



Influence of surface alignment on the orientation behavior of a liquid crystal cell near nanoscale grooved surfaces

Scientific research paper

Saeedeh Shoarinejad^{1*}, Zahra Keikavousi¹, Mohammad Reza Mozaffari²

¹Department of Theoretical Physics and Nanophysics, Faculty of Physics, Alzahra University, Tehran, Iran,

²Department of Physics, University of Qom, Qom, Iran

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ABSTRACT

In this work, we investigate the anchoring energy of a nematic liquid crystal cell with one patterned and one unpatterned surface. Surface reorientation effects are studied both in the absence of an external electric field and under the action of an external field. We consider the contribution of the saddle-splay surface energy and obtain the anchoring energies of the system. Director profiles are determined and the influence of the geometry, as well as the pitch values of the sinusoidal surface, are discussed. The reorientation of liquid crystal molecules in the vicinity of a nano-size grooved surface and the effect of different surface energy terms on the orientational behavior of a liquid crystal near the surfaces are investigated. Our calculations were performed using the Oseen-Frank theory based on nano-scale groove models. Our results reveal the crucial effects of surface and external fields on nematic reorientational behavior near a patterned surface. Also, our findings highlight the importance of the saddle-splay surface energy when comparing the Fukuda and Berreman models. Besides, it turns out that the presence of an external electric field significantly affects the results reported by these models.

1 Introduction

Surface anchoring in liquid crystals (LCs) has been the subject of intense research due to its fundamental importance and many applications in industry, such as high-tech-liquid crystal display devices and bio-inspired liquid crystal research [1-4]. Indeed, thanks to the fascinating fundamental and technological aspects, an increasing number of publications have been devoted to studying the different anchoring conditions in LCs [1, 2, 5-8]. Some desirable anchoring properties by surfaces tailored with submicron-scale grooves or geometrical patterns have been investigated by many experimental researchers [1, 2, 5, 6, 8-12]. Moreover, many

researchers have theoretically investigated the mechanism of the reorientation process of liquid crystal (LC) molecules on a treated interface [7, 13-16]. The surface anchoring strength is a crucial parameter in determining the orientational behavior of LC molecules [14, 17, 18]. As well known, the elongated molecules tend to align on average in a common direction called director $\mathbf{n}(r)$ in a nematic medium, the simplest LC phase. Actually, in the vicinity of a surface, it costs energy to change the direction of the LC director from its preferred anchoring direction. To describe the anchoring strength of a nematic LC, Rapini and Papoular have introduced a simple expression for the interfacial energy per unit area for a one-dimensional

*Corresponding author.

Email address: sshoari@alzahra.ac.ir

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(1D) deformation [19]: $f_s = (1/2)W \sin^2 \alpha$, in which, W represents the anchoring strength and α is the angle between the director and easy boundary direction on the surface [19-21]. Although this equation provides an excellent approximation for a one-dimensional surface with only one easy axis, it does not apply to a system with an anchoring competition [20]. For instance, large director deviations or arbitrary surface patterns are agents that require a different model to describe the surface anchoring effects. Berreman [22, 23], proposed a model for nematic LC mesogens in contact with a sinusoidal wavy surface. He assumed that the director is always parallel to the surface and calculated the free energy due to the induced distortions by a sinusoidal surface [22]. It is a simple model for geometry-induced surface anchoring that appears in most theoretical studies on the surface anchoring effects. Based on Berreman's model, the anchoring energy per unit area is given by $(1/4)K A^2 q^3 \sin^2 \phi$, in which K , A , and $q = 2\pi/\lambda$, are the elastic constant in one-constant approximation, the amplitude and the wavenumber of the sinusoidal surface, respectively [21, 24]. Also, ϕ is the angle between the director and the groove direction [22, 24]. Afterward, J. I. Fukuda et al. [24, 25], reexamined the theoretical treatment of Berreman for the surface anchoring induced by grooves. They found that the anchoring energy behaves as $\sin^4 \phi$, as a function of the angle between the groove direction and the director at infinity [24]. They argued that the small negligible assumption of azimuthal distortions in the theory of Berreman is not valid for general ϕ . The tilt distortions are comparable in magnitude to the azimuthal distortions. The obtained anchoring energies as a function of ϕ show a significant difference compared to Berreman's energy for $K_1 = K_3$, which is a dominant contribution in splay and twist modes near the easy axis [24]. They have the same values only at $\phi = 0, \pm(\pi/2)$, while the energy is always smaller than Berreman's energy [24]. Moreover, J. I. Fukuda et al. [6, 24, 25], have investigated the influence of surface-like elasticity, which has an essential role in the surface-groove-induced anchoring energy of a nematic LC.

In this work, we have studied the anchoring energy effects of a nematic LC sandwiched between two surfaces with a patterned and an unpatterned surface. Our study is based on the Oseen-Frank theory. We have considered the contribution of the surface-like elastic energy in the vicinity of the surfaces and investigated

the influence of the cell geometry. The effect of the groove pitch on the surface anchoring strength has attracted the attention of theoretical and experimental researchers [1, 6]. Therefore, it prompted us to examine the reorientation of LC molecules near the nano-size grooved surfaces with different pitches more closely.

The article is organized as follows. In Section 2, we have presented the basic equations based on the Oseen-Frank theory in three subsections. The formulation of the problem using the Oseen-Frank theory in the absence and presence of an external electric field is given in the first two subsections respectively, and the effects of field and surface-like elastic energy are discussed in the third subsection. In Section 3, we have studied the influence of the groove pitches on the reorientation of the director and surface energy. Finally, our conclusions are presented in section 4.

2 LC molecular reorientation near the grooved surface

2.1 Effects of surface-like energy in the director field and anchoring energy in the absence of an electric field

We consider a confined nematic cell with one patterned and one flat surface, which have different anchoring conditions. As shown in Fig. 1, one of the surfaces has a sinusoidal pattern with one-dimensional parallel grooves along the x-direction, and the other is a flat plane ($z = L_z$). The sinusoidal-shaped surface is described by $z = A \sin [q(x \sin \phi + y \cos \phi)]$, where ϕ is the angle between director \mathbf{n} and x-axis, A and q show the amplitude and the wavenumber of the sinusoidal surface, respectively [21].

