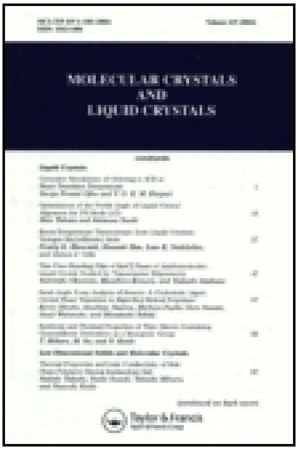

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Electric Field Control of Diffraction Efficiency in Holographic Polymer Dispersed Liquid Crystal

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We report on theoretical study of diffraction efficiency of holographic polymer dispersed liquid crystals (H-PDLCs) subject to externally applied electric field. To find the director profile within single liquid crystal (LC) droplet under externally applied voltage we used Monte Carlo simulations, Lebwohl-Lasher (LL) lattice model, strong tangential (bipolar droplets) and normal (radial droplets) anchoring conditions. The coupled-wave theory is then used to describe the diffraction properties of anisotropic holographic gratings under the action of the electric field.

Keywords: electric switch; Monte Carlo simulation; polymer dispersed liquid crystals

1. INTRODUCTION

Polymer dispersed liquid crystals (PDLC) are materials that consist of liquid crystal submicron droplets, with typical radii ranging from few hundred angstroms to more than micrometers, embedded in a polymer matrix. These systems are interesting both for technical purposes, in view of their applications in optical devices, such as optical storage, variable focus lenses, etc, and also for studying the behavior of mesophases in confined environments [1–5]. These materials allow the

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Address correspondence to V. Reshetnyak, Physics Faculty, Kyiv National Taras Shevchenko University, Prospect Glushkova, 6, Kyiv, 03680, Ukraine. E-mail: reshet@iop.kiev.ua recording of high spatial frequencies with real-time response, with low energy exposures and without wet processing, in contrast with classical recording materials, such as photographic materials (photoresist or dichromated gelatin).

Recently the interest to H-PDLC materials has been continuously growing due to the large anisotropy and large electric field-induced birefringence change in LC droplets that allow the easy control of optical properties of components. H-PDLC materials are formed exposing a light-sensitive homogeneous monomer and LC mixture to an interference pattern. The number of monomers is reduced in the illuminated zones with the polymerization and monomers from the dark regions diffuse into the bright zones [6]. LC density is higher in the dark zones, the effective refractive index there is determined mainly by LC director profile within the droplet volume. The bright zones have higher polymer density and the effective refractive index there is close to the polymer refractive index. The aggregation of LC molecules into LC droplets in H-PDLC materials provides the potential of post-exposure control over the diffraction efficiency. Due to the large electric field-induced birefringence change in those droplets it is easy to control optical properties of the components made of these materials. The refractive index modulation as well as the diffraction efficiency of such H-PDLC materials strongly depends on LC director orientation within the droplet.

Recently Harbour and co-authors have reported on diffraction efficiency study of H-PDLC films [6]. In the theoretical part of their study they assumed perfect homogeneous alignment of LC director within the droplet volume. In the present work we take into account that LC director profile in each LC droplet is inhomogeneous and controlled by the balance of elastic energy associated with the director inhomogeneity within the droplet, anchoring energy at the droplet surface, and the magnitude of the externally applied electric field.

2. DIFFRACTION EFFICIENCY OF H-PDLC FILM AND DIRECTOR PROFILE WITHIN LC DROPS

Recently Montemezzani and Zgonik [7] have extended the coupled wave theory of Kogelnik [8] to the case of anisotropic materials with grating vector and medium oriented in arbitrary directions. The authors of Ref. [6] used this theory for the evaluation of diffraction efficiency when the director within each LC droplet is uniformly aligned along the grating wave vector:

$$\varepsilon_{||} = \varepsilon_{||}^{LC}, \quad \varepsilon_{\perp} = \varepsilon_{\perp}^{LC} \tag{1}$$

They assumed that the relative-permittivity tensor of H-PDLC film varies in the sinusoidal form along the x axis and that the main axis of the local optical indicatrix of the uniaxial medium lies along the same axis such that the relative permittivity of the film is given by

$$\hat{\varepsilon} = \hat{\varepsilon}^0 + \hat{\varepsilon}^1 \cos(Kx) \tag{2}$$

where $\hat{\varepsilon}^0$ is the average (over volume) relative permittivity tensor, $\hat{\varepsilon}^1$ is the modulation depth of the relative permittivity tensor. Taking into account these simplifications for their H-PDLC material the diagonal form of the relative permittivity tensor

