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Studying the Electrically Driven Switching of the Planar Light Guide

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Liquid crystalline materials can be used as an active media for the new generation of planar light guides. The main characteristics which governs light-guiding and switching abilities of such devices are the spatial distributions of the refraction indices (defined via the distribution of nematic director) for the liquid crystal confined within a light-guiding pore. We aim to obtain these distributions from the molecular dynamics simulation of the liquid crystalline cell with the homeotropic boundary conditions being applied. We discuss the reorientation kinetics of the homeotropic-planar transition and obtain the equilibrium director profile upon application of the planar reorienting field.

Keywords Planar light guides; liquid crystals; molecular dynamics

Introduction

Planar light guides are used as both passive and connecting elements in optical circles targeted on effective information processing and transmitting of data. At present, various solid materials with suitable optical properties are used as active and passive elements in such light guides. This has the shortcoming that a considerable amount of light intensity is lost due to reflection off the interface layer. One of the ways to overcome this problem is to use the same material with switchable optical properties as both active and passive media. The choice, quite naturally is the liquid crystalline (LC) material, which is characterized by high anisotropy of refractive index, high sensitivity to external electric and magnetic fields and a wide interval of working temperatures. The LC cell can exhibit various inhomogeneous orientational distributions depending on the surface anchoring and on external stimuli [1, 2].

However, the development of the LC based light guides requires thorough studies of the properties of confined LC layer that are related to the light propagation (especially at the wavelengths typical for laser beams). These properties include both light scattering and

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light propagation through the inhomogeneously oriented LC layers. These studies can be aided efficiently by performing computer simulations on the molecular models of various complexity [3]. In particular, the molecular dynamics (MD) simulations is well suited to study the LC cell confined inside a pore with initially homeotropic boundary conditions [3, 4]. Application of the external planar field will mimic the process of switching of the cell from homeotropic into a planar state. This is exactly what is occurring in the LC based gradient light guide. The director profile obtained by means of the MD can be used then for the analysis of light transmitting properties of the model planar light guide [5].

Here we concentrate on the first step of this broad and technologically important program. We consider popular Gay-Berne potential [6] and study the behavior of the LC cell with homeotropic boundary conditions under the influence of the temperature and external electric field. However, in external electric field the minimum of the free energy of nematic liquid crystals with negative dielectric anisotropy are determined not in director direction but in perpendicularly to applying field. We can not predict the reorientation direction of liquid crystal layer. We propose to determine this direction by means of initial pretilt of homeotropic nematic liquid crystalline texture. As the result, we obtained the director distribution inside a cell that can be used as an input in the future analysis. The outline is as follows. In section 2 we give a brief account on the modeling technique, section 3 contains results being obtained, conclusions are drawn in section 4.

Modeling Technique

To model LC systems, similar methods can be applied as for the simulation of simple liquids [3,4]. In this study we use the MD approach in canonical, *NVT*, ensemble [4]. In this case a number of particles N, the volume V, and the temperature T are constrained. All the N particles are contained within a simulation box.

To model the interaction between LC particles we use the well known Gay-Berne potential [6]:

$$U_{ij}^{GB}(\hat{u}_1, \hat{u}_2, \vec{r}_{12}) = \varepsilon(\hat{u}_1, \hat{u}_2, \hat{r}_{12}) \left[\left(\frac{\sigma_0}{r_{12} - \sigma(\hat{u}_1, \hat{u}_2, \vec{r}_{12}) + \sigma_0} \right)^{12} - \left(\frac{\sigma_0}{r_{12} - \sigma(\hat{u}_1, \hat{u}_2, \vec{r}_{12}) + \sigma_0} \right)^{6} \right] \quad (1)$$

where $\hat{u}_1$, $\hat{u}_2$ are unit vectors that define the orientations of i-th та j-th particle, respectively; $\hat{r}_{12} = \vec{r}_{12}/r_{12}$ is a unit vector along the radius-vector $\vec{r}_{12}$ that connects their centers. $\varepsilon(\hat{u}_1, \hat{u}_2, \hat{r}_{12})$ is the energy parameter, whereas $\sigma(\hat{u}_1, \hat{u}_2, \vec{r}_{12})$has a meaning of an effective separation between i-th та j-th particle, respectively. Both depend on mutual arrangement between the pair of particles and their orientations [6]. Gay-Berne potential is being well studied and its phase diagram in (ρ,T) space is known at various parameters such as asphericity of the particles, attractive well anisotropy, etc. [8,9]. We use the following set of parameters, $k = 3$, $k' = 0.2$, $\mu = 1$, $\nu = 2$, $\sigma_0 = 5$Å, $\varepsilon_0 = 0.561 \cdot 10^{-20} J$, for more details see Ref. [6–9].

Simulation box of dimensions L_x, L_y, and L_z, has periodic boundary conditions applied along *X, Y* axes and two impenetrable walls along Z axis, at $z = 0$ and $z = L_z$. In the simulations of confined liquids, the interaction between the particle and the wall is usually described via so-called 9–3 Lennard-Jones potential [10] (obtained as the result of integration over all interactions of a given particle with frozen wall particles). This form of

the potential is crucial for studying adsorption and wetting-related phenomena in confined liquids. In the case of confined LC, more emphasize is put on the orientational anchoring of mesogens and the exact form of a mesogen-wall repulsion is of lesser importance, providing the potential it repulsive enough to provide confinement of mesogens. Therefore, we opted to use the form of smoothed Weeks-Chandler-Andersen potential [11]:

$$U_{WCA}(z) = \begin{cases} 4\varepsilon[(\sigma_0/\Delta z)^{12} - (\sigma_0/\Delta z)^6] + \varepsilon, & \Delta z < 2^{1/6}\sigma_0 \\ 0, & \Delta z \geq 2^{1/6}\sigma_0 \end{cases} \quad (2)$$

which is evaluated in respect to the shortest distance between the center of the particle and the surface, Δz. This repulsive potential prevents mesogens from crossing the walls at $z = 0$ and $z = L_z$. To model the homeotropic anchoring of mesogens orientation near walls, one can use either a step-like $V_{srf}^{(1)}$ or exponentially decaying $V_{srf}^{(2)}$ local orientation potentials defined as:

$$V_{srf}^{(1)}(z) = \begin{cases} f_{srf}\, u_z^2, & \Delta z < \Delta z_{\max} \\ 0, & \Delta z \geq \Delta z_{\max} \end{cases} \quad (3)$$

$$V_{srf}^{(2)}(z) = f_{srf} e^{-z/\xi} u_z^2, \quad (4)$$

where f_{srf} is the strength of anchoring, Δz is a shortest distance from particle center to the wall, u_z is the component of the particle orientation $\hat{u}$ along the surface normal. In this paper we used the step-like potential (5) with the cutoff distance of $\Delta z_{max} = 19$Å from each wall.

The bulk external electric field has a similar form but affects all the mesogens within the simulation box, the interaction energy has the form:

$$V_{el} = -f_{el}(\hat{u} \cdot \hat{e})^2 \quad (5)$$

where f_{el} is the field strength and the unit vector $\hat{e}$ defines its direction. In the case of $f_{el}>0$ the field prescribes the preferential axis for particle $\hat{u}$, whereas for $f_{el}<0$ all $\hat{u}$ vectors confined within the plane perpendicular to $\hat{e}$ will have the same energy (see, Fig. 1). This mimics the case of the transverse dipole case. Differentiation of expressions (5–7) over $\hat{u}$ yields torques which enter the equations of motion for the orientational degrees of freedom.

The main property of interest in this study is the distribution of the nematic order inside the pore. The box is split into a grid of cuboidal domains and both nematic order and director are evaluated in each domain using a standard method. One first evaluates an average order tensor:

$$S_{\alpha\beta} = \frac{3}{2}\begin{pmatrix} < u_x u_x > -\frac{1}{3} & < u_x u_y > & < u_x u_z > \\ < u_y u_x > & < u_y u_y > -\frac{1}{3} & < u_x u_z > \\ < u_z u_x > & < u_z u_y > & < u_z u_z > -\frac{1}{3} \end{pmatrix}, \quad (6)$$

where the averaging is performed over all particles within the domain. The tensor $S_{\alpha\beta}$ is then diagonalized [12, 13]. Its largest eigenvalue S defines the scalar order parameter, whereas the eigenvector related to this eigenvalue defines the nematic director within a domain. To evaluate global order, the evaluations are performed within the whole simulation box. Alternatively, one can use approach based on evaluation of long-ranged correlations between LC particles [14].

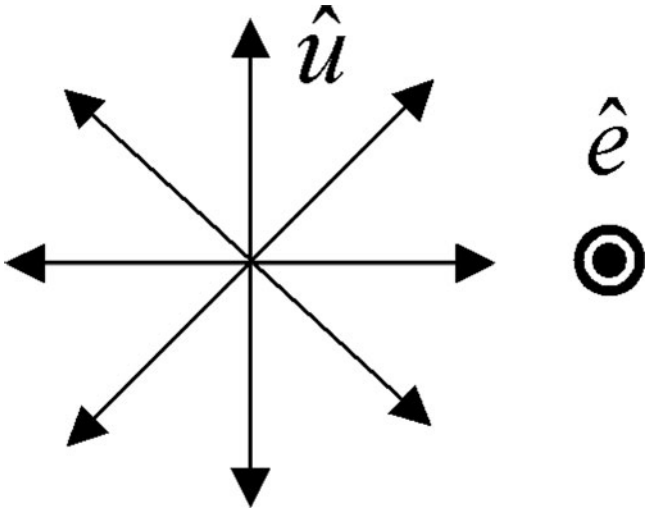


Figure 1. Symmetry for the mesogen orientation $\hat{u}$ within the plane perpendicular to the bulk field orientation defined via unit vector $\hat{e}$ (see, Eq. (7)).

One can also introduce an order parameter in respect to a given axis (e.g. the direction of external electric field) defined via the unit vector $\hat{f}$:

$$S_f = \frac{3}{2}\left\langle (\hat{u}\cdot\hat{f})^2 - \frac{1}{3}\right\rangle, \tag{7}$$

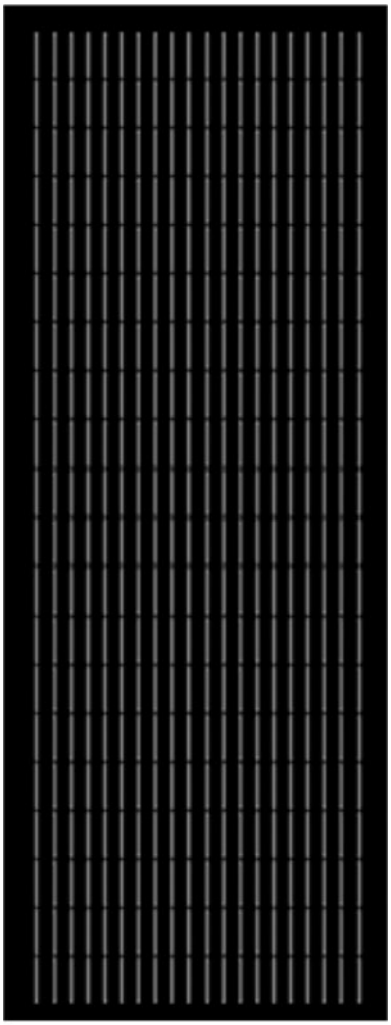
where averaging is performed over all mesogens orientations $\hat{u}$. The profile for the order parameter along Z axis, $S_f(z)$, is evaluated by binning the simulations box along this axis and evaluating S_f in each bin.

Results and Discussion

All the simulations are performed using the GBMOLDD program developed for the more general case of LC polymers [15, 16]. It was extended to include the surface potentials (5), (7) introduced above. We used the *NVT* ensemble. The start-up configuration is built as a simple cubic lattice of $20 \times 20 \times 20$ sites, all $N = 8000$ mesogens perfectly aligned along Z axis (see, Fig.2). The size of the simulation box is $L_x = L_y = 111.5$Å$, L_z = 321.5$Å, the density equal to $\rho = 0.751$g/cm^3. The homeotropic boundary conditions at the surfaces are applied via the potential form of (5) with $f_{srf} = 2$ and $z_{max} = 19$Å. The time step of 20 ns was used, and the simulations of runs length of The sketch sequence of the phases being observed are as follows. At $T = 400$ K the LC exhibits regular smectic A phase with the nematic order parameter $S = 0.82$.

With the increase of the temperature up to $T = 450$ K, the bulk region turns into the nematic phase while the surface particles stay layered due to surface anchoring. The order parameter averaged over the entire simulation box is equal to $S = 0.6$.