According to the continuum elastic theory, the Oseen-Frank elastic free energy, in the presence of the saddle-splay energy, is given by the following expression [7, 25, 26]:

$$F_{el} = \frac{1}{2} \int dr [K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 - K_s \nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n})], \quad (1)$$

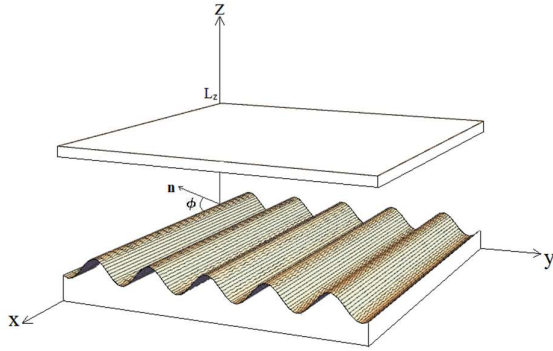


Figure 1. The geometry of a confined nematic LC between two surfaces, ϕ is the angle between director \mathbf{n} and x -axis

where, K_1 , K_2 , and K_3 are respectively the splay, twist, and bend elastic constants. The fourth term is known as saddle-splay energy. It describes the contribution of the surface interaction, in which $K_s \equiv 4K_1K_2/(K_1 + K_2)$ shows the surface-like elastic constant [1, 7, 27-29]. On the basis of the Fukuda model, the director is approximately written down as $\mathbf{n} = (\sqrt{1 - n_y^2 - n_z^2}, n_y, n_z) \approx (1, n_y, n_z)$. The Frank elastic energy can be expressed in terms of spatial derivatives of n_y and n_z , as follows [22, 26]:

$$F_{el} = \frac{1}{2} \int dr \left[K_1(\partial_y n_y + \partial_z n_z)^2 + K_2(\partial_y n_z - \partial_z n_y)^2 + K_3[(\partial_x n_y)^2 + (\partial_x n_z)^2] - 2K_s(\partial_y n_y \partial_z n_z - \partial_y n_z \partial_z n_y) \right]. \tag{2}$$

Here, we have used the full variational principle ($\delta F = 0$), and the Euler-Lagrange equations are achieved. To determine the director field components near the sinusoidal grooved surface, we can use the Euler-Lagrange equations and apply boundary conditions ($n_x = Aq \sin \phi \cos[q(x \sin \phi + y \cos \phi)]$ and $\partial_y n_z - \partial_z n_y = 0$). The resulting expressions for the director field components are as follows [25, 30]:

$$n_x = 1, \tag{3}$$

$$n_y = Aq \sin \phi \sin[q(x \sin \phi + y \cos \phi)] \left(\frac{\cos \phi}{g_1} e^{-qz g_1} + \frac{K_s}{K_3} \cot^2 \phi \left(\frac{\cos \phi}{g_1} e^{-qz g_1} - \frac{\cos \phi}{g_2} e^{-qz g_2} \right) \right), \tag{4}$$

$$n_z = Aq \sin \phi \cos[q(x \sin \phi + y \cos \phi)] \left(e^{-qz g_1} + \frac{K_s}{K_3} \cot^2 \phi (e^{-qz g_1} - e^{-qz g_2}) \right). \tag{5}$$

In these equations, g_i is defined as $g_i = \sqrt{\cos^2 \phi + (K_3/K_i) \sin^2 \phi}$; ($i = 1, 2$). Nevertheless, the director has a specific orientation on the flat surface as $(1, 0, 0)$, which is parallel to the direction of the grooves. We calculate the anchoring energy in this situation. We first obtain the anchoring energy per unit area without the effect of the surface-like elastic term (K_s). Using Fukuda's equations and supposing the groove's direction in the x -axis, as considered by Fukuda et al. [24], the surface anchoring energy per unit area leads to

$$F_s = -\frac{1}{4} A^2 (-1 + e^{-2L_z q}) K_3 q^3 \sin^4 \phi, \tag{6}$$

where the effect of finite thickness in the z -direction clearly is presented. Next, we consider the effect of the surface-like elastic term (K_s). For this end, we similarly substitute Eqs. (4) and (5) in Eq. (2), and calculate $\int_{x=0}^1 \int_{y=0}^1 \int_{z=0}^{L_z} f \, dx \, dy \, dz$. The anchoring energy per unit area is given by

$$F_{K_s} = \frac{1}{8} A^2 q^3 K_3 \sin^2 \phi \left(-1 + e^{-2L_z q} \right) \left((\cos 2\phi - 1) - \frac{2K_s}{K_3} (\cos 2\phi + 1) \right). \tag{7}$$

2-2. Effects of surface-like energy and anchoring energy under an applied electric field

In this subsection, we investigate the molecular reorientation of the LC system under the action of an external electric field. As considered in the previous section, we rewrite the total free energy density in the presence of surface-like elastic energy as well as the contribution of interaction between the electric field and the director field. Then, the total density of free energy is written as follows [31]:

$$\begin{aligned}
 f_{tot} &= \frac{1}{2} [K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 \\
 &+ K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 - K_s \nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n})] \\
 &- \frac{1}{2} \frac{\epsilon_a}{4\pi} (\mathbf{n} \cdot \mathbf{E})^2, \tag{8}
 \end{aligned}$$

where ϵ_a indicates the dielectric anisotropy of the system. We assume that the external electric field is applied along the z-axis, that is perpendicular to the direction of grooves, i.e., perpendicular to the x-direction [32]. Therefore, $\mathbf{E} = (0, 0, E) = E\hat{z}$, and so the total free energy of the system takes the form

$$\begin{aligned}
 F_{tot} = \int dr & \left(\frac{1}{2} (K_1(\partial_y n_y + \partial_z n_z)^2 \right. \\
 &+ K_2(\partial_y n_z - \partial_z n_y)^2 \\
 &+ K_3 [(\partial_x n_y)^2 + (\partial_x n_z)^2] \\
 &- 2K_s(\partial_y n_y \partial_z n_z - \partial_y n_z \partial_z n_y) \\
 &\left. - \frac{1}{2} \frac{\epsilon_a}{4\pi} (n_z E)^2 \right). \tag{9}
 \end{aligned}$$

