23.2: Q-Tensor Based Numerical Modeling of Blue-Phase LCDs

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Abstract

We have developed a novel numerical modeling software for calculation of the molecular orientation within layers of liquid crystal material in the blue phase and for the optical properties of blue phase LCDs including additional optical components like polarizers and retarder sheets.

The calculation of the molecular orientation within the blue phase layer is based on the Q-tensor approach. Equilibrium and time dependent states are obtained with a relaxation method that minimizes the total energy of the system. Mutual coupling of the electrostatic potential and molecular orientation is taken into account. The geometry is mapped onto a 3d-grid, periodic boundary conditions are assigned to the faces of the bounding box. The grid is extended on top and bottom side of the bounding box to apply suitable boundary conditions for the electric potential.

The finite difference time domain method is applied to calculate reflectance and transmittance of blue-phase LCDs with uniaxial perfectly matched layers on top and bottom sides of the bounding box to mitigate spurious reflections from the grid boundaries. The grid used for the Q-tensor calculation is also chosen for the optics calculation.

1. Introduction

Liquid crystal displays based on (polymer stabilized) blue phases (BP LCDs) seem to be promising with respect to very fast switching which enables field sequential color control, thus avoiding expensive color filters, as well as improved display of moving images (refer to e.g. [1] and the references given therein). On the way to mass production of such displays some obstacles like high operating voltages and electro-optical hysteresis effects remain to be investigated and removed.

In order to support research and development activities in this emerging field of LCD-technology we have developed a novel numerical model for both the field induced elastic deformation and for the corresponding optical properties.

2. Numerical Modeling of LCDs

Simulation of liquid crystal display devices (LCDs) via numerical modeling has become an indispensable part of the research and development of new electro-optical effects in LCs (i.e. development of novel display types) and of the optimization of existing display effects, because it allows exact and individual control of all model parameters, fast results and thus, it ideally parallels the laboratory workbench. Complex optimization schemes can be used together with the numerical model in order to find special parameter combinations and to analyze parameter sensitivities. Numerical modeling of LCDs was successfully employed by van Doorn [2] and Berreman [3] in 1975 to explain the “bounce” in the dynamical optical response of TN-cells. At the time of its release in 1987, **DIMOS** was the first commercial software for numerical modeling of display systems with LCDs [4].

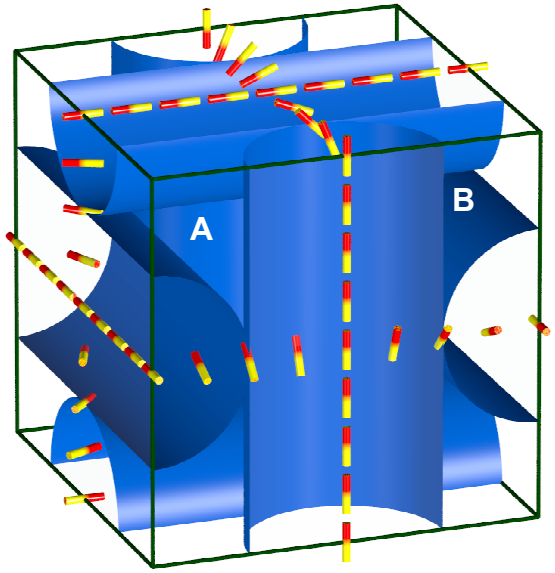

Figure 1: Elementary cell of a BPII configuration illustrating the involved double-twist cylinders and the local orientation of the LC-director (eigenvectors of Q-tensor with largest eigenvalue).

Depending on the complexity of the display and on the targets of optimization, the simulation effort can be as small as typing in a few numbers into a pocket calculator (e.g. transmittance of a TN-cell in the quiescent state at normal light incidence) or on the other hand it requires high-end PCs or even workstation computers when lateral effects cannot he neglected as in the case of high resolution TFT-LCDs or in devices using the in-plane-switching effect (IPS) or fringe-field switching effects (FFS). In a first approximation, the LCD is composed of plane parallel layers like glass substrates, LC layer, polarizes etc. As long as the lateral extensions are much larger compared to the thickness of the individual layers and if sufficient homogeneity of the material and cell parameters along the surface can be assumed, a one-dimensional model is the adequate approximation. In this case the LCD model is composed of layers with infinite lateral extension. Refractive indices and the director orientation vary only along one direction, usually the LCD normal. The amount of numerical calculations for the determination of the director configuration and the optical quantities like transmittance and reflectance is moderate compared to two- or three-dimensional problems. This simple model allows performance optimization with simultaneous

variation of several material and cell parameters. High-resolution displays with small pixels and complex electrode structures require two- or three-dimensional modeling, since "fringing field" effects cannot he neglected. In those cases the director orientation strongly depends on the lateral position.