Upon further heating of the system up to $T = 500$ K, the bulk turns into the isotropic phase. Well ordered surface layers prevent the average order parameter of approaching zero, it is equal to $S = 0.2$ instead. To compare obtained phase diagram with another simulation studies one needs to switch to the reduced density and temperature, which are



a)

Figure 2. Initial lattice structure.

$\rho^* = N(\sigma_0)^3/V = 0.25$ and $T^* = kT/\varepsilon_0 = 0.984$, 1.107, 1.23 (for $T = 400$ K, 450 K, 500 K, respectively). As follows from the phase diagram by de Miguel et al. [9], similar temperature sequence of phases is observed at higher reduced density, $\rho^* \sim 0.31$ (however, they used a bit different form of the Gay-Berne potential with $\mu = 2$, $\nu = 1$). Therefore, the shift of the phase boundaries to lower densities in our case can be attributed to both the effects of another set of (μ, ν), and to the presence of the anchoring potential.

Let considerate the initial configuration with pretilt along the X-axis (15° and 30°) but with the presence of bulk external field of the form (7) with $f_{el} = 0.2$ applied along the

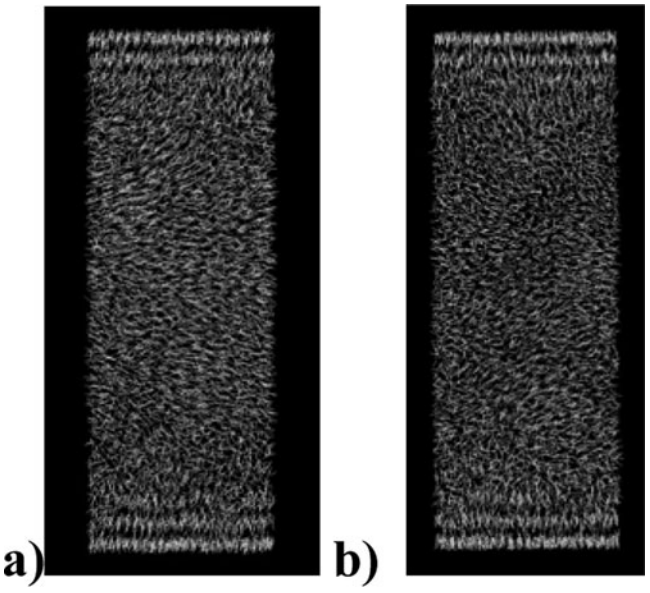


Figure 3. The nematic texture (pretilt 15°) upon application of the electric field with fel = 0.2 at the temperature T = 500 K after t = 300 ps: a) in parallel to pretilt direction b) in perpendicular to pretilt direction.

Z-axis. At the temperature $T = 500$ K the orientational perturbations are started to build up in the middle of the pore,

Further on in time, the center of the pore is gradually reoriented pretilt direction. After $t = 300ps$, most of the particles in bulk are reoriented along the field. One observes formation of a planar layer with the homeotropic anchoring of one or two layers next to the surfaces (Fig.3,4). Such orientational distribution of particles in a pore is observed experimentally in a gradient wave guide. The refractive index difference, $\Delta n = n_{\parallel}$ - $n_{\perp}$, (where $n_{\parallel}$ is measured along the global director) changes from its minimum value near the surface to its maximum one in the middle of the pore.

The simulations allow one to obtain the distribution of the local nematic director within the pore. It can be characterized by the value of the order parameter $S_f(z)$ (9) which is evaluated along the electric field. At $S_f(z)>0$ the local director at z is oriented along the field (homeotropic arrangement) whereas at $S_f(z)<0$ it is oriented perpendicularly to it (planar arrangement). The distribution obtained at $T = 500$ K, $f = 0.2$ and averaged over the time interval $t = 200$–300 ps is shown in Fig. 5, 6.

To reduce the fluctuations of the profile a wider pore can be used but it incurs longer simulation runs. The profile of $S_e(z)$ can be used to predict the transmission of the light in the LC planar light guide. The resulting direction of long molecular axes orientation makes it possible to determine the refractive index profile in the liquid crystal layer since nematic LC has properties of a uniaxial with an optical axis direcrion matching the long axis of a molecule. The refractive index profile will give an opportunity to study processes of propagation of optical radiation, including laser, in planar liquid crystal fiber by the means of Zemax software tool, especially the phenomenon of light scattering and the effects occurring during light propagation in inhomogeneously oriented layers of liquid crystals.

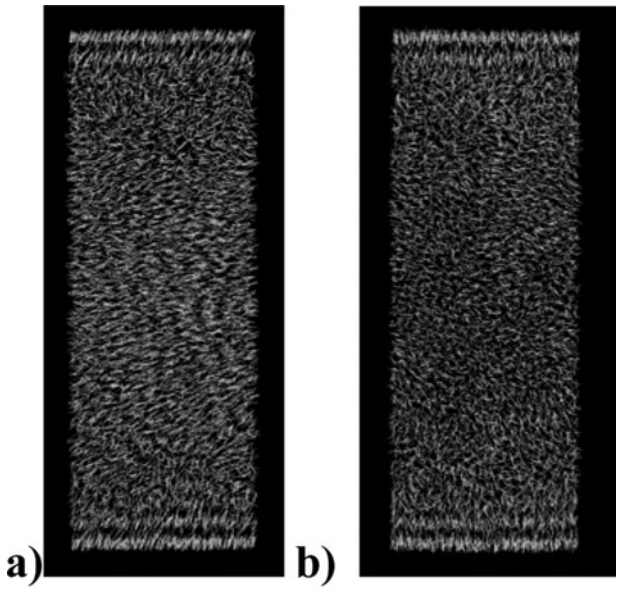


Figure 4. The nematic texture (pretilt 30°) upon application of the electric field with fel = 0.2 at the temperature T = 500 K after t = 300 ps: a) in parallel to pretilt direction б) in perpendicular to pretilt direction.

Experimental Conoscopic Studies

In this section we present experimental conoscopic studies of the reorientation of the LC molecules in MBBA-based LC cell under external electric field. The details of the experiment are given elsewhere [5]. The pretilt of initial homeotropic nematic texture was

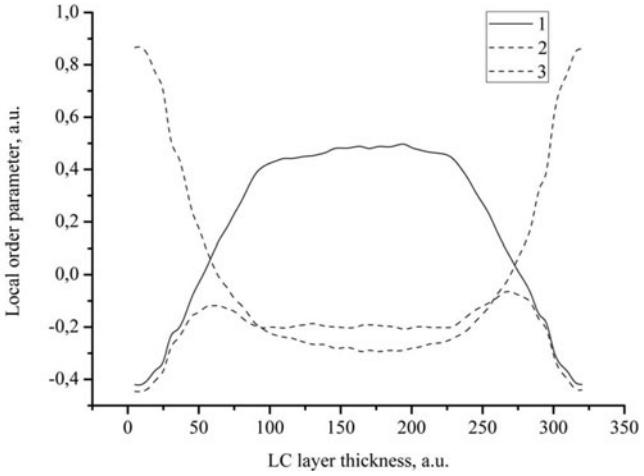


Figure 5. Equilibrium distribution of the local order parameters $S_x(z)$-(1), $S_y(z)$- (2), $S_z(z)$- (3). *Z*-axis coincides with the field and surface normal vector, *X* is the direction of spontaneous arrangement of LC molecules inside the pore. Temperature is T = 500 K, the field (f_{el} = 0.2) is applied along *Z*-axis, (pretilt 15°).

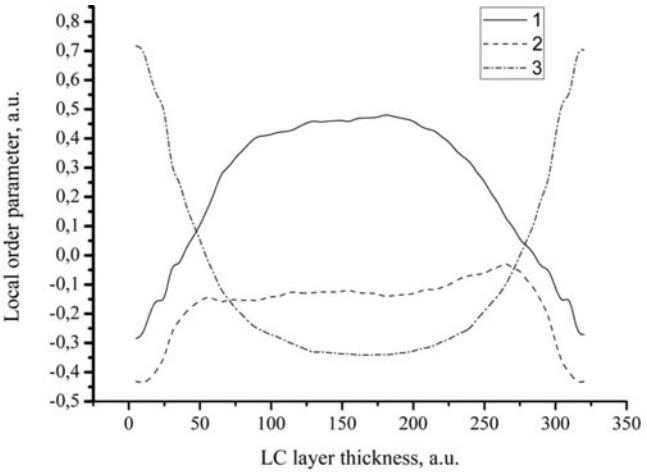


Figure 6. Equilibrium distribution of the local order parameters $S_x(z)$-(1), $S_y(z)$- (2), $S_z(z)$- (3). *i*-axis coincides with the field and surface normal vector, *X* is the direction of spontaneous arrangement of LC molecules inside the pore. Temperature is T = 500 K, the field ($f_{el} = 0.2$) is applied along *Z*-axis, (pretilt 30°).

obtained under the flow of nemetic liquid crystal on polymer oriented layer during the LC-cell filling. Analysis of conoscopic pictures was carried out corresponding to theoretical conoscopic pictures described in [7].

Initial arrangement of the LC molecules is homogeneous homeotropic as indicated by a conoscopic picture which contatins characteristic dark cross in the center (Fig.1).

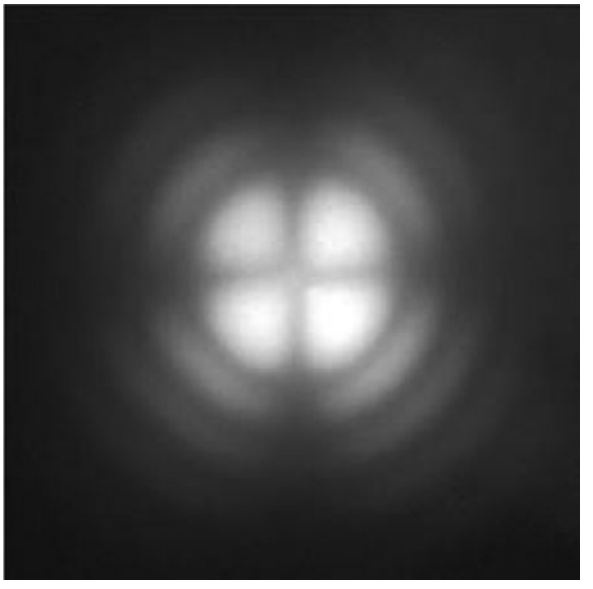


Figure 7. Experimental conoscopic pictures of a sample with initial homeotropic orientation.

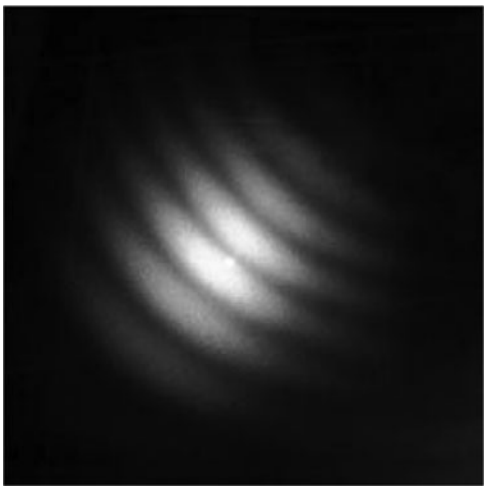


Figure 8. Experimental conoscopic pictures (applied voltage 9V) of a sample with initial homeotropic orientation.

The direction of reorientation of central part of LC sample corresponds to cross shifting in central part of conoscopic pictures. Upon application of a weak electric field, the LC molecules are reoriented in the middle of the cell. Further increase of the potential to 2–15V leads to the enlargement of planarly oriented region in the bulk, this is indicated by the changes in a conoscopic picture shown in Fig.2. Further voltage increase leads to the formation of izochroms of hyperbolic type and to the formation of conoscopic picture typical for planar nematic liquid crystal orientation. However, the lack of symmetry of conoscopic picture along the axis of radiation propagation (U $=$ 50V, see Fig. 3) indicates

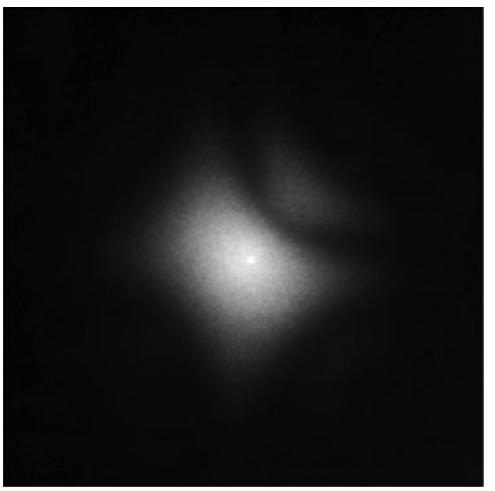


Figure 9. Experimental conoscopic pictures (applied voltage 50V) of a sample with initial homeotropic orientation.

about the presence of thin homeotropicly oriented near surface layers in the sample. Further voltage increase does not affect the appearance of conoscopic picture.

