Electrically Controlled Phase Gratings for Terahertz Radiation Based on Nematic Liquid Crystal

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Abstract. A mathematical model of a new type of liquid crystal (LC) based diffraction grating for the terahertz frequency range is proposed. Numerical time-integration by the finite-difference time-domain (FDTD) method of Maxwell-equation systems, describing the proposed structure, has been performed. The partial differential equation, describing the electro-optical induced orientation of the LC molecule in the external electric field, is calculated by the method of lines (MOL). The dependence of induced birefringence vs. external control voltage is obtained for 6CB nematic liquid crystal (NLC).

1. Introduction
Terahertz (THz) waves attracted a lot of attention due to a number of applications ranging from basic research to industrial quality control and security applications [1], THz spectroscopy and THz imaging systems. A very promising class of THz devices is those which contain LC. Liquid crystal components for terahertz radiation are in high demand due to the recent rapid progress in THz science and technology [2, 3]. The possibility for gratings with liquid-crystal-enabled functionalities was recognized [4]. Various tunable THz devices employing nematic liquid crystals, such as phase shifters, filters, and switches that are controlled either electrically or magnetically were demonstrated [5]. For manipulating THz waves by changing the effective refractive index of the NLC, recently demonstrated a magnetically controlled phase grating [6]. In [7], proposed and demonstrated an electrically controlled phase grating (PG) using NLC for THz waves, which contains alternate sections of two materials with different refractive indices – fused silica and NLC. In this paper we propose the all NLC based electrically controlled phase grating for terahertz radiation. This type of gratings can be used also for study the birefringence of NLC in THz domain.

2. Theoretical and numerical model of phase grating. Simulation results
We propose the electrically controlled phase grating (ECPG) consisting from the structured NLC layers (Figure 1). The device is the cell with thickness d, where the liquid crystal layer is sandwiched between two glass substrates coated by transparent ITO electrodes. One of the substrates is a structured conductive layer of parallel electrodes electrically connected with each others. The distance...
between the parallel electrodes and width of them are \( L \). The second one is continuum ITO film. Applying the voltage between the substrates will result to periodically orientation of NLC molecules.

![Schematic cross-section view of liquid crystal based phase grating](image)

**Figure 1** Schematic cross-section view of liquid crystal based phase grating

Taking into account the viscosity of NLC for the given value of controlled voltage, above the Frederik threshold value, the molecule’s spatial periodic orientation along the substrates can be approximated as a sinusoidal function. By control voltage the spatially periodical modulation of refraction index is generated due to electro-optically induced orientation of liquid crystal molecules. The phase difference between THz waves at wavelength \( \lambda_{THz} \), propagated through the neighbor layers with the difference values of refraction indexes controlled by the control voltage. Such a sinusoidal phase grating can be represented as a layer of nematic liquid crystal with a periodically varying refractive index. As shown in [8], for phase grating with sinusoidal refraction index modulation, at the modulation index value \( \pi d (n_{eff}(V) − n_e) / \lambda_{THz} = 2 \), which corresponds to the root of the Bessel function \( J_0 \), the maximum of the diffraction zero-order disappears. For a fixed value of the induced birefringence and the grating thickness in order to eliminate the zero order the wavelength of the terahertz radiation should be chosen so that the depth of modulation was equal to 2. For obtaining the dependences of induced birefringence vs. the control voltage numerical modelling of the process of electro-optical induced reorientation of NLC molecules was done. The NLC cell with planar orientation along the axis \( y \) and control voltage applied along the axis \( z \) was considered (Figure 2). By the method of lines (MOL) [9] was obtained numerical solution of Erikson-Leslie equation, which described the dynamics of NLC director rotation in the case when the backflow and inertial effects are ignored

\[
\frac{\partial \theta}{\partial t} = \left[ K_{11} \sin^2(\theta) + K_{33} \cos^2(\theta) \right] \frac{\partial^2 \theta}{\partial z^2} + \frac{1}{2} \left( K_{11} - K_{33} \right) \sin(2\theta) \frac{\partial \theta}{\partial z} - \frac{\varepsilon_0}{8\pi} \Delta \varepsilon E_z^2(t) \sin(2\theta) \tag{1}
\]