The boundary conditions at the surface are the same as in the previous section. Then using the Euler-Lagrange equation yields:

$$\begin{aligned}
 K_1 \partial_z (\partial_y n_y + \partial_z n_z) + K_2 \partial_y (\partial_y n_z - \partial_z n_y) \\
 + K_3 \partial_x^2 n_z + \frac{\epsilon_a}{4\pi} n_z E^2 = 0, \tag{10}
 \end{aligned}$$

$$\begin{aligned}
 K_1 \partial_y (\partial_y n_y + \partial_z n_z) - K_2 \partial_z (\partial_y n_z - \partial_z n_y) \\
 + K_3 \partial_x^2 n_y = 0. \tag{11}
 \end{aligned}$$

Applying the boundary condition to Eqs. (10) and (11), one can obtain the components of the director field in the presence of an external electric field as [33]:

$$\begin{aligned}
 n_y &= Aq \sin\phi \sin[q(x \sin\phi \\
 &+ y \cos\phi)] \left[\left(\frac{\cos\phi}{g_1} e^{-qz g_1} \right. \right. \\
 &+ \left. \left. \frac{K_s}{K_3} \cot^2\phi \left(\frac{\cos\phi}{g_1} e^{-qz g_1} - \frac{\cos\phi}{g_2} e^{-qz g_2} \right) \right) \right. \\
 &\left. - \frac{\epsilon_a z}{K_1 4\pi} E^2 \frac{1}{q \cos\phi} \right], \tag{12}
 \end{aligned}$$

and

$$\begin{aligned}
 n_z &= Aq \sin\phi \cos(q(x \sin\phi + y \cos\phi)) \left[\left(e^{-qz g_1} \right. \right. \\
 &+ \left. \left. \frac{K_s}{K_3} \cot^2\phi (e^{-qz g_1} - e^{-qz g_2}) \right) \right. \\
 &\left. + \frac{\epsilon_a}{K_1 4\pi} E^2 \frac{1}{q^2 \cos^2\phi} \right]. \tag{13}
 \end{aligned}$$

In the presence of an external electric field, a distortion occurs due to a competition between restoring elastic forces induced by the alignment at the surfaces and the destabilizing torques produced by the applied field [34]. In fact, the applied electric field causes the reorientation of the director, so that the director tends to reorient along the external field direction because of the positive dielectric anisotropy ($\epsilon_a > 0$) [35]. The parameter η is the angle between the electric field and the director, which is a function of z , $\eta = \eta(z)$ and $n_E = \mathbf{n} \cdot \mathbf{E} = nE \cos\eta(z)$ [36]. As the distance from the sinusoidal surfaces increases, the angle η changes, so that the η is 90° at the upper surface, i.e., the director has tangential anchoring.

Now, to calculate the anchoring energy of the system under an applied electric field, we use the Frank model with one constant approximation ($K_1 = K_2 = K_3$). Substituting Eqs. (12) and (13) in Eq. (9), and integrating the free energy density

$\int_{x=0}^1 \int_{y=0}^1 \int_{z=0}^{L_z} f \, dx \, dy \, dz$, then the following expression is obtained:

$$\begin{aligned}
 F_{tot} &= -\frac{1}{64\pi q} A^2 e^{-2L_z q} (-1 + e^{2L_z q}) \sin \phi [2q^2 (\varepsilon_a E^2 - 4\pi q^2 ((K_3 + 2K_s) + (K_3 - 2K_s) \cos(2\phi))) \sin \phi + \varepsilon_a E^2 \sec \phi \sin(q \cos \phi) (-\sin(q \cos \phi) + \sin(q(\cos \phi + 2\sin \phi)))] \quad (14)
 \end{aligned}$$

2.3 Director profiles and anchoring energy

Now, we have found the two-dimensional (2D) and three-dimensional (3D) director profiles in the presence of surface-like elastic energy. Near the sinusoidal surface, the director profile appears in Figs. 2 and 3, for $\phi = 45^\circ$ and $\phi = 90^\circ$ by using Eqs. (3), (4), and (5). The results were achieved through the numerical method, utilizing parameter values that are typical and match the parameters of 5CB liquid crystal. Moreover, we have also used the typical values for A and q , which represent the amplitude and the wavenumber of the sinusoidal surface respectively. Specifically, we set A to 0.5 nm and q to $\frac{3\pi}{8} \text{ (nm)}^{-1}$ for the sinusoidal surface [7]. As illustrated by Figs. 2 and 3, in the vicinity of the sinusoidal wavy surface, the results are indeed consistent with those reported by Fukuda et al. [24].

As can be seen from Figs. 2a and 2b, the director field follows the pattern of the sinusoidal-shaped surface and tends to be perpendicular to the direction of the grooves near the lower surface ($z = 0$). It makes the angle ϕ with the surface grooves. This angle approaches zero as moving away from the surface. Therefore, the director field completely follows the easy axis of the surface adjacent to the upper surface. Obviously, this is due to the surface torques exerted on the LC molecules due to the presence of confining surfaces of the cell [27, 34].