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix} \tag{3}$$

has the following components: $\varepsilon_{xx} = \varepsilon_{\text{II}}$ is the dielectric permittivity for the light with polarization that is parallel to the grating vector, $\varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_\perp$ are dielectric permitivities for the light with polarization that is perpendicular to the grating vector. Thus in Eq. (2) they assumed

$$\varepsilon^0_{\perp,\text{II}} = \varepsilon^{LC}_{\perp,\text{II}} c + \varepsilon_{Pol}(1-c), \varepsilon^1_{\perp,\text{II}} = (\varepsilon^{LC}_{\perp,\text{II}} - \varepsilon_{Pol})c \tag{4}$$

where c is the volume concentration of the LC, $\varepsilon^{LC}_{\text{II}}$ and $\varepsilon^{LC}_{\perp}$ are relative permitivities of LC for light polarized parallel and perpendicular to the director orientation, respectively, ε_{Pol} is the relative permitivity of the polymer.

In the present work we use the same form for the dielectric permitivity of H-PDLC film with the difference that now instead of liquid crystal material permittivity in (4) the more realistic, averaged over droplet volume, value of LC permitivity will be used

$$\langle \hat{\varepsilon}^{LC} \rangle = \frac{1}{\text{V}} \int \hat{\varepsilon}^{LC}(\vec{r}, \vec{E}) d\vec{r} \tag{5}$$

where

$$\varepsilon_{ij}(\vec{E}) = \varepsilon_\perp \delta_{ij} + (\varepsilon_\rceil - \varepsilon_\perp) n_i(\vec{E}) n_j(\vec{E}) \tag{6}$$

To calculate the diffraction efficiency η of grating (2) we shall use results of papers [6,7]:

$$\eta = \frac{\sin^2 \sqrt{\xi^2 + \nu^2}}{1 + \xi^2/\nu^2} \tag{7}$$

with $\nu = d\sqrt{\chi_i\chi_d}$ is a parameter governing the coupling constant, ξ is the Bragg mismatching parameter, $\chi_{i,d}$ are coupling constants:

$$\xi = \frac{dg_d\Delta k_i}{2\cos(\varphi_d)k_d}, \ \chi_{i,d} = \frac{k_0 A}{4n_{i,d}g_{i,d}\cos(\varphi_{i,d})} \tag{8}$$

In Eq. (8), $\varphi_{i,d}$ are angles between the normal to the surface of H-PDLC (axis OY) and Poynting vectors for incident and diffracted waves, respectively, $n_{i,d}$ are average refractive indexes for incident and diffracted waves, $k_{i,d} = k_0 n_{i,d}$ are wave vectors inside H-PDLC material, walk-off parameters $g_{\mathrm{i,d}}$ are cosines of angles between the energy propagation direction and wave vector directions in the incident and diffracted beams, $A = e_i\hat{\varepsilon}^1 e_d = e_d\hat{\varepsilon}^1 e_i$, e_i and e_d are unit vectors along incident and diffracted electric fields, respectively, Δ is small dephasing measure from Bragg condition, which is defined according to Kogelnik [8].

$$\Delta = \frac{(K^2 - 2k_0 K n_i \sin(\theta_i))}{2k_0 n_i} \tag{9}$$

To find the director profile inside LC droplet we used a lattice model of LC, where the particles are treated as interaction sites (“spins”) with continuously varying orientation but with fixed positions. In this work we choose the simplest Monte Carlo simulations model, which is based on the Lebwohl-Lasher (LL) lattice model. In this model vector spins are confined to the sites of a cubic lattice. In the model system each spin represents a closely packed group of molecules that maintains its short range order across the nematic/isotropic phase transition. The anisotropic potential among the nearest neighbors sites depends only on their relative orientations. The total interaction energy for our model system consisting of nematic spins was calculated as

$$U = -\sum_{\substack{i,j\\ i<j}} \varepsilon_{ij} P_2(\cos\beta_{ij}) - \varepsilon\xi\sum_{i=1}^{N} P_2(\cos\beta_i) \tag{10}$$

with $P_2(x) = 1/2(3x^2 - 1)$ (second rank Legendre polynomial), $\cos\beta_{ij} = u_i u_j$. Here u_i denotes the unit vector giving the orientation of the spin located at the i-th lattice site, β_i is the angle between the field direction and the molecular symmetry axis. The sum in Eq. (1) is taken over nearest neighbors only. The first term in (10) is responsible for interaction between LC molecules. The ε_{ij} constant represents the interaction strengths and is denoted by ε for nearest-neighbors particles i and j and zero otherwise. The second term in (10) describes interaction between LC and external electric field [9]:

$$\varepsilon\xi = \frac{\varepsilon_0}{3}\Delta\alpha \mathrm{E}^2 \tag{11}$$

The quantity ξ determines the strength of coupling with the external electric field **E**, which is assumed to be homogeneous across the drop, $\Delta\alpha$ is the microscopic polarizability anisotropy.

