represents a crystalline solid, and $\theta = 1$ represents a completely isotropic liquid. Most crystals in the nematic phase have an order parameter vary between 0.3 and 0.8. To see the crystalline structure rather than optical microscopy, polarisation microscopy relies on the birefringence of the liquid crystals; see [A.1](#).

2.2.2 The Smectic Phase

The smectic phase is similar to the nematic phase; however, an additional structure is involved in the smectic phase. Over the directional anisotropy, a layer structure is formed, and these layers form a 2D crystal structure. As can be seen in the toy example below, there is certain directionality to the nematic liquid crystals in one dimension only, whereas in the smectic phase, the dipoles arrange themselves in a layer structure as well.

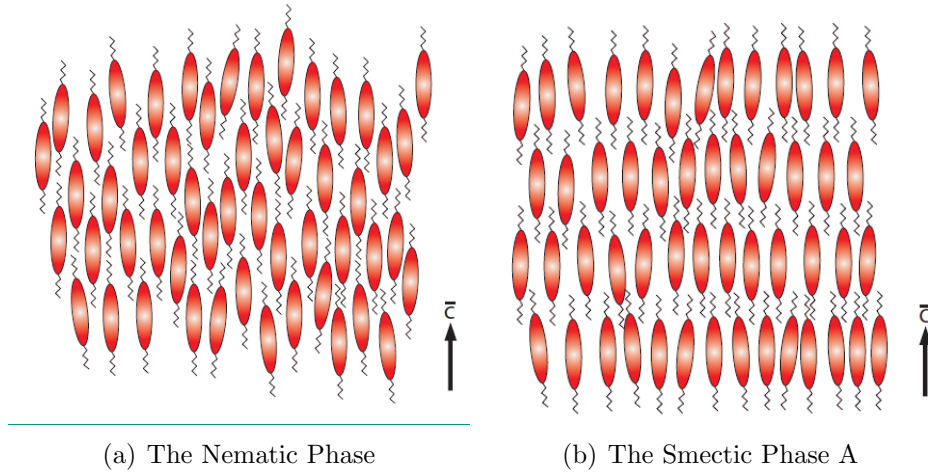


Figure 1: Comparison between Nematic and Smectic Phases [3]

The comparison above shows the layer order between the simplest of the two Liquid crystal phases. The figure above shows the layer structure over the directionality in the smectic Phase A of the liquid crystal. The director of the smectic phase is written as:

$$s = \frac{1}{2} \left\langle \cos \left(\frac{2\pi z}{d} \right) (3\cos^2(\theta) - 2) \right\rangle \quad (2)$$

where z is the direction of the molecule parallel to the layer. If the molecules align parallel to the z -axis, the molecule forms the layers.

2.3 Chirality in Liquid Crystal Phases

we have now restricted ourselves to talks about axial arrangement of the molecules in liquid crystal. Since we are arranging dipoles in the molecules, it also requires us to consider the orientation of the molecules when packing them. Due to this preferred orientation also known as "handedness", we see twisting in Liquid Crystal Phases, introducing a new class of Liquid crystal phases.

2.3.1 The Chiral Nematic Phase

Also Known as the cholesteric phase, is again the simplest of the chiral Liquid Crystal Phases. In this phase over the directional treatment of the molecules, twisting is involved, and the orientations of the dipoles change perpendicular to the axis of anisotropy. As shown in the figure below, one whole phase of molecular twisting forms a pitch. Although Chirality is also seen in the smectic phases, we will primarily focus on the chiral nematic phase.

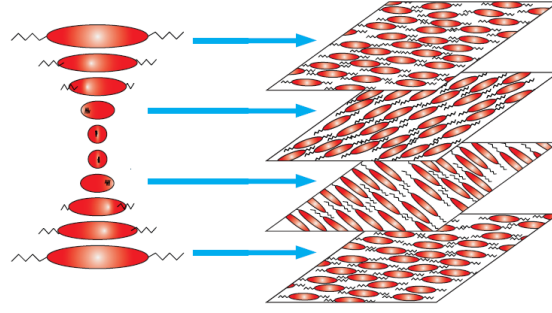


Figure 2: The Chiral Nematic Phase [3]

The distance in which the liquid crystal molecules in their helical arrangement perpendicular to the director, return to their original position is known as the pitch. The magnitude of the pitch has a significant role in the optical properties of the liquid crystal as it changes the optical properties of the material.

3 Photonic Bands

Photonic crystals are periodically arranged dielectric media, which, like normal crystals with ions arranged periodically, have a periodic dielectric potential. In the electronic band theory, we found that if we scatter electrons through a periodic potential, they form a band gap, and disallow certain energies of electrons. Furthermore, the electrons being fermions can not have unlimited particles in finite energy states. Similarly, Photonic crystals also scatter photons and form photonic bands. They also form a band gap, and photons of energies in the bandgap cannot propagate through the crystal.