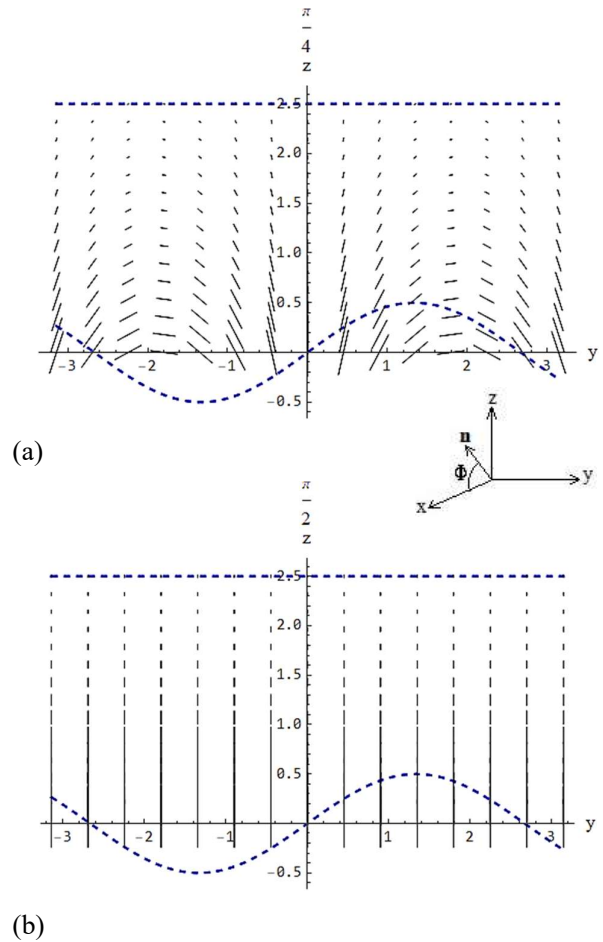


Figure 2. 2D model of director profile (n_y, n_z) at $x=0$, in the presence of surface-like elastic energy for (a) $\phi = 45^\circ$ and (b) $\phi = 90^\circ$.

Then, to investigate the influence of the surface-like elastic term in the director field deformation, we plotted the anchoring energy of the grooved surface as a function of the deviation angle ϕ , for both cases with and without K_s term. The results are presented in Fig. 4. These results clearly indicate the significant role of the K_s term in the director field reorientation. The difference demonstrates the anchoring energies in the Fukuda model.

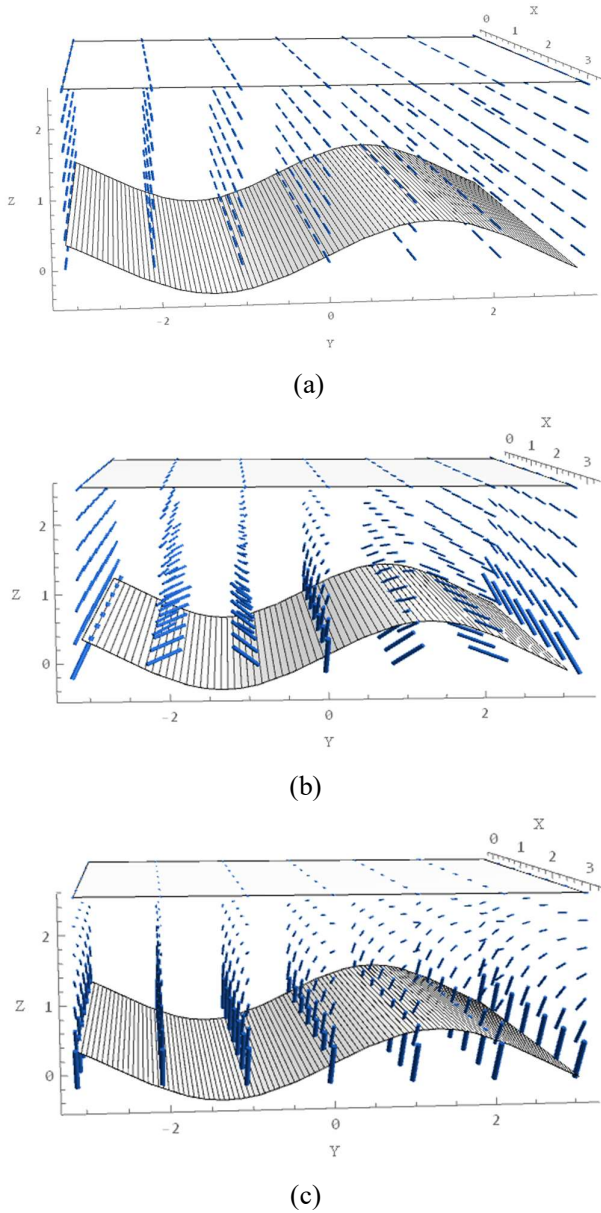


Figure 3. 3D director profile (n_x, n_y, n_z) , in the presence of surface-like elastic energy for (a) $\phi = 0^\circ$, (b) $\phi = 45^\circ$ and (c) $\phi = 90^\circ$.

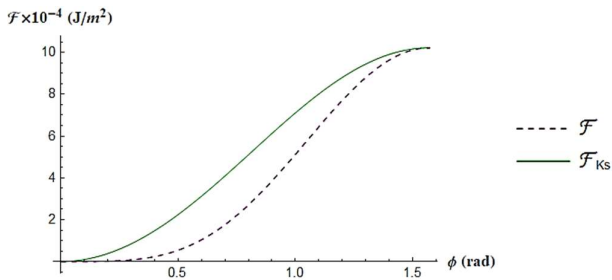


Figure 4. The anchoring energies, with K_s term (thick curve), and without K_s term (dashed curve).

As shown in Fig. 4, both curves have the lowest energy with different slopes at $\phi = 0^\circ$ and the same behavior at $\phi = 90^\circ$. When the anchoring energy is minimum, the LC director would be along the easy axis, so at $\phi = 0^\circ$, the energy per unit area would be minimum, and the easy axis coincides with the surface groove direction. While, with the deviation of the director axis relative to the easy axis the angle between \mathbf{n} and \mathbf{e} changes, and the anchoring energy increases, depending on the anchoring strength of the nematic LC ($f_s = \frac{1}{2} W \sin^2 \alpha$). Therefore, when the angle is 90° , $\sin \alpha = 1$ and the surface energy will have the maximum value. However, in the presence of the surface-like term, the increase occurs with a higher slope. In fact, these results confirm that the effect of surface-like elastic term on texture deformation is not really negligible. As well as the model of Fukuda, we have plotted the anchoring energy based on the model of Berreman. Figure 5 shows the results of both models. In the presence of the surface-like term, the result is consistent with the results of Berreman [22]. It has a slight change that occurs at angles close to zero.

