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Orientation of nematic liquid crystals with spatially periodic anchoring

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Abstract

Development of biosensors is one among many biomedical applications of liquid crystals. Recent simulation studies show that interactions at the interface between a nematic and a confining substrate (anchoring) enable us to detect sensitively the presence of biomolecules in complex samples.Yet, to the best of our knowledge, there is a scarcity of systematic studies of the effect of periodic modulation of surface anchoring for this kind of applications.Through simulations the final orientation fields can be predicted given certain initial conditions and detect the presence of disclinations in the liquid crystal. From the simulations carried out in this work, it is possible to predict the final corientation that the liquid crystal will present when it reaches the equilibrium as a function of the initial configuration which is very important for the development of biosensors

Nematic liquid crystals, periodic anchoring, biosensors, biomolecules

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Introduction

In the field of liquid crystal based (CL) biosensors development, recent simulations and experiments have shown that the interactions at the interface between a nematic and the confining surface allow sensitively to detect the presence of biomolecules on the surface in very small concentrations.

By using numerical simulations and using coarse grain models, they suggest the possibility of controlling such sensitivity by spatially periodic anchoring patterns, however such simulations assume that the origin of such anchor is the periodic placement of binding sites for the biomolecules with a more precise beyond the current experimental techniques. As an alternative, it has been proposed to directly modify the chemical composition of the substrates to obtain anchor bands perpendicular and parallel to the substrate, alternately and periodically.

In addition to evaluating the effect of this type of anchoring conditions on the sensitivity of CL biosensors, periodic structures of the field of nematic orientation are of interest in the field of photonics. However, the nematic characteristically possess topological defects (disclinations) that can destroy the periodicity of the directing field.

To explore and understand the behavior of systems under such anchoring conditions at the CL interface with the confining surface, it is proposed to study the effect on the structure of the orientation field of the liquid crystal in models for CL biosensors.

Specifically, this work simulates the temporal evolution of the liquid crystal system from controlled initial conditions, observing the effect on the final orientation structure of the LC associated with three classes of initial configuration: homeotropic, planar and random. The temporal evolution numerically solved the Beris-Edwards equations for a nematic by the finite difference method.

The methods and programs developed in this project can be applied later to problems of photonics, if they are combined with methods to calculate the structure of bands corresponding to different wavelengths of incident light in this type of devices.

Cementitious Fluid Crystals

The main characteristic of Nemethic Liquid Crystals (NLC) is that its molecules are highly anisotropic, usually they can be elongated in bar form, flattened in the form of disc or other more complex as banana form, besides being highly sensitive To electric and magnetic fields.

Another important aspect of NLC is that its molecules have no positional order, but they do tend to be oriented in the same direction (uniaxial), that is, the mass centers of the molecules are placed as in a liquid (without order) and the axes Principal molecules point, on average, along a particular direction called director n as seen in Figure 1.

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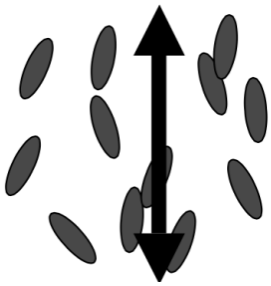

Figure 1 Vector director **n**.

One way of describing how ordered the molecules are is by the order parameter S.

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

$$= \int \frac{1}{2}(3\cos^2\theta - 1) f(\theta) d\Omega$$

Where θ is the angle of the principal axis of each molecule with respect to the director and the average is performed on the orientation Ω of all molecules of the system. The value S = 1 represents a total order of the molecules while S = 0 means that the molecules are totally disordered.

Periodic Space Anchors

With regard to anchoring, this refers to how the director is oriented on the surface that confines the liquid crystal. Thus, when referring to spatially periodic anchoring we mean that there will be alternating regions on the surface that confines to the NLC where the anchorage is of one or the other type.

Basically in this project we will focus on two types of alignment of the director on the surfaces that confine the LC: homeotropic anchorage, where the alignment is perpendicular to the surface, and homogeneous anchorage where the alignment is parallel to the surface (also called planar anchorage). Figure 2 shows a system confined to two surfaces (one at the top and one at the bottom). Each surface has two types of anchor: on the left side the anchorage is homeotropic and the right side is homogeneous. Applying periodic boundary conditions in the horizontal direction to this device will yield an infinite system with spatially periodic anchorage.