Comparing experimental and theoretical conoscopic pictures, we can conclude that the application of external electric field to a liquid crystal cell with an initial homeotropic orientation filled with a liquid crystal with a negative dielectric anisotropy leads to the formation of a section with a planar orientation of liquid crystal in the center of the cell. In the investigated range of voltages the application of an external electric field does not lead to a complete reorientation of the LC layer, ie with the maximum voltage applied (U = 50V) near surface layers with homeotropic orientation are observed in the LC cell. Based on the foregoing, it can be argued that in a standard sandwich-cell with initial homeotropic orientation and liquid crystal with negative dielectric anisotropy and positive refractive index anisotropy under the affect of applied electric field there is formed a texture with optical properties which satisfy the conditions of planar light guide. At the same time, the size of the core of such planar light guide can be changed within wide limits by changing the control voltage. The direction of reorientation of central part of LC layer corresponds to pretilt direction of initial nematic texture obtained at LC cell filling.

Conclusions

We use in this study a simple molecular model based on the Gay-Berne potential to describe the liquid crystal based planar wave guide. Orientational anchoring of homeotropic type is applied on both surfaces of the pore. At first, the isotropic, nematic and smectic *A* phases were found by varying the temperature. To model switching of the light guide from homogeneous homeotropic state into the state with planar state in the bulk the planar external field is applied. As the result, the following kinetics of switching is observed. Orientational perturbation due to application of the field starts from the center of the pore and then propagates into the rest bulk region of the pore. Final equilibrium director profile has a bell-like shape and is planned to be used in further studies aimed on modeling the light propagating properties of the proposed light guide. The results being obtained form a sceleton scheme towards the development of electrically controlled integrated liquid crystalline optical circuits for data processing systems, transmission and displaying of optical information.

References

[1] Brzdakiewicz K. A., Karpierz M. A., Fratalocchi A. [et al.] (2005). *Opto-Electronics Review, No. 2*, V. *13*, 107.
[2] Tyszkiewicz C., Pustelny T. (2004). *Optika Applicata, No. 4*, V.*34*, 507.
[3] Frenkel D., Smit B., (2002). *Understanding molecular simulation, from algorithms to applications, 2nd edition*. New York, Academic.
[4] Allen M., Tildesley D. (1991). *Computer simulation of liquids*. Oxford, Oxford University Press.
[5] Mykytyuk Z., Fechan A., Sushynsky O. [et al.] (2010). *Acta Physica Polonica A, No 1*, V. *117*, 248.
[6] Gay J. G., Berne B. J. (1981). *J. Chem. Phys.*, *74*, 3316.
[7] Nastishin Ya., Dovgyj O. B., Vlokh O. G. (2002). *Ukrainian journal of physical optics, No. 3*, V.*3*, 98–106.
[8] de Miguel E. *et al.* (1996). *J. Chem. Phys.*, *105*, 4234.
[9] Brown J.T. *et al.* (1998). *Phys. Rev.*, *E 57*, 6685.
[10] F.F. Abraham, Y. Singh, (1977). *J. Chem. Phys. 67*, 2384.

[11] Weeks J. D., Chandler D. and Andersen H. C. (1971). *J. Chem. Phys.*, *54*, 5237.
[12] Vieillard-Baron J. (1974). *Mol. Phys.*, *28*, 809.
[13] Eppenga R. and Frenkel D. (1984). *Mol. Phys.*, *58*, 1303.
[14] Zannoni C. (1979). *Molecular Physics of Liquid Crystals*, *191–220*, 139.
[15] Ilnytskyi J. and Wilson M. R. (2001). *Comput. Phys. Commun.*, *134*, 23.
[16] Ilnytskyi J. and Wilson M. R. (2002). *Comput. Phys. Commun.*, *148*, 43.