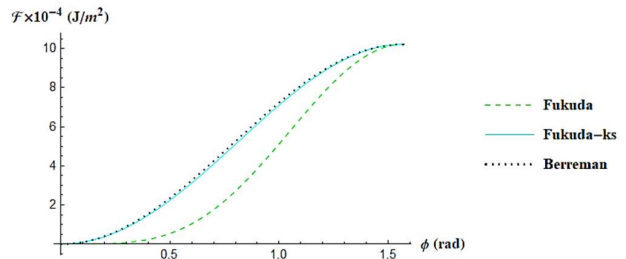


Figure 5. The difference between anchoring energies in Berreman's model (dotted curve), Fukuda's model without K_s term (dashed curve), and Fukuda's model with K_s term (thick curve).

Also, the director profiles of the system under an external electric field ($\mathbf{E} = (0,0,E) = E\hat{z}$) can be obtained using Eqs. (12) and (13) at $\phi = 45^\circ$. The results of two- and three- dimensional models are shown in Figs. 6 and 7, respectively. We have used the typical values of $\epsilon_a = 11$ and $E = 4 \times 10^{-2} \text{ V/nm}$ [37-39]. In these cases, the torque caused by the external electric field also has an impact in addition to the surface torques mentioned earlier. In fact, the competition between the director field, applied electric field, and surface fields, affects the profile of the director. This competition plays a crucial role in the system's orientation behavior and ultimately changes the director profiles. This is evidenced by comparing the

results presented in Figs. 6 and 7 with previous findings (Figs. 2 and 3).

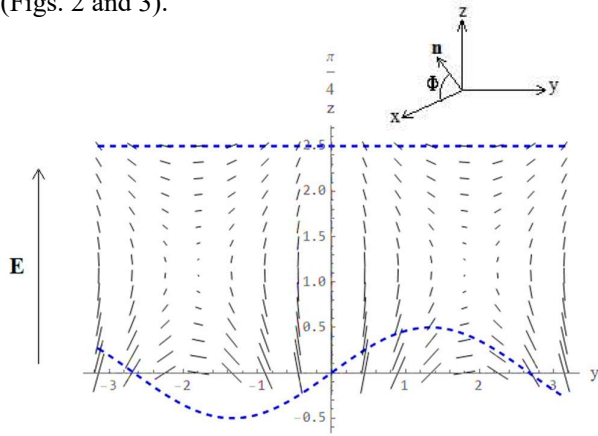


Figure 6. 2D director profile (n_y, n_z) at $x=0$, in the presence of an external electric field ($E = 4 \times 10^{-2}$ V/nm) for $\phi = 45^\circ$.

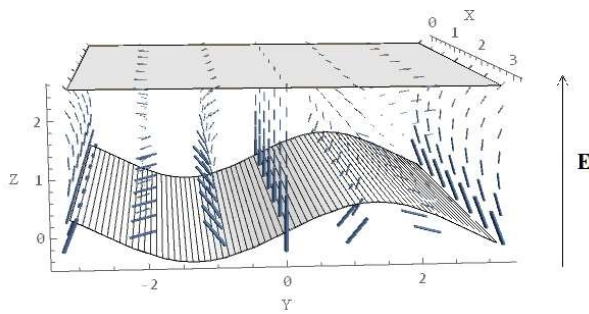


Figure 7. 3D director profile near the grooved surface at $\phi = 45^\circ$, in the presence of an external electric field ($E = 4 \times 10^{-2}$ V/nm).

To better insight, we compare the anchoring energy after and before applying the electric field. We have plotted the energy diagrams using Eqs. (7) and (14) for both systems in Fig. 8. This figure actually illustrates the difference in the anchoring energy of the system under the action of an electric field compared to its energy without exposure.

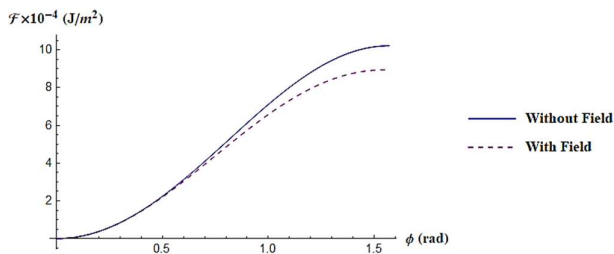


Figure 8. The energy diagrams of nematic LC under an external electric field (dashed curve, $E = 4 \times 10^{-2}$ V/nm) and in the absence of external electric field (thick curve), in the framework of Fukuda's model.

As shown in Fig. 8, applying an external electric field leads to a reduction in the surface energy of the system. We have assumed a positive dielectric anisotropy ($\epsilon_a > 0$), which means that the nematic orientation tends to align with the electric field direction [40], resulting in a zero angle between them ($\mathbf{n} \parallel \mathbf{E}$). Then, it is expected that the anchoring energy will reach its maximum value at this particular angle [37]. Since the electric field is in the z-axis direction, the director should also align in this direction for \mathbf{n} and \mathbf{E} to be aligned. This occurs only when the angle between the director and the surface groove, ϕ , is equal to 90° . Therefore, we expect maximum energy for this angle. Clearly, as the electric field strength increases the energy reduction would be more significant [33].

3 LC molecular reorientation near the grooved surface with different pitches

In this section, we consider a cell with a sinusoidal surface with different pitches. The geometry of the cell is shown in Fig. 9. In this geometry, we assume that the grooves are along the x-direction (Fig. 9).

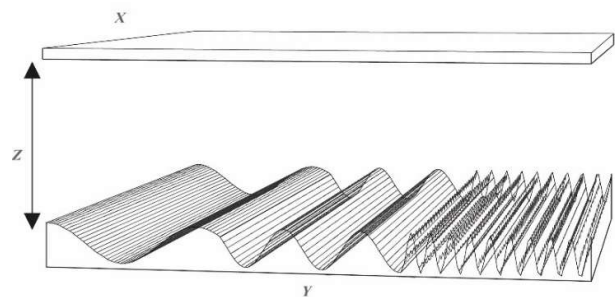


Figure 9. The sinusoidal surface with different pitches. x-axis is the direction of the grooves.