Prior to calculating the optical properties of LCDs all parameters describing the model (refractive indices, layer thickness and optic axis orientation in case of birefringent materials) must be known. On the molecular level chiral-nematic liquid crystals are composed of rod-shaped molecules with the long axes of neighboring molecules in the same layer aligned approximately parallel to one another. Deviations from the ideal parallel alignment are due to thermal fluctuations that are reducing the state of nematic order, which is usually quantified by a scalar *order parameter*. The *director*, represented by a unit vector *n*, is the average of the molecular axes over a small volume at any location within the liquid crystal. The orientation of the director is allowed to change continuously within the medium, except at singularities, where the distances over which orientational changes occur are no longer much larger than the molecular dimensions. The orientation within the bulk of the LC-layer is not directly available in the general case. Oseen, Frank, Leslie and Ericksen, and others, developed theories [4, 5, 6, 7, 8] that are the basis for computation of static and dynamic LC-configurations. In the corresponding expressions for the free energy of the system the orientation of the *director* can be expressed in terms of two polar angles or by the respective cartesian components.

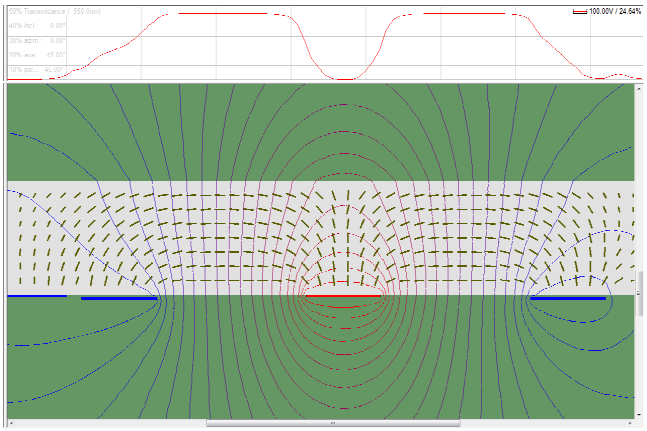

Figure 2: Simple BP-LCD model with interdigital electrodes based on the Kerr effect. Electrical-field induced birefringence in an isotropic LC-medium (Δn ~ length of rods) with equi-potential lines and transmittance (λ = 550 nm) between crossed polarizers (red curve on top). The applied voltage is 100 V (red electrode).

Alternatively, the free energy of the liquid crystal (here the sum of *distortional*, *electric* and *surface energy*) can be written in terms of the order parameter tensor, Q. This "tensor approach" maintains the physical equivalence of *n* and -*n* and thus has sometimes been believed to be more "realistic" in the numerical modeling of LCDs. However, this approach can give rise to spontaneous transitions between topologically nonequivalent states without generation of disclinations (e.g. inversion walls), solely caused by discretization, which is unrealistic from the viewpoint of LC-physics [9].

3. Novel Numerical Model

The calculation of the molecular orientation within the BP layer in this model is based on the Q-tensor approach [10, 11]. The total energy of the chiral-nematic LC is described as follows:

$$F = F_{dist} + F_{thermo} + F_{el} + F_{surf}$$

$$F = \int_V \left(f_{dist} + f_{thermo} + f_{el}\right) dv + \int_S \left(f_{surf}\right) ds \quad (1)$$

with

F_{dist}	*elastic (distortional) energy*
F_{thermo}	*thermotropic energy*
F_{el}	*electric field energy*
F_{surf}	*surface energy*

The thermotropic energy, F_{thermo}, is a potential function which determines the state which the liquid crystal adopts, i.e. a uniaxial, biaxial or the isotropic state. At sufficiently high temperature this potential should have one minimum of energy in the isotropic state, whereas at lower temperatures there are minima at different uniaxial and biaxial states.