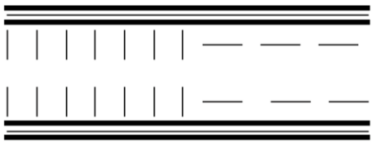

Figure 2 Spatially Periodic Anchorage Schematic

Topological Defects

Another characteristic of NLCs is that they often present topological defects, commonly known as dysclinations, which relate to the head fields mentioned above. When there are abrupt changes of the directors or there is a very noticeable discontinuity, then we can say that there are disclinations.

There are two important types of dysclinations in an NLC: D = 1/2 intensity disclination and S = -1 / 2 disclination to determine the intensity of a disclination in a CLN surrounds the defect region by plotting a circumference and Then it runs in the clockwise direction.

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Analyzing how a vector tangent to the directing field rotates at each point in the path. In this way we can know how many turns the vector rotated (which indicates the magnitude of the disclination) and whether it did in the positive or negative direction (ie clockwise or counterclockwise).

System to Simulate

The systems we simulate are thought of as working NLC in the experimental field, where a liquid crystal Pentil-cyano-biphenyl (5CB) is confined between two parallel plates separated by a distance of the order of microns, which are covered by a Layer on the inside very thin, ie a thin film of gold that can hold fixed the alternating anchorage between planar and perpendicular on the inner surfaces of both plates.

In the diagram of figure 3 we can observe the cell that we will use for our simulations: the vertical vectors in the first half represent the anchorage perpendicular to the plates and the horizontal vectors of the second half represent the planar anchorage, note that the anchorage is located In the horizontal direction (x-axis) and the plates that confine the liquid crystal are located in the vertical direction (normal to the z-axis). The angle θ that determines the orientation of the planar anchor is measured with respect to the x-axis.

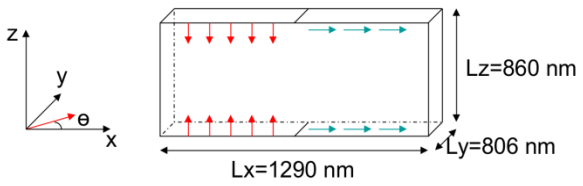

Figure 3 Simulation Cell

Model

In order to predict the final orientation fields given certain initial conditions and to observe if they presented topological defects, we used a relaxation model that is a particular case of the Beris-Edwards model, which allows us to describe how the field of the order parameter evolves as it passes the time, by means of the alignment tensioner ***Q*:**

$$\frac{\partial Q}{\partial t} = -\frac{1}{\gamma}\left[\frac{\delta F}{\delta Q}\right] \qquad (2)$$

In the above equation, the alignment tensor ***Q*** is related to the directing field n as follows ***Q*** = S (nn - I / 3), where S is the order parameter, I is the identity tensor, δ denotes the functional derivative , F is the free energy functional and γ is a constant related to the coefficient of rotational diffusivity.

The free energy consists of two parts; the free energy of Landau de Gennes and elastic energy**.**

$$F[Q(r)] = \int A\, trQ^2 + B\, trQ^3 + C\, trQ^4 + L(\partial k\, Q_{ij})^2 dr \qquad (3)$$

The coefficients A, B and C are functions of temperature and L is the elastic constant that is related to the three types of distortion Aperture, Twist and Bend (Splay, Twist and Bend).

In this model equilibrium properties are described by the free energy of Landau de Gennes, in the following figure 4 we can observe the three types of distortions that appear in the liquid crystals, these are Torsion, Fold and Opening from left to right respectively

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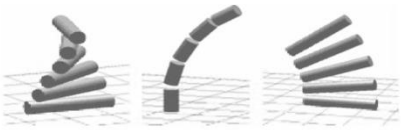

Figure 4 Tipos de distorsiones

Stationary solutions

In this project we are interested in the long-term stationary solutions in the relaxation model. To ensure that the simulations reached equilibrium, we took simulation times t much larger than the relaxation time τ of the CL, which in the case of 5CB implies that $t = 50\ s >> \tau = 0.01\ s$.

An additional complication is that random initial conditions were analyzed in the project, so that multiple realizations of these systems had to be performed.

By performing multiple simulations for the random cases we can rely more or make sure that the results were obtained with a high degree of precision compared to the current experimental techniques.

Numerical Method

The algorithm used to solve the differential equations that were presented in the development of this research was that of Euler and the derivatives were evaluated with the numerical method of finite differences, on domains with a rectangular prism shape.

Solutions were calculated on periodic systems, to study the effect of finite size on the orientation structure obtained finally.

Control Variables for Simulations

In general, the following cases were analyzed for the liquid crystal:

- Uniform Initial Configuration (homogeneous and homeotropic),
- Random Initial Setup

In each case the perpendicular fraction was modified in the x-direction, as well as the angle of the planar orientation with respect to the x-axis. That is, the main variables were the following illustrated in the diagram of figure 5.

- perpendicular fraction of the anchor in the x-direction (frac-perp)
- angle of the director n with respect to the x-axis (angle)
- initial direction of the directors between the plates (homeotropic, homogeneous and random)

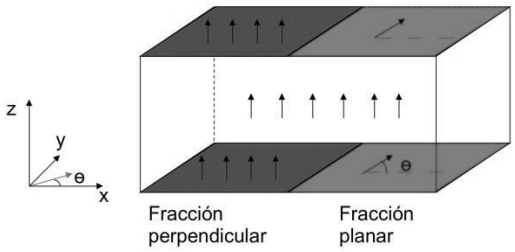

Figure 5 Diagrama de las variables de control

Program code

For the development of this research we rely on the articles "Multiscale Simulations of Liquid Crystals" and "Monte Carlo simulations and dynamic field theory for suspended particles in liquid crystalline systems," focused on the Beris-Edwards liquid crystal relaxation model. These articles exploit computational techniques to simulate the evolution of a liquid crystal confined by a surface.

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Based on the aforementioned articles, changes were made to the programs developed by their authors: mainly a fixTensorAtPlates subroutine was modified to establish the periodic and alternating anchor, adding the new parameters (control variables, perpendicular fraction, angle of planar anchor and initial configuration of the liquid crystal) necessary to fulfill our objectives.

In order to make these changes to the basic programs, the knowledge of the Fortran 77 programming language had to be deepened.In the subroutine that establishes the parameters of the simulation from an input data file, the perpendicular limit that delimits the planar and perpendicular anchorage is added, as well as the angle of the planar orientation with respect to the x-axis.Variables were also introduced to represent the initial configuration of the liquid crystal.

We implemented a subroutine that fixes the initial condition of the liquid crystal inside the cell that is, start with the liquid crystal with a homeotropic, planar, and random configuration to study its behavior.

The execution of the program displays a table of numbers that represent the free energy of Landau, the elastic energy and the total energy with respect to the time, being difficult its interpretation, then with the help of software "Paraview" we were able to visualize both the parameter of order and the Directors and thus to make a more complete analysis regarding the degree of ordering as possible distortions in the liquid crystal.

Results

Simulated Cases

Basically, the following cases were analyzed for the liquid crystal: homogeneous homeotropic, planar and random initial configuration.

For each type of simulation, the control variables were changed: the perpendicular fraction was set at 25, 50 and 75 percent of the length of the cell in the x direction, while with respect to the angle of the planar orientation were used 30, 60 and 90 degrees with respect to the x-axis.

The size of the sides of the fundamental cell of said periodic arrangement was Lx = 1290 nm, Ly = 20 nm and Lz = 806 nm.

Liquid crystal initially homeotropic

As one of the objectives is to investigate the orientation of liquid crystals in devices that can be used in photonics, it is convenient to study the effect of varying the size of the cell to reach dimensions comparable to the wavelength of visible light.

We begin by studying the effect of varying the perpendicular anchorage fraction (fracperp) and the planar anchorage angle q when the initial condition in the cell is homeotropic.

In the case of the initial homeotropic configuration, it was observed that the initial orientation of the liquid crystal is preserved and that the perpendicular anchorage portion and the orientation of the planar anchorage are not relevant.

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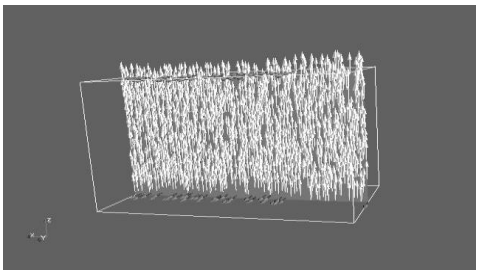

Figure 6 frac-perp=0.25, angle=60º

Pulmonary fluid crystal

In the second system studied, the initial configuration was planar at an angle of zero degrees with respect to the x-axis, with a planar anchor at 60 degrees. The following figures illustrate the results for anchoring angle of 60 and 90 degrees.

A reorientation of the liquid crystal was observed in the same direction as the planar anchorage, regardless of the magnitude of the perpendicular fraction.

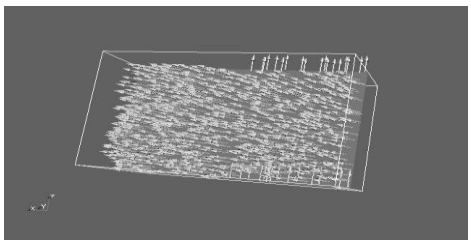

Figure 7 frac-perp=0.50, angle=60º

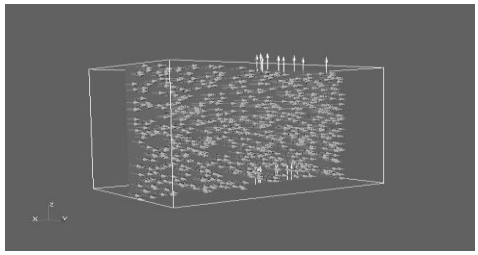

Figure 8 frac-perp=0.50, angle=90º

Random liquid crystal

Finally, for the case where the initial configuration is random, the liquid crystal is reoriented according to the majority anchorage, be it planar or perpendicular. The following figure 9 shows this behavior:

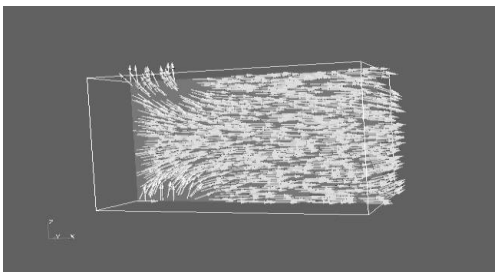

Figure 9 frac-perp=0.25, angle=0º

Finally, when we have an initially random configuration and a non-zero planar anchorage angle, we observe a reorientation of the liquid crystal in the direction of the majority anchorage.

Simultaneously we observe that the director deflects out of the x-plane and, noting that the director aligns partially with the z-axis. Figure 10 shows this effect (note the right end of the cell and how the directors do not point horizontally).

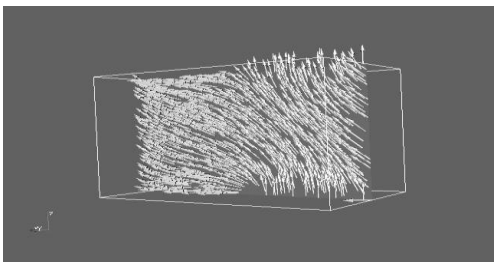

Figure 10 frac-perp=0.50, angle=30º

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Conclusions

From the simulations made, we are already prepared to be able to predict the final configuration that will be presented when arriving at the equilibrium for different initial configurations given.

The results can be reduced to three cases, according to the initial state of the liquid crystal between the plates: planar, homeotropic or random.

The final state depends on the initial state of the liquid crystal.

- If it starts with a homogeneous perpendicular configuration, no change is presented: that is, the initial configuration of the system is preserved, neither the perpendicular fraction of the anchor nor the planar part is oriented at a certain angle.

- If initially we have a planarly oriented medium, then the final orientation of the directing field ends aligned with the orientation of the planar anchorage and the perpendicular fraction is not relevant.

- Finally, if the initial configuration of the liquid crystal is random, the equilibrium is reached with a final configuration aligned in the direction of the majority anchorage. In addition, if the orientation of the planar anchorage is different from zero then a partial alignment with the vertical axis z is also present.

Another important aspect of the final configurations is that we could notice the presence of distortions in the double-aperture liquid crystal.

Finally it is very important to mention that through the simulations made it is possible to know the final orientation that the liquid crystals will take when reaching equilibrium, which is of great importance for the development of biomolecule detectors

Prospects

The consequence of applying electric fields allowing to align the CL is very interesting. In the case of a parallel dipole, if the conductor adjusts to the applied field, then the electric field in the material is reduced by polarization effects and it turns out that the total energy of the system is also reduced. This is why it is intended in the near future to apply electromagnetic fields to the CLN system and determine what effects are observed in the presence of static electric and magnetic fields for different intensities.

Another important point is that, although this research does not take into account the effects of hydrodynamics of liquid crystals, this work can be used to make comparisons to those who work in the hydrodynamics of liquid crystals, since when comparing the results Obtained with and without hydrodynamic effects, a more complete analysis of the latter can be obtained, based on this work.

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