Computer Simulation of the Impact Magnitude of Applied Field and Surface Anchoring Force on Gradient Lightguide Formation in the Layer of Nematic Liquid Crystal

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Abstract – **There were investigated phase diagram and distribution profile of the director field of simulated liquid crystal which is kept in the pore with homeotropic boundary conditions in different phases. By the means of molecular dynamics method there was performed the computer simulation of the changes of refractive index profile in gradient lightguide under the surface anchoring force and applied electric field.**

Keywords - **planar lightguides, liquid crystals, molecular dynamics.**

I. INTRODUCTION

Planar lightguides are used in optical circuits for processing and transfer of information as passive, active as well as interface circuits elements. Nowadays for their production most of all solid matter is used. In solid-state planar lightguide systems there is a problem with creating active and passive elements on the basis of the same material. When using media with different optical properties a significant loss of optical radiation is observed on their interface. One way to solve this problem is the application of liquid crystal (LC) materials as an active medium of a planar lightguides, which are characterized by high refractive index anisotropy, high sensitivity to external electric and magnetic fields and a wide range of operating temperatures.

However, in order to be able to use these devices an investigation of propagation of optical radiation (including laser emission in visible range of spectrum) in a fiber with liquid crystal core, including the phenomenon of light scattering effects that occur during the passage of light in inhomogeneously aligned liquid crystal layers. Therefore, simulation of the effect of applied electric field magnitude and surface anchoring force on the director field distribution in nematic liquid crystal (NLC) layer with the initial homeotropic alignment will provide the ability for fundamental study of gradient lightguide with liquid crystal core.

II. COMPUTER SIMULATION

For LC systems simulation it is possible to use the same methods as for investigation of the properties of fluids [1-2]. Thus, at first there should be obtained appropriate thermodynamic ensemble [2]: a certain number of molecules are injected in the cell and are imposed to boundary conditions, such as fixed number of particles N, volume V (or pressure P) and temperature T. For investigation of volumetric properties periodic boundary conditions are usually used, during the investigation of surface phenomena in the direction of one of the spatial axes creates atomic or continuous wall. For description of the isotropic and nematic phases the cell with a fixed shape is enough (in NVT, as well as in NPT ensembles). Smectic phases are characterized by large anisotropy, and their self-assembly can be complicated by noncompatibility of phase' metric with the shape of the cell. The indicator of this phenomenon is significant anisotropy of pressure tensor in the case of placing such a system in the cell with fixed shape. In such cases more efficient are ensembles with variable cell shape, for example, in the most general Parrinello-Raman form, or in more simple $NP_{xx}P_{yy}P_{zz}T$ form, which provides constant each of diagonal pressure components.

The main task of orientation ordering simulation is to determine the nematic order parameter and direction orientation. They are calculated by the method according to which initially order parameter tensor is calculated, and then obtained order parameter tensor is being diagonalized. An alternative method is based on the long-range orientational correlations calculations. For the analysis of the structure of the phase with inherent translational ordering the calculation of coupled correlation functions should be done. Computer simulation of molecular models in this paper is made by the means of GBMOLDD software [3]. In the basis of computer simulation there is the interaction potential, which describes the microscopic characteristic energy of the system. For LC systems simulation is used classical bi-particular potentials that take into account quantum-mechanical effects only in an effective manner. In this paper we used the potential of the Gay-Berne:

$$U_{ij}^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij}) = C_{ij}^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})\left[\left(r_{ij}^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})\right)^{12} - \left(r_{ij}^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})\right)^{6}\right] \quad (1)$$

where u_i, u_j – orientations of i and j molecules long axes, respectively, r_{ij} – unit radius-vector between the centers of these molecules,

$$r_{ij}^{(GB)} = \frac{s_0^{(GB)}}{\hat{r}_{ij} - s^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij}) + s_0^{(GB)}}$$

shifted contact separation between molecules, and

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$$\varepsilon_{ij}^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij}),\ s^{(GB)}(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})$$

respectively energy parameter and effective separation between *i* and *j* molecules, which are functions of their mutual location and orientation [Gay-Berne].