where \( K_{11}, K_{22}, K_{33} \) are the elastic constants associated with splay, twist and bend deformation respectively, \( \gamma \) - rotational viscosity, \( \varepsilon_0 \Delta \varepsilon E_z^2 \) is the electric energy density, \( \Delta \varepsilon \) is the NLC dielectric anisotropy, and \( \theta(z, t) \) is the tilt angle of the NLC directors. On base of numerical solution was determined the effective refractive index of NLC vs. applied voltage \( V = E_z d \)

\[
n_{eff} = \frac{1}{d} \int_{z=0}^{z}=2 \sqrt{\frac{\varepsilon_0 \varepsilon_z}{\varepsilon_z \cos^2(\theta(z, t \rightarrow \infty)) + \varepsilon_{zz} \sin^2(\theta(z, t \rightarrow \infty))}} \, dz \tag{2}
\]
for NLC layer of thickness $d$ and with $z=0$ at the centre of the layer, $\theta(z, t \to \infty) = \theta_t$ - is the value of the tilt angle in steady-state regime, $\varepsilon_{\perp}, \varepsilon_{\parallel}$ - dielectric permittivity’s for extraordinary and ordinary waves.

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To demonstrate the dependence of electro-optically induced birefringence vs. the control external voltage, we carried out a numerical integration for 6CB NLC with the 200 um thickness, 180 um grating period, 60 um THz radiation wavelength and with the following parameters: $\varepsilon_{\parallel} = 12$, $\varepsilon_{\perp} = 4$, $K_{11} = 8.57 \text{ pN}$, $K_{33} = 3.7 \text{ pN}$, $\gamma = 13.3 \text{ kg/m} \cdot \text{s}$. The dependence of induced birefringence and derivative of induced birefringence for the different sub ranges vs. control voltage are shown on the Figure 3. As seen from figure the Frederiks threshold value is about 11V.

$$\text{Figure 2 Geometry of interaction of NLC director with the controlled external electric field.}$$

$$\text{Figure 3 Electro-optically induced birefringence vs. external control voltage.}$$

In the FDTD numerical model we pass from continuous space to discrete one with spatial discretization step $\lambda_{\text{THz}}/50$ and the inverse dielectric tensor of considered grating was presented as

$$\bar{\varepsilon}^{-1} = \begin{bmatrix} \varepsilon_{\parallel} + (\varepsilon_{\parallel} - \varepsilon_{\perp})\sin^2(\theta_{\parallel}(x)) & \varepsilon_{\perp} \\ \varepsilon_{\parallel} & \varepsilon_{\perp} \end{bmatrix},$$

$$\bar{\varepsilon}^{-1} = \begin{bmatrix} -(\varepsilon_{\parallel} - \varepsilon_{\perp})\cos(\theta_{\parallel}(x))\sin(\theta_{\parallel}(x)) & \varepsilon_{\perp} \\ -\varepsilon_{\parallel} & \varepsilon_{\perp} \end{bmatrix},$$

$$\bar{\varepsilon}^{-1} = \begin{bmatrix} \varepsilon_{\parallel} + (\varepsilon_{\parallel} - \varepsilon_{\perp})\cos^2(\theta_{\parallel}(x)) & \varepsilon_{\perp} \\ \varepsilon_{\parallel} & \varepsilon_{\perp} \end{bmatrix},$$

$$\bar{\varepsilon}^{-1} = \varepsilon_{\perp}^{-1}.$$

In the Figure 4 is shown the two-dimensional spatial distribution of $E_x$ component of the diffracted field, obtained by numerical solution of Maxwell equations systems by FDTD method for the linearly
polarized field \((E_{\omega}, 0, 0)\). The boundaries of grating are shown by white lines. According to the figure, the diffracted field which is formed on the output of grating, start to distribute between ±1 and 0 diffraction orders.

**Figure 4** Two-dimensional spatial distribution of \(E_x\) component of the diffracted field.

For determination the diffracted far field, as the initial value, the field distribution directly at the grating's output was used. Comparison shows that the obtained numerically by FDTD and analytically far field distributions practically are same.

**Conclusion**

In this paper a mathematical model of a new type of phase liquid crystal diffraction grating for the terahertz frequency range is proposed. Since the diffraction efficiency will depend on absorption of NLC at THz, the proposed phase grating can be used for study the dielectric permittivity of NLC in the THz.

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