3. NUMERICAL RESULTS AND CONCLUSIONS

We have studied two types of boundary conditions at the nematic spherical droplet-polymer matrix interface, namely tangential boundary conditions, for which the ghost spins are oriented tangential to the droplet surface and radial boundary conditions, the spins are oriented normally to the local surface, so that they point towards the center of the droplet. In the first case we have so-called bipolar droplets and in the second–radial droplets.

Our simulations started from a random configuration of the nematic spins. Then the standard Metropolis scheme was employed to update nematic spins orientations, maintaining a rejection ratio close to 0.5. The final result doesn't depend on the choice of the starting configuration.

We have performed a complete set of Monte Carlo simulations for different values of field strength, $\xi = (0, 0.2, 0.4, 0.6, 0.8, 1)$. Our simulation system consisted of $N = 150000$ spins.

For numerical calculations of diffraction efficiency we used the following values of LC and polymer matrix parameters $\varepsilon_{\perp}^{LC} = 2.3, \varepsilon_{||}^{LC} = 2.95$, $\varepsilon_{pol} = 2.4$, concentrations of LC – 30% [6]. Diffraction efficiency was calculated for a probe light with $\lambda = 0.628\,\mu\text{m}$, incident on the grating with a period $\Lambda = 1.0\,\mu\text{m}$ and a cell thickness $d = 27.4\,\mu\text{m}$ [6].

On Figure 1a we show angular selectivity of diffraction efficiency for *s*-polarized reading beam, for different electric field strength. Figure 1b presents angular selectivity of diffraction efficiency for *p*-polarized reading beam, for different electric field strength. Both results are for bipolar droplets. It can be seen that the electric field influences the maximums of diffraction efficiency and its position. The droplet order parameter $S_{ij} = \frac{1}{V}\int S(n_i(\vec{r},\vec{E})n_j(\vec{r},\vec{E}) - \frac{1}{3}\delta_{ij})d\vec{r}$ is represented at Figure 1c. Diffraction efficiency and order parameter for radial droplets are presented on Figures 2a–c.

From Figures 1 and 2 one can see that by applying electric field it is possible to control the diffraction efficiency of H-PDLC films. Electric