Equilibrium and time dependent states in our model are calculated using a relaxation method that minimizes the total energy comprising elastic, electrostatic, and thermotropic energy. Mutual coupling of the electrostatic potential and molecular orientation is taken into account. The geometry of the cell is mapped onto a 3d grid. Periodic boundary conditions are assigned to left and right face and to front and back face of the bounding box. The grid is extended on top and bottom side of the bounding box to apply suitable boundary conditions for the electric potential (i.e. electrodes for application of a driving voltage).

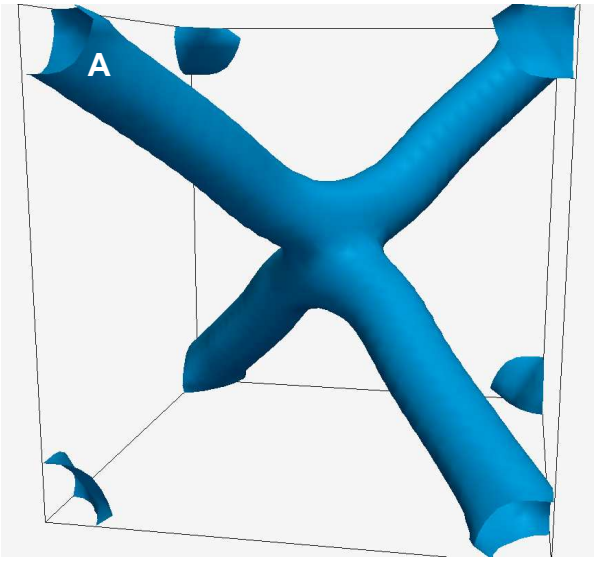

Figure 3: Elementary cell of the BPII disclination lattice corresponding to the arrangement of double twist cylinders illustrated in Fig.1. At the core of the blue tubes representing the disclinations the order parameter is significantly reduced.

4. Results

4.1. Network of Disclinations

We are first considering an initial configuration of six double-twist cylinders (DTCs) which are axially bisected so that six half-cylinders are contained in one single elementary unit cell. This arrangement, as illustrated in Fig. 1, represents the arrangement of DTCs in the Blue-Phase-II. For every triple of DTCs there are two ways of coming in to pairwise contact: either they form a continuous junction (when the local molecular orientations match) or a disclination is formed in the gusset (region A in Fig.1). In the latter case, the disclination continues as a line through the volume of the unit cell as illustrated by the blue tubes in Fig. 3. In the gusset B of Fig. 1, the local molecular orientations match pairwise and no disclination line is generated.

The situation resulting from two elementary BPII cells that are in contact (vertically stacked) is illustrated in Fig. 4. The local molecular alignment of the liquid crystal is represented by the eigenvector of the Q-tensor with the largest eigenvalue. The local state of molecular order is specified by the corresponding scalar order parameter S_1 and represented by colors ranging from red to blue (lowest order). In the plane where the two elementary cells are in contact the order parameter is highest in the center, i.e. where the distance to the disclination lines is a maximum. At the locations where the disclination lines intersect the contact plane the order parameter has a minimum value (blue color).

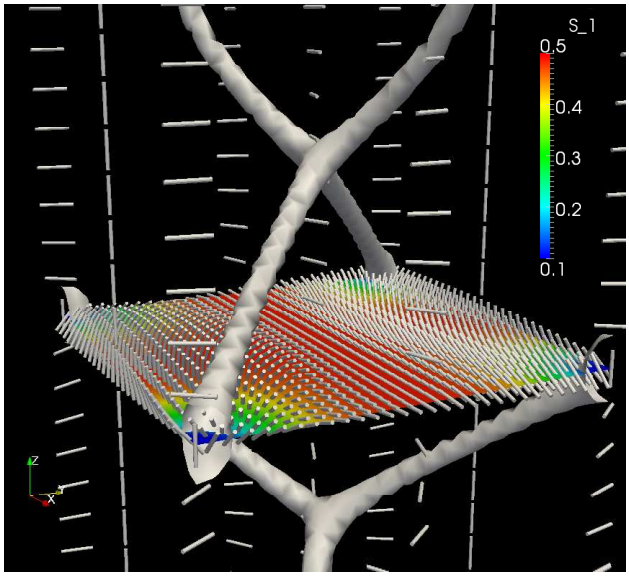

Figure 4: Local molecular orientation within two adjacent elementary BPII cells illustrated by the eigenvectors of the Q-tensor with the largest eigenvalue, together with the local molecular order specified by the order parameter S_1 (red → blue).