Then, the components of the director field of the nematic LC cell near the grooved surface are given by:

$$n_x = 1, \tag{15}$$

$$n_y = A q_i \sin\phi \sin [q_i(x \sin\phi + y \cos\phi)] \left(\frac{\cos\phi}{g_1} e^{-q_i z g_1} + \frac{K_s}{K_3} \cot^2\phi \left(\frac{\cos\phi}{g_1} e^{-q_2 z g_1} - \frac{\cos\phi}{g_2} e^{-q_2 z g_2} \right) \right), \quad (16)$$

and

$$n_z = A q_i \sin\phi \cos [q_i(x \sin\phi + y \cos\phi)] \left(e^{-q_i z g_1} + \frac{K_s}{K_3} \cot^2\phi \left(e^{-q_i z g_1} - e^{-q_i z g_2} \right) \right), \quad (17)$$

where q_i is the wavenumber for different pitches. In fact, in the vicinity of the grooved surface, the LC molecules are affected by various reorientation effects due to the influence of the different pitches of the grooves. To realize the influence of different pitches of the grooves, we have drawn the 2D and 3D profiles of the director field near the grooved surface for two ϕ angles (Figs. 10 and 11).

Figures 10 and 11 clearly show the strong influence of groove pitches on the orientation of the director field. Actually, the LC molecules tend to be aligned with the direction of the grooves in the smooth regions. While, with the increasing roughness of the pitch, the aligning effect of adjacent molecules would be more dominant than the surface field of the grooves. Indeed, there is competition between these effects in the alignment of the director field. Thus, the resultant orientation of the director field would strongly depend on both aligning efficacies [41]. Therefore, the geometry of the surface plays a key role in determining

the free energy of the system and significantly changes the surface energy.

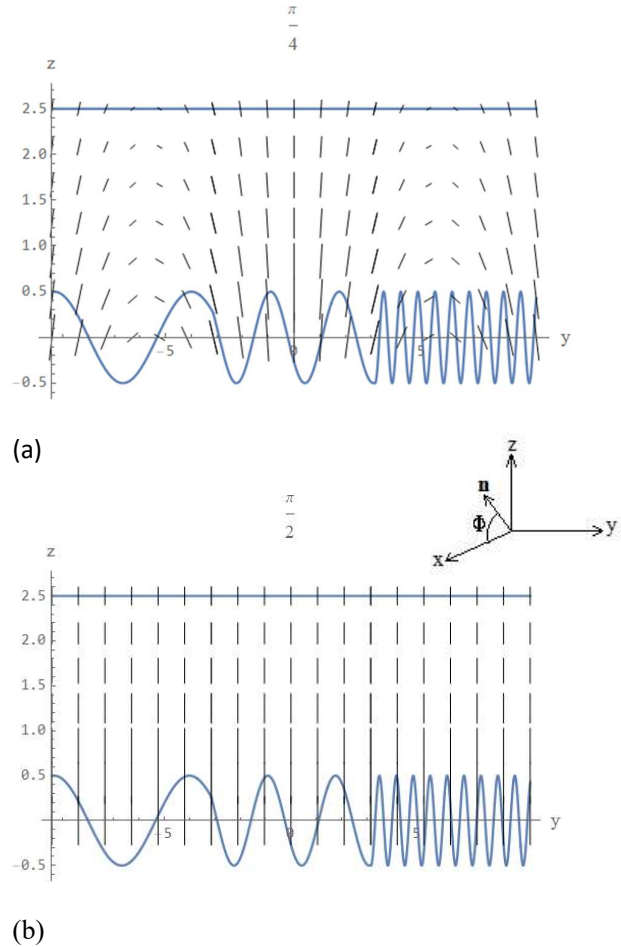


Figure 10. The 2D director profiles (n_y, n_z) near the grooved surfaces ($x=0$), with different groove pitches, (a) $\phi = 45^\circ$ and (b) $\phi = 90^\circ$.

In fact, the shape of the cell walls greatly influences the equilibrium configurations of nematics. For instance, sinusoidal surfaces have a continuous curvature compared to triangular surfaces, and therefore have a smoother surface. It enables a better alignment of liquid crystal molecules and thus improves its properties.

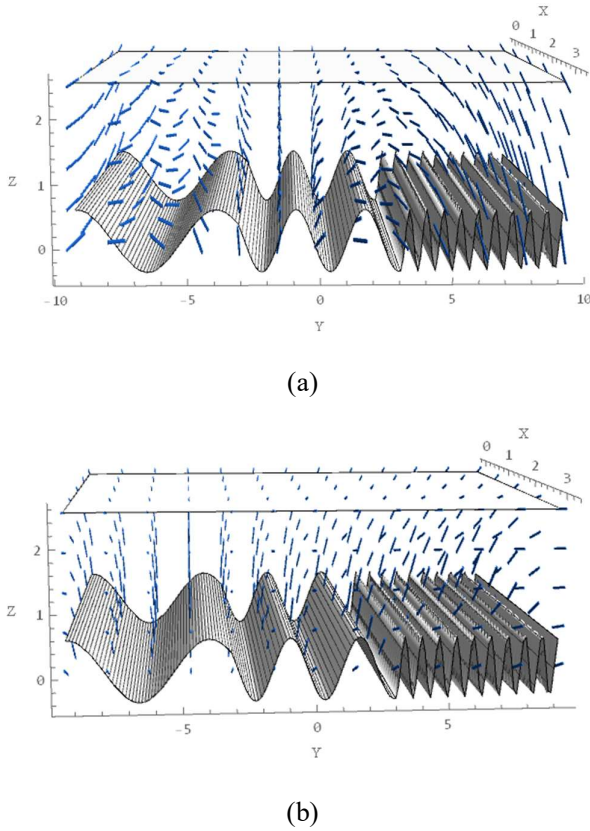


Figure 11. The 3D of the director profile near the grooved surface with different groove pitches, (a) $\phi = 45^\circ$ and (b) $\phi = 90^\circ$.

Now, we obtain the anchoring energy of the nematic LC cell with a grooved surface. For this purpose, we have used Eqs. (2), (16) and (17), and three-dimensional integration of $\int_{x=0}^1 \int_{y=0}^1 \int_{z=0}^{L_z} dx dy dz$. Then, taking into account the influence of the saddle-splay energy, we found the following expression:

$$F_{K_s} = \frac{1}{8} A^2 q_i^3 K_3 \sin^2 \phi \left(-1 + e^{-2L_z q_i} \left((\cos 2\phi - 1) - \frac{2K_s}{K_3} (\cos 2\phi + 1) \right) \right). \quad (18)$$

The obtained surface energy reflects the relationship between the shell extrinsic curvature and nematic order parameters, which are not typically explored in LC investigations with such a defined geometry.

In the next stage, to study the effect of the pitch of the grooves, we plotted the variation of the anchoring energy as a function of the angle ϕ at different pitch values. The results are shown in Fig. 12. This figure

demonstrates how the order of pitch length affects the anchoring energy of the system. By referring to Fig. 12, it is evident that decreasing the pitch of the grooves results in higher costs for anchoring energy. Hence, as mentioned above, the pitch value of the grooved surface and the geometry of the patterned surface of the LC cell significantly may change the reorientational behavior of the system.

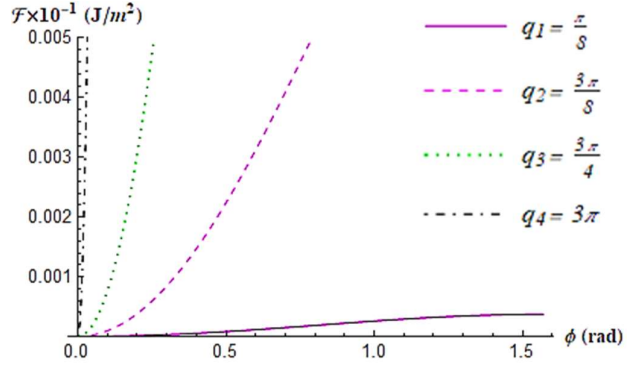


Figure 12. The anchoring energy at different pitch values, $q_1 = (\pi/8) \text{ (nm)}^{-1}$, $q_2 = (3\pi/8) \text{ (nm)}^{-1}$, $q_3 = (3\pi/4) \text{ (nm)}^{-1}$, $q_4 = 3\pi \text{ (nm)}^{-1}$.

4 Conclusions

The elastic surface-like elastic term has a fundamental role in the anchoring energy near the sinusoidal grooved surfaces. Considering the influence of this energy, we found that the model proposed by Fukuda leads to the same results as the Berreman model. However, it does not significantly affect the director profile, although the system undergoes changes in molecular reorientation under an external electric field. Since the pitch of the grooves on the patterned surfaces has a key role in the anchoring energy, we determined the 2D and 3D director profiles by considering the grooved surface with different pitches. We concluded that decreasing the pitch of the grooves leads to increased anchoring energy. The geometry and pitch values of the grooves on the surface were investigated as the significant property of nematic cells. It turned out that, as expected, choosing the appropriate pitches of the layers crucially affects the LC molecular reorientation. Definitely, these parameters are among the effective and determining parameters in the fabrication of nematic LC based-devices and experimental studies.

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Declarations

Competing interests: the authors declare no competing interest.

References

- [1] Y. Choi, H. Yokoyama, J. Seog Gwag, "Determination of surface nematic liquid crystal anchoring strength using nano-scale surface grooves." *Optics Express*, **21** (2013) 12135.
- [2] K. Haruna, H. Okada, "Alignment of liquid crystals with 200 nm-sized V-shaped groove structure fabricated by nano-imprint lithography." *Journal of Molecular Liquids*, **286** (2019) 110830.
- [3] P. J. Collings, J. S. Patel, *Handbook of Liquid Crystal Research*, Oxford University Press, Oxford, 1997, Chap. 6.
- [4] Y. Shang, J. Wang, T. Ikeda, L. Jiang, "Bio-inspired Liquid crystal Actuator materials." *Journal of Materials chemistry C*, **7** (2019) 3413.
- [5] C. Gear, K. Diest, V. Liberman, M. Rothschild, "Engineered liquid crystal anchoring energies with nanopatterned surfaces." *Optics Express*, **23** (2015) 807.
- [6] J. S. Gwag, J. Hyuk Kwon, M. Oh-e, J.-i. Niitsuma, M. Yoneya, H. Yokoyama, "Higher-order surface free energy in azimuthal nematic anchoring on nanopatterned grooves." *Applied Physics Letters*, **95** (2009) 103101.
- [7] J. i. Fukuda, Yoneya Makoto, H. Yokoyama, "Anchoring of a nematic liquid crystal induced by surface grooves: A numerical study." *Physical Review E*, **77** (2008) 030701.
- [8] Y. T. Kim, S. Hwang, J. H. Hong, S. D. Lee, "Alignment layerless flexible liquid crystal display fabricated by an imprinting technique at ambient temperature." *Applied Physics Letters*, **89** (2006) 173506.
- [9] D. C. Flanders, D. C. Shaver, H. I. Smith, "Alignment of liquid crystals using submicrometer periodicity gratings." *Applied Physics Letters*, **32** (1978) 597.
- [10] D. H. Kim, D. Wook Lee, J. Young Oh, J. Won, D.-S. Seo, "Nanopatterning of polymer/Gallium Oxide thin films by UV-Curing Nanoimprint Lithography for Liquid Crystal Alignment." *ACS Applied Nano Materials*, **5** (2022) 1435.
- [11] P. Kumar, C. Jaggi, V. Sharma, K. Kumar Raina, "Advancements of vertically aligned liquid crystal displays." *Micron*, **81** (2016) 34.
- [12] D. H. Kim, J. Hwan Lee, D. Wook Lee, J. Young Oh, J. Won, Y. Liu, D.-S. Seo, "Controlled nano structures on solution-processed inorganic/organic film for liquid crystal application." *Journal of Sol-Gel Science and Technology*, **104** (2022) 412.
- [13] B. Zhang, F. K. Lee, O. K. C. Tsui, P. Sheng, "Liquid Crystal orientation transition on microtextured substrates." *Physical Review Letters*, **91** (2003) 215501.
- [14] H. Chen, C. Xu, G. Xiao, Z. Chen, M. Yi, J. Zhang, "Surface anchoring behavior of 5CB liquid crystal confined between iron surfaces: A molecular dynamic study." *Applied Surface Science*, **508** (2020) 145284.
- [15] H. Chen, Q. sun, G. Xiao, Z. Chen, M. Yi, J. Zhang, C. Xu, "Molecular Dynamic simulations on the flow behavior of 5CB liquid crystal sandwiched between iron walls." *Advanced Theory and Simulation*, **5** (2022) 2200346.
- [16] J. Yang, Y. Yuan, K. Li, T. Amann, C. Wang, C. Yuan, A. Neville, "Ultralow friction of 5CB liquid crystal on steel surfaces using a 1,3-diketone additive", *Wear*, **480-481** (2021) 203934.
- [17] J. Prakash, A. Kumar, S. Chauhan, "Aligning Liquid Crystal Materials through Nanoparticles: A review of recent progress." *Liquids*, **2** (2022) 50.