3.1 The solutions to Maxwell's equations in matter

The photonic bandgap, as discussed, occurs due to the dielectric potential, which disallows certain wavelengths from propagating in the medium. One way to achieve this would be to solve for Maxwell's equations in matter, in particular, this equation:

$$\nabla \times \frac{1}{\epsilon} \nabla \times \vec{H} = \left(\frac{\omega}{c}\right)^2 \vec{H}. \quad (3)$$

This is an eigenvalue problem. We can find the values of ω corresponding to it. Although the equation may look solvable directly, some factors need to be considered to solve it, such as the dielectric potentials encoded into the H fields. Additionally, we have periodic dielectric potentials, such that: $\epsilon(\vec{x}) = \epsilon(x + R_i)$ where R_i are the primitive lattice vectors. Bloch theorem, due to the periodic potential, allows us to assume solutions for the H field to be of the kind: $\vec{H}(\vec{x}) = e^{ik \cdot x} \vec{H}_{n,k}(x)$ Where the n represents the eigenvector corresponding to each eigenvalue of the modified eigenvalue equation that equations of this form satisfy:

$$(\nabla + i\vec{k}) \times \frac{1}{\epsilon} ((\nabla + i\vec{k}) \times \vec{H}_{n,k}) = \left(\frac{\omega_n(k)}{c}\right)^2 \vec{H}_{n,k}. \quad (4)$$

Each eigenvalue $\omega_n(k)$ represents a continuous function of k . Still, they set up discrete bands corresponding to each eigenvalue. The bandgap depends on the dielectric

potential entirely. It is reasoned by the removal of degeneracy in propagating states and the response of the dielectric material. A wavevector having a different energy from its negative wavevector will produce a band gap at the boundaries of the Brillouin zones[1].

Future Work

- Understanding the dielectric potential of the Cholesteric Liquid Crystal Phases.
- Understanding the Pitch measurements techniques, and their influence on the dielectric potential.
- Extrinsically applying forces on the Nematic liquid crystals and remeasuring their optical properties as a measure of change in their pitch.

A Appendix

A.1 Polarization Microscopy

Unlike optical microscopy, which relies on magnifying the objects using lenses and shining light on the sample, in order to discern between the conventional liquid phases and the liquid crystal phases, a technique called Polarization microscopy turns out to be more helpful to image the molecular arrangement of these crystals.

Since the Liquid crystals are anisotropic, and their packing is favoured along a certain direction, the axis of direction can also serve as the polarization axis. The light of a mixed state, when passed through a twisted nematic phase as can be seen in the image below[4] :

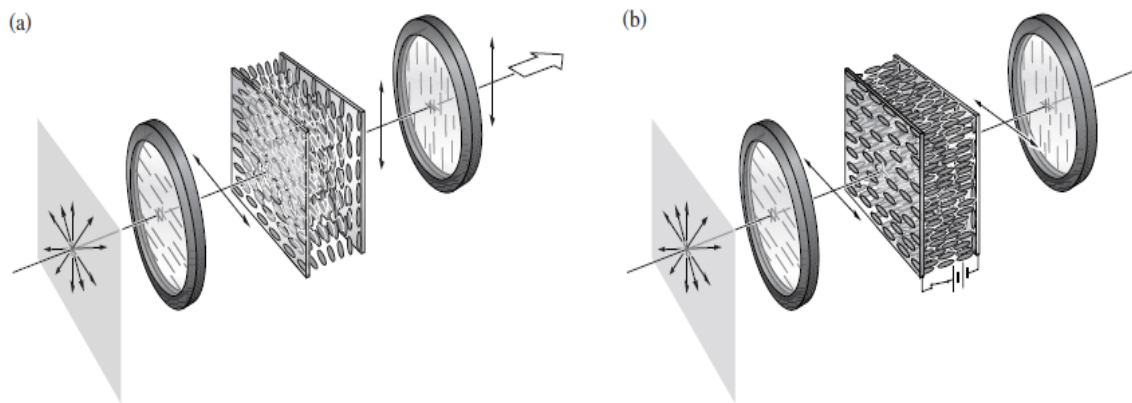


Figure 3: Polarizing Nematic Liquid Crystal Phases

The images above show how a twisted nematic phase can be used as a polariser, as it will polarise the light along its own axis, and when not the light is along the axis of the liquid crystal, the polarization remains unchanged. Using the polarisation of the output light from the liquid crystal sample, the nematic phase's directionality can be figured out.

References

- [1] Steven G. Johnson and J. D. Joannopoulos, *Introduction to Photonic Crystals: Bloch's Theorem, Band Diagrams, and Gaps*, (MIT, 2003).
- [2] Syed Furqan Hashmi, *Switchable Photon Sources based on the 2D Semiconductor-Liquid Crystal Interface*, (LUMS,2021)
- [3] Linda S. Hirst, *Fundamentals of Soft matter Science*, (CRC Press 2020).
- [4] Eugene Hecht *Optics*, (Pearson 2017.)