ANCHORING ANGLE INFLUENCE ON MAGNETIC FREEDERICKSZ TRANSITION THRESHOLD

Zabreanu Andrei[1], Luncanu Stefan Valentin[1], Ana Dondera[2], Cristina Cirtoaje[3]

To Professor Emil Petrescu

The paper presents a theoretical analysis of the influence of the anchoring angle on the Freedericksz transition threshold in a magnetic field. The study is based on Frank's elastic continuum theory and the effect of the magnetic field on the molecules of nematic liquid crystal in cells with planar alignment. The numerical simulations conducted for the nematic phase indicated a consistent variation in the ratio between the applied magnetic field and the critical Freedericksz transition field in the case of flexible anchoring with an initial angle different from zero. For an angle of 10^o*, the ratio* B/B_c *can be reduced to* $1/2$ *of its initial value*

Keywords: liquid crystal, magnetic Freedericksz transition, anchoring angle

1. Introduction

Liquid crystals consist of molecules of organic compounds or metallomesogens exhibiting orientational order with or without position order ([1, 2, 3, 4, 5]). They are widely used in electronic devices such as LCDs, photonic systems or phase modulator due to their combined flexibility given by the fluid state and orientational order present in crystalline solids. Sometimes, to improve their performances, they are mixed with various nanoparticles including carbon nanotubes, ferroelectric particles, ferromagnetic particles, quantum dots or carbon based particles ([6, 7, 8, 9, 10]). Sometimes these methods don't provide the expected results so other methods based on the inner structure of liquid crystals or on the nature of the constituents as well as on external parameters such as temperature or solvents [11, 12] must be found. The nematic phase has been widely studied and applied among other phases because

[1] Student, Faculty of Applied Sciences Politehnica Bucharest, Romania, *andrei.zabreanu@stud.fsa.upb.ro*

[1] Student, Faculty of Applied Sciences Politehnica Bucharest, Romania, *stefan.luncanu@stud.fsa.upb.ro*

[2] Ph.D Student, Faculty of Applied Sciences Politehnica Bucharest, Romania, *ana_dondera@yahoo.com*

[3] coresponding author, Asoc. Professor, Physics Department Politehnica Bucharest, Romania, *cristina.cirtoaje@upb.ro*

it is present in a wide temperature range and it can be used for many devices [13, 14, 2] The most important property of nematic liquid crystals is anisotropy, determined by their lower symmetry compared to liquids. Quantitatively