Surface is specified in the direction of the Z axis, so at $z = 0$ and $z = Lz$ there is introduced smoothed repulsive potential of Chandersa Weeks-Anderson type, acting between the surface and molecules and keeping molecules inside the cell. In other axes direction there were used periodic boundary conditions. In order to provide homeotropic boundary conditions we used the step orientation function, which act on each molecule at distances in the order of 19Å from both surfaces and introduced by with surface rotating energy:

$$V_{srf}=f_{srf}\cdot(e_z)^2 \quad (2)$$

where – $f_{srf}>0$ characterizes anchoring force of near-surface layers, e_z – component of orientation of the molecule with respect to normal direction to the surface.

The influence of electric field is simulated by a similar three-dimensional orientation field which is introduced through reorientation energy:

$$V_{el}=f_{el}\cdot(e_z)^2 \quad (3)$$

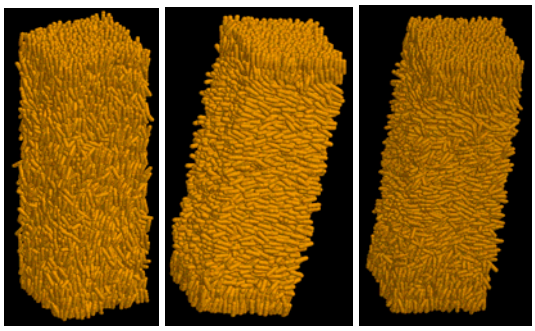
where – f_{el} characterizes the reorientation force. This field acts on all molecules in the cell and case $f_{el}>0$ corresponds to longitudinal dipole, and $f_{el}<0$ - transverse. Differentiation of equations (2), (3) with respect to e_z gives rotational torques which are parts of rotational motion equations in molecular dynamics. GBMOLDD software tool gives ability to receive the distribution of director direction in any point of the cell and the corresponding value of the order parameter that directly associated with the refractive index value.

The basic input data for the program are: n_x, n_y, n_z – the number of molecules in *x*, *y* and *z* axes; f_{srf} – the magnitude of the anchoring force of near-surface layers; T – the simulation temperature; f_{el} – the magnitude of applied to LC molecules field;

The output data from the program is recorded in files of two types: *.coord and *.lst. Files of the type of *.coord allow to display visually the reorientation of molecules in the LC layer, and therefore the direction of molecules director. *.lst files contains the numerical values of the distribution of the director orientation, which are further processed in order to obtain a change of refractive index in LC layer under the influence of electric field. In Fig. 1 - 2 there is shown the results of simulation in the mentioned above software.

As it is possible to see under the influence of electric field there is observed orientation change of the central part of LC layer and the speed of formation of the planar part and its thickness are greater for large values of applied field magnitude and minimum surface anchoring force (Fig. 1b). This assembly of molecules (Fig.1b and Fig.2) is an evident of the formation of gradient lightguide in the layer of nematic liquid crystal.

Simulated textures allow obtaining distribution of director orientation in NLC layer, which is depicted in Fig. 2. In this model the director orientation can have values from 1 (homeotropic orientation) to -0.5 (planar orientation). Further, taking into account the anisotropy of refractive index obtained dependence values used for calculation distribution of the refractive index in NLC layer.



1 2 3

Fig.1. Simulated textures of NLC with different values of the magnitude of applied field and anchoring force: 1) 0.1 and 0.2; 2) 0.6 and 0.2; 3) 0.6 and 0.6.

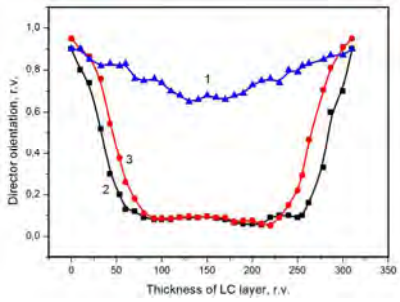


Fig.2. Distribution of director orientation with different values of applied field magnitude and anchoring force: 1) 0.1 and 0.2; 2) 0.6 and 0.2;3) 0.6 and 0.6.

III. Conclusion

Results of simulation showed:

1. Application of the electric field to the LC material with negative dielectric anisotropy and with the initial homeotropic orientation leads to the formation of a stable layer with planar orientation, with a width directly proportional to the magnitude of applied field.

2. The increase of anchoring force, at a constant value of the magnitude of applied field leads to an increase of the thickness of near-surface homeotropic aligned layer. Simulation confirms that the change of the applied field magnitude and near-surface anchoring force can induce the change of distribution of planar lightguide refractive index and thus tune its optical characteristics.

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