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Investigating electro-optical properties of a nematic liquid crystal cell with planar anchoring boundary condition for various thicknesses: A Monte Carlo study

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ABSTRACT

Monte Carlo (MC) simulations and the Mueller matrix formalism were applied to investigate electro optical properties of a LC cell with planar boundary conditions for various thicknesses. Field dependent global order parameter and the optical transmissions were analyzed in common. Three characteristic regions of the periodicity of optical transmissions as a function of polarizer angle and the external field were identified.

1. Introduction

Liquid crystals (LCs) are known to be anisotropic fluids, thermodynamically located in between isotropic liquid and crystalline solid [1]. The most extensively studied liquid crystalline phase, both theoretically and experimentally is the nematic (N) phase, which is characterized by long-range orientational order, where the molecules tend to align along a prefered direction so-called director (abbreviated as $\hat{n}$), without any long-range positional order [2]. Such an order imparts anisotropic behavior in the elastic, electric, magnetic and optical properties of a liquid crystalline material. Among these, the optical anisotropy, namely birefringence, plays an important role in applications of liquid crystals, since an optimum birefringence value is required to get a maximum optical contrast in each type of nematic liquid crystal display (LCD). As liquid crystal molecules (LCMs) respond to even weak external fields (electric, magnetic etc.), one can tune the birefringence in LCMs [3,4]. So field dependent characteristics of optical transmission in LCs can be measured.

Due to their anisotropic and self-assembling nature, LCs holds an important place in electro-optical applications of many devices [5–8]. In literature, one can find numerous experimental and computational studies on electro-optical behavior, especially transmittance–voltage characteristics of LCs and LC dispersions, e.g. carbon nanotube or nanoparticle doped LCs [6,7,9–12]. Computer simulation studies on electro-optical properties of LCs also are of great importance to make a comparison with both theoretical models and experimental results.

It is well known that the LC cell thickness is a critical parameter determining the electro-optical response of LC materials. In this work, our aim is to find out electro optical characteristics of nematic LCs with planar boundary conditions via MC Metropolis equilibrium sampling technique. For this purpose, the optical transmission rate and the LC director angle with respect to the polarizer direction have been studied for varying thicknesses.

2. Model and simulation details

We consider a planarly aligned liquid crystal cell such that LCMs are located at nodes of a simple cubic lattice. The lattice is sandwiched between two planar plates. Planar alignment directions of both plates are parallel to Ox-axis. We also placed two crossed linear polarizers both side of the cell parallel to xy-plane and considered that the light, passing through the cell, propagates parallel to Oz-axis. A representation of this configuration is given in Fig. 1.

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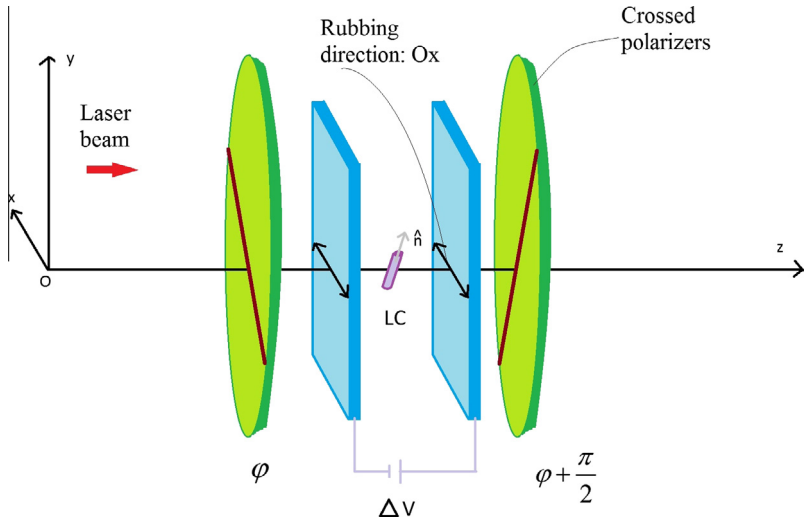

Fig. 1. Schematic representation of the simulated system.