4.2. Pitch Variations - Redshift

The chiral-nematic pitch, i.e. the distance over which the director performs a rotation of 360°, is usually measured in a wedge-cell with the axis of the chiral helix basically perpendicular to the substrate planes. In this configuration the chiral pitch is measured without torques acting on the molecules, and thus it is called the free or natural pitch of the chiral-nematic material. In a macroscopic volume containing a chiral-nematic material with a free pitch in the range of some 100 nm, forming a blue phase, complex molecular interactions shift the equilibrium pitch, p_e, to a value that is larger that the natural free pitch of the material in the planar twisted configuration, p_0. As a consequence, the dimensions of the disclination network and the lattice constant of the blue-phase increases and the center wavelength of Bragg reflections from this configuration is shifted to longer wavelengths. This effect has been observed experimentally by Grebel et al. in 1983 [12].

A consequence of that effect for the numerical modeling of BP LCDs is the repeated adjustment of the initial configuration to a unit cell dimension that yields a minimum of energy.

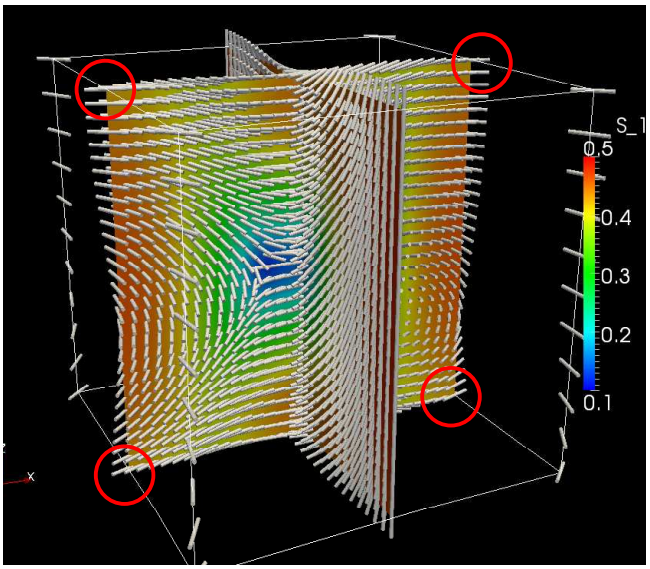

Figure 5: Molecular alignment in a BPII unit cell with edge length = $p_0/2$ (free chiral pitch, p_0 = 270,4 nm, unit cell dimensions = 135,2 nm). The molecular orientation on top and bottom planes (red circles) indicate a twist <180°.

Figure 5 illustrates the molecular alignment when the unit cell dimensions are chosen according to the free chiral pitch, p_0 (i.e. the length of the edges of the unit cell are equal to $p_0/2$). In that case the twist angle between bottom and top plane is smaller that the expected 180° as illustrated in Fig. 5. Variation of the edge dimensions of the unit cell until a minimum of energy is obtained leads to a matched length of the unit cell edges of 160,2 nm in this example as illustrated in Fig. 6.

5. Optics

The *finite difference time domain* (FDTD) method [13] is applied here to calculate reflectance and transmittance of the BP LC-cell, since this is a very versatile approach without any approximations and assumptions apart from the discretization. Uniaxial perfectly matched layers (UPML) are used on the top and bottom sides of the bounding box to mitigate spurious reflections coming from the grid boundaries. The grid used for the Q-tensor calculation is also chosen for the optics calculation.