- [18] B. Jerome, "Surface effects and anchoring in liquid crystals." Reports on progress in physics, **54**, (1991) 391.
- [19] A. Rapini, M. Papoular, "Distorsion d'une lamelle ne'matique sous champ magne'tique conditions d'ancrage aux parois." Le Journal de Physique Colloques, **30** (1969) C4-54.
- [20] Y. Guo-chen, Z. Shu-jing, h. Li-jun, G. Rong-Hua, "the formula of anchoring energy for a nematic liquid crystal." Liq. Cryst., **31** (2004) 1093.
- [21] G. Babakhanova, O. D.Laverntovich, "The Techniques of Surface Alignment of Liquid Crystals." Modern Problems of the Physics of Liquid Systems, Selected Reviews from the 8th International Conference "Physics of Liquid Matter: Modern Problems." Kyiv, Ukraine, May 18-22, 2018, Springer International Publishing, 2019.
- [22] D. W. Berreman, "Alignment of liquid crystals by grooved surfaces." Molecular Crystals and Liquid Crystals, **23** (1973) 215.
- [23] D. W. Berreman, "Solid surface shape and the alignment of an adjacent nematic liquid crystal." Physical Review Letters, **28** (1972) 1683.
- [24] J. i. Fukuda, M. Yoneya, H. Yokoyama, "Surface-groove induced azimuthal anchoring of a nematic liquid crystal: Berreman's model reexamined." Physical Review Letters, **98** (2007) 187803.
- [25] J. I. Fukuda, M. Yoneya, H. Yokoyama, "Erratum: Surface-groove-induced azimuthal anchoring of a nematic liquid crystal: Berreman's Model Reexamined [Phys.Rev.Lett.98,187803 (2007)]." Physical Review Letters, **99** (2007) 139902.
- [26] O. A. Rojas-Gomez, M. M. Telo da Gama, J. M. Romero-Enrique, "Wetting of Nematic Liquid crystals on crenellated substrates: A Frank-Oseen Approach." Crytals, **9** (2019) 430.
- [27] D.Demus, J. Goodby, G. Gray, H. Spiess, V. Vill, Handbook of liquid crystals, vol. 2 A: Low molecular weight liquid crystals I, Wiley-VCH, 1998.
- [28] S. Kralj, S. Zumer, D. Allender, "Nematic-isotropic phase transition in a liquid-crystal droplet." Physical Review A, **43** (1991) 2943.
- [29] J. Nehring, A. Saupe, "On the elastic theory of uniaxial liquid crystals." Journal of Chemical Physics, **54** (1971) 337.
- [30] J. i. Fukuda, M. Yoneya and H. Yokoyama, "Consistent numerical evaluation of the anchoring energy of a grooved surface." Physical Review E, **79** (2009) 011705.
- [31] D. G. Ryu, G. J. Choi, R. Kumar Mishra, J. Seog Gwag, "Anchoring energy of nematic liquid crystals on zinc oxide film." Journal of the Korean Physival Society, **78** (2021) 307.
- [32] M.Emdadi, J. Poursamad, M. Sahrai, F. Moghaddas, "Behaviour of nematic liquid crystals doped with ferroelectric nanoparticles in the presence of an electric field." Molecular Physics, **116**, (2018) 1650.
- [33] Z. Keikavousi, S. Shoarinejad, M. R. Mozaffari, "Adjusted Structures in Nematic Liquid Crystals." Iranian Journal of Applied Physics, **10** (2020) 29.
- [34] S. Shoarinejad and M. Shahzamanian, "On the numerical study of Frederick transition in nematic liquid crystals." Journal of Molecular Liquids, **138** (2008) 14.
- [35] S. Khosla, S. Lal, A. Devi, "Review of Blue phase liquid crystal devices." AIP Conference Proceedings, **2352** (2021) 020037.
- [36] R. H. Self, C. Please, T. Sluckin, "Deformation of nematic liquid crystals in an electric field." European Journal of Applied Mathematics, **13**, (2002) 1.
- [37] D. K. Yang, S. T. Wu, "Fundamentals of liquid crystal devices", second ed., Willey, England, 2014.

- [38] M. Ravnik, "Colloidal structures confined to thin nematic layers: doctoral thesis", M. Ravnik, 2009.
- [39] J. i. Fukuda, S. Zumer, "Field-induced dynamics and structures in a cholesteric-blue-phase cell." *Physical Review E*, **87** (2013) 042506.
- [40] M. Kleman, O. D. Lavrentovich, "Soft matter physics: an introduction", NY: Springer New York, 2003.
- [41] U. Wolff, W. Greubel, H. Kruger, "The homogeneous alignment of liquid crystal layers." *Molecular Crystals and Liquid Crystals*, **23** (1973) 187.