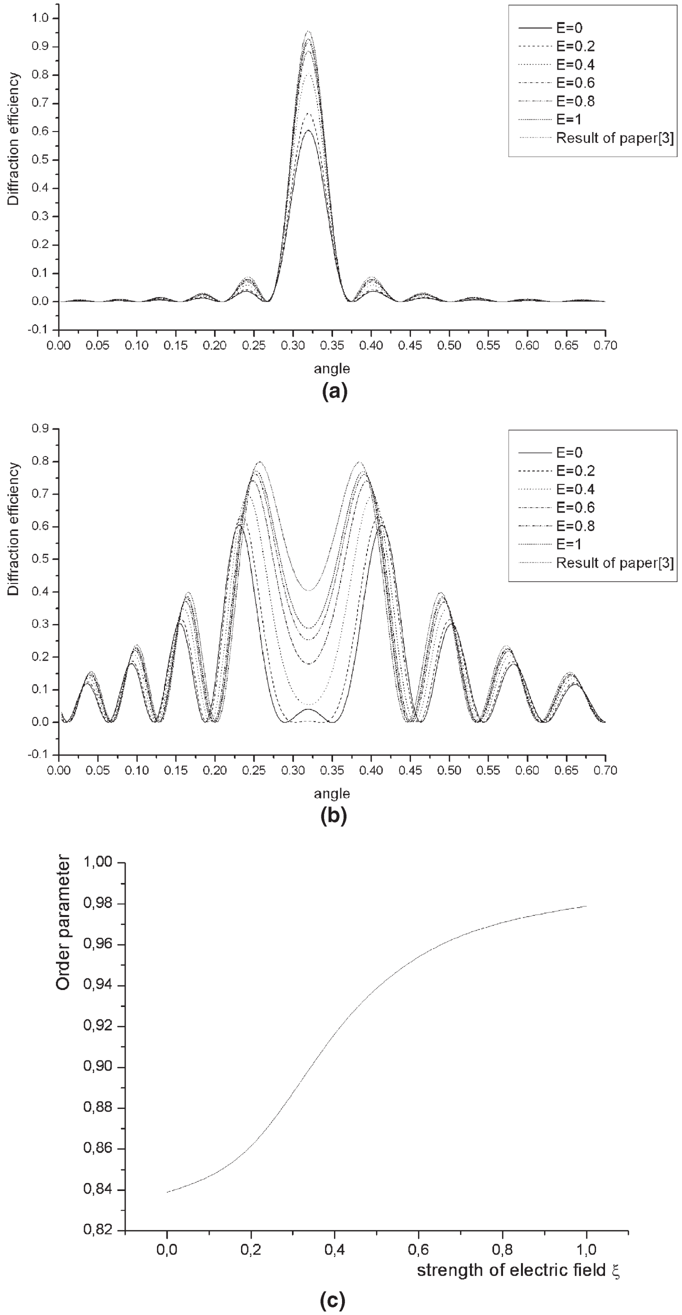

FIGURE 1 Angular selectivity of diffraction efficiency for different electric field strength: a)for *s*-polarized reading beam; b) for *p*-polarized reading beam. Both results are for bipolar droplets. Figure 1c represents the droplet order parameter.

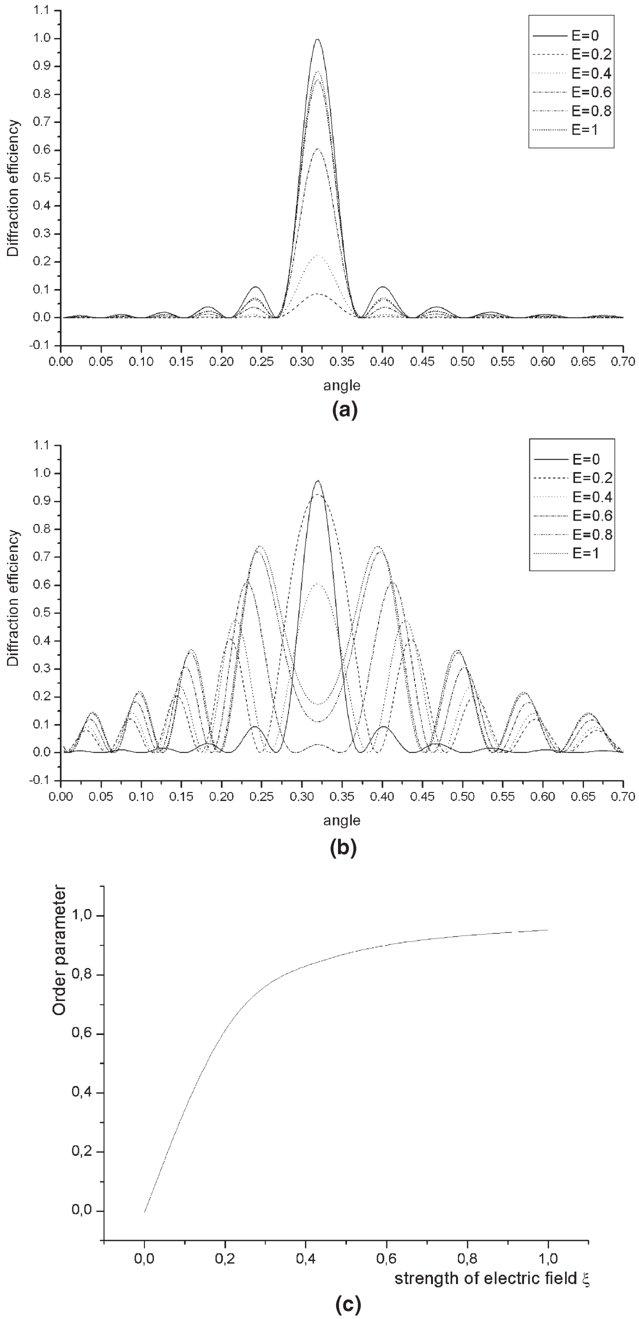

FIGURE 2 The same as Figure 1 for radial droplet.

field influence is more pronounced for radial droplets. This fact agrees with higher change of droplet order parameter for radial droplet upon applying electric field.

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