

Simulating Liquid Crystals

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(Dated: June 7, 2020)

I simulate the response of liquid crystal molecules to the electric field between non-uniformly charged capacitor plates.

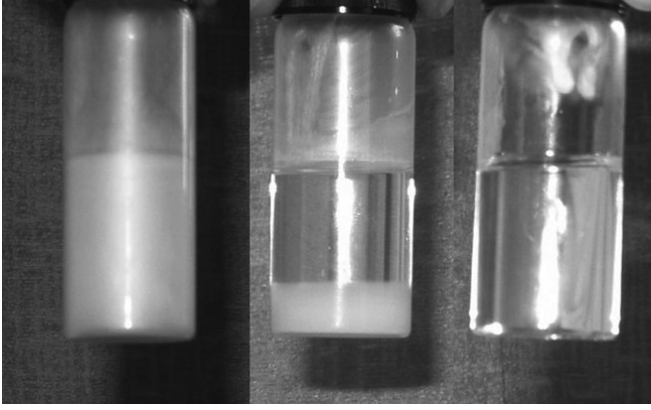


FIG. 1: Double melting: [?] A vial of liquid crystal being warmed from room temperature. A phase transition from liquid crystal (opaque) to isotropic liquid (clear) appears at the upper surface of the liquid and moves downward.

INTRODUCTION - LIQUID CRYSTALS

History

The first liquid crystal, cholesteryl benzoate, was identified by Austrian botanical physiologist Friedrich Reinitzer, and further characterized by German physicist Otto Lehmann. [?] Reinitzer observed that the substance had two melting points: it melted from a solid into a cloudy liquid at 418.65 K, and melted again into a clear liquid at 451.65 K (Figure 1). He also found that the cloudy phase reflected circularly polarized light and had the ability to change the polarization of light, while the clear phase had the properties of an isotropic liquid. Lehmann observed that the cloudy phase contained crystallites and exhibited birefringence like a crystalline solid. Later, {talk about Georges Friedel, Charles Mauguin = magnetism, de Gennes, Leslie = modern theory, others; picture of Schlieren phenomenon }

Formal Definition

A liquid crystal can be formally defined using the density-density correlation function $\langle \rho(\mathbf{x})\rho(\mathbf{x}') \rangle$ of statistical mechanics. [?] Let \mathbf{x}_0 be the position of a molecule or some other feature; we want to know the probability

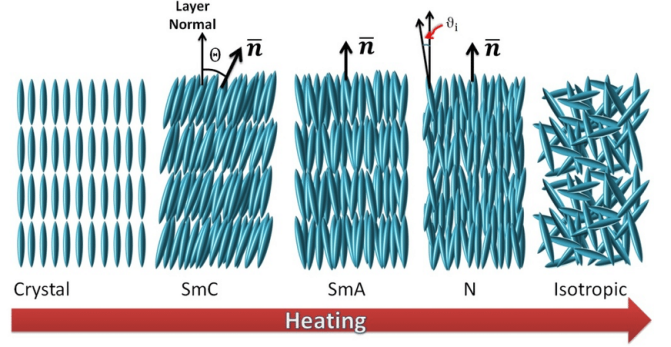


FIG. 2: Multiple mesophases: [?] A thermotropic liquid crystal showing two smectic phases (SmC, SmA) and a nematic phase (N) in the transition from crystalline solid to isotropic liquid. Notice the molecular layers present in the smectic phases but not the nematic.

of finding an equivalent molecule or feature at position $\mathbf{x} = \mathbf{x}_0 + n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ for n_i integers and \mathbf{a}_i basis vectors. A crystal is defined by the fact that it is periodic in space, so its correlation function remains periodic even as $|\mathbf{x} - \mathbf{x}_0| \rightarrow \infty$. For a crystalline solid,

$$\lim_{|\mathbf{x} - \mathbf{x}_0| \rightarrow \infty} \langle \rho(\mathbf{x})\rho(\mathbf{x}_0) \rangle = F(\mathbf{x} - \mathbf{x}_0) \quad (1)$$

where $F(\mathbf{x})$ is a periodic function of basis vector \mathbf{a}_i .

On the other hand, in an isotropic liquid the correlation function tends toward a constant, the square of the average density $\bar{\rho}$:

$$\lim_{|\mathbf{x} - \mathbf{x}_0| \rightarrow \infty} \langle \rho(\mathbf{x})\rho(\mathbf{x}_0) \rangle \simeq \bar{\rho}^2 \quad (2)$$

Note that in an isotropic liquid, there is a length scale ξ over which correlations decay. (X-ray diffraction of isotropic liquid results in diffuse peaks of typical width ξ^{-1} .)

A liquid crystal (LC) is a *system in which a liquid-like order exists in at least one direction of space and in which some degree of anisotropy is present.* [?] (By 'some degree of anisotropy,' we mean that the LC has a correlation function that depends not solely on the magnitude of $(\mathbf{x} - \mathbf{x}_0)$, but also on its direction.)

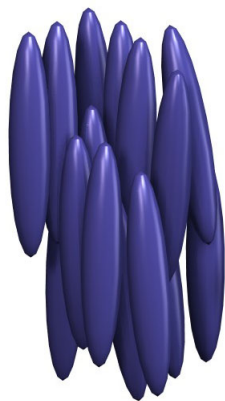


FIG. 3: Uniaxial nematic phase



FIG. 4: Cholesteric (a.k.a. chiral nematic) phase

Types of Liquid Crystals

The nature of the anisotropy in an LC determines its classification into one of several *mesophases* between crystalline solid and isotropic liquid; several distinct mesophases can exist between the two extremes. (Figure ??) Phase transitions are called *thermotropic* if they occur with changing temperature and *lyotropic* if they occur with changing LC molecule concentration in the solvent. The three known types of LC mesophases are

nematic, *smectic*, and *columnar*.

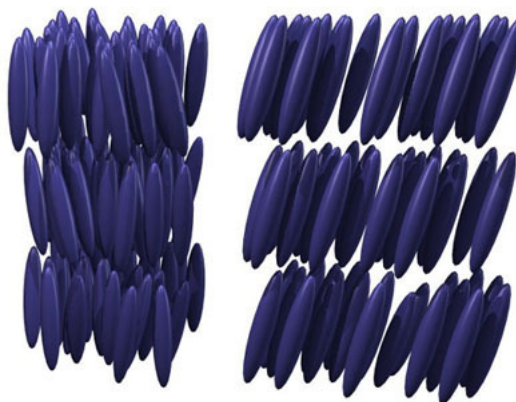


FIG. 5: Smectic A and C phases

Nematics

In *nematic* LCs, the only difference from the isotropic liquid is that there are two distinct length scales, ξ_{\parallel} and ξ_{\perp} , over which the correlation function decays at different rates. This corresponds to a simple alignment of the LC molecules along a single axis, known as a *director*, throughout the entire bulk of the liquid.³

If a molecule that has a nematic phase in an achiral or racemic solvent is instead dissolved in a chiral solvent, the nematic phase becomes *cholesteric*, also known as *twisted* or *chiral nematic*. ("Cholesteric" because cholesterol esters, including cholesteryl benzoate, form this type of LC.) This is a nematic in which the director changes over space and the molecules line up along helices.⁴

Smectics

Columnar phases

(TO BE COMPLETED)