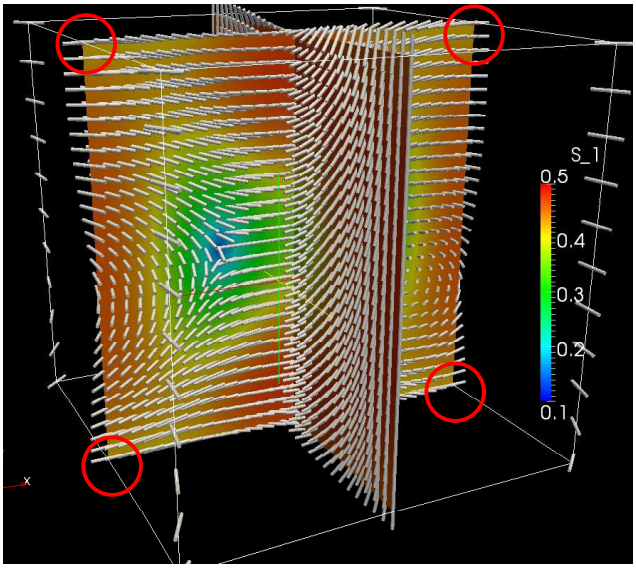

Figure 6: Molecular alignment in a BPII unit cell with adapted unit cell edge length ≠ $p_0/2$ (free chiral pitch, p_0 = 270,4 nm, unit cell dimensions = 160,2 nm). The molecular orientation on top and bottom planes (red circles) indicate a twist of 180°.

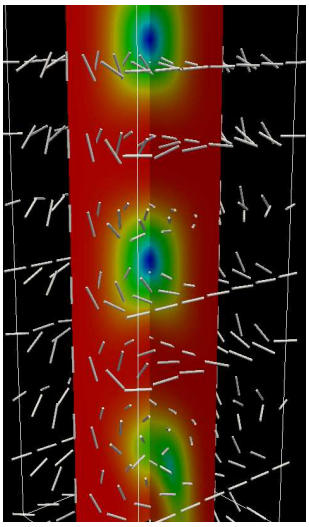

Figure 7a: Stack of 8 PBII unit cells with molecular alignment and color-coded order parameter S_1.

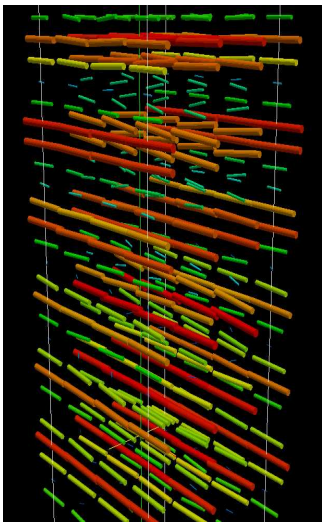

Figure 7b: Snapshot in time of electrical field vector for monochromatic light (λ = 200 nm) incident on the stack of Fig. 7a.

The light propagation inside a stack of eight elementary BPII cells as shown in Fig. 7a is illustrated in Fig. 7b by the vector of the electric field shown for one moment in time. The value of the electric field vector is represented by the thickness of the rods and by their color (red = maximum). The electro-magnetic wave is assumed to have a wavelength of 200 nm, it is incident on the stack from below. The electric field vector does not exhibit pronounced variations since the BPII volume is not distorted by external electrical fields in this example and thus the BPII volume basically is optically isotropic.

6. Discussion

The field of numerical simulation of the blue phase of chiral nematic liquid crystals has been quite busy in the past years and many details have thus been explored and analyzed (see e.g. 11, 13 and the references therein). While the model of Fukuda [14] uses a one-constant approximation of the LC-eleasticity, our model handles the full elastic anisotropy of chiral-nematic LCs. Also in extension to Fukudas model which takes into account the effect of a constant external electrical field, our model allows for definition of electrodes and it reproduces the mutual coupling of electrostatic potential and molecular orientation inside the LC.

7. Conclusion

According to the knowledge of the authors this is the first realization of a numerical model for simulation of display devices with chiral-nematic LCs in the blue phase, comprising calculation of the molecular orientation within the liquid crystal material and the optical properties of blue phase LCDs including additional optical components like polarizers and retarder sheets in a commercial modeling software package.

8. References

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