To get the equilibrium configurations of LCs, we used standard MC Metropolis algorithm [13] with the following model Hamiltonian given in [14]:

$$H = -\xi \sum_{<i,\ j>} P_2(\cos\beta_{ij}) - E^2 \sum_{i=1}^{N} P_2(\cos\varphi_i) + \alpha \sum_{k_w} \sin^2(\gamma_{k_w}) \qquad (1)$$

where P_2 is the second order Legendre polynomial. The first term in Eq. (1) is known as the Lebwohl–Lasher potential [15] and it describes the interaction energy between the nearest neighbor LCMs with strength ξ. Each LCM is represented by a simple cylindrical rod. Alignment of the long axis of those rods is considered as a three dimensional headless spins [16]. Here, β_{ij} refers to the angle between long axes of nearest neighbor molecules "***-i***" and "***-j***". The second term is the electric field coupling of the molecule-***i***, where ***E*** is the electric field strength along *Oz*-axis and, φ_i is the angle between electric field vector and the long axis of the molecule-***i***. In the third term of Eq. (1), which is known as the Rapini term [17,18]. α is the anchoring force strength between molecules and the cell walls, k_w identifies the nearest molecules to the cell walls and, γ_{k_w} is the angle between planar alignment direction of the cell walls and the long axis of molecule-k_w. It is worthwhile noting that the model Hamiltonian in Eq. (1) has proven to be able to reveal various characteristics of nematic LCs via MC simulations [14,19,20]. Here all coupling constants, namely ξ, $\boldsymbol{E^2}$, and α, are expressed in units k_BT where k_B and T refer Boltzman constant and absolute temperature respectively.

We applied periodic boundary conditions through the *xy*-plane and, planar boundary conditions by means of anchoring forces through the *Oz*-axis. In this work, we have performed MC simulations under the conditions that the anchoring force is spatially homogenous and the temperature of the nematic LC cell under investigation is in the nematic region [21,22]. We set $\xi = 1.0k_BT$, $\alpha = 11.08k_BT$, and $0 \leqslant E^2 < 3.5^2 k_BT$ for all simulations. It has been considered that there are $N = L_x \times L_y \times L_z = 22 \times 22 \times 6(7,\ldots,18)$ number of molecules in all simulations. Besides, in order to calculate the relevant observables such as order parameters, directors and light transmission rates for the corresponding parameters, we have performed more than 400 MC simulations by varying the cell thicknesses and the applied fields. We arranged the number of Monte Carlo steps (NMCs) as a function of the number of molecules (N) in the corresponding simulation. We set "NMCs = $1100 \times N$" for the equilibration procedure and "NMCs = $484 \times N$" for the sampling procedure. It took approximately "3.2×10^6 < NMCs < 9.6×10^6" and "1.4×10^5 < NMCs < 4.2×10^6" for the equilibration procedure and the sampling procedure respectively, depending on the cell thickness by means of the number of molecules in the simulation.

LCMs are considered as headless spins. They have no heads or tails but they have some spatial alignments. Because of this situation, the order in LCMs represented in a matrix form [23], called order tensor-$Q(C)$, and a measurement of this alignment is called order parameter-S. The director and the orientational order parameter of the orientation of the system over microstates can be calculated with the following matrix diagonalization procedure [23–25] for each simulation. For a given *microstate-C*, the projection matrix over all molecules is given by:

$$A(C) = \frac{1}{N} \sum_{i=1}^{N} |u_i\rangle\langle u_i| \qquad (2)$$

where $N = L_x \times L_y \times L_z$ is the number of molecules, $|u_i\rangle$ is the director of molecule-*i*. Then, a traceless second rank tensor $Q(C)$ can be calculated as:

$$Q(C) = A(C) - \frac{1}{3} trace(A) \times I_3 \qquad (3)$$

where I_3 is the third-order unit matrix. If η is the largest eigenvalue of $Q(C)$, then the order parameter takes the value $S = 3\eta/2$ and the corresponding eigenvector $|n\rangle$ (or represented by $\hat{n}$) is the director of this *microstate-C*.

The homogeneity of a system of LCMs decays with boundary conditions (anchoring effects: planar, twist) and the external fields. Although, global order parameter is typically used for uniaxial homogeneous systems, we prefer to use it rather than local order parameter. By choosing global order parameter, we aim to have some general panorama on a system of LCMs with anisotropic conditions. A nice discussion on the limitation of global order parameter can be found in [26].

We used Mueller formalism to investigate electro-optical properties of optical transmission. It is well known that Mueller formalism can deal with all polarization states including depolarization as well, as opposed to Jones formalism which treats only totally polarized light. In Mueller formalism, LCMs are considered as linear retarders and represented by Mueller matrices M_i through the path of the incoming light. Crossed polarizer and analyzer are also represented by Mueller matrices P_{in} and P_{out} respectively. Then, the outgoing polarized light can be evaluated as a Stokes vector by the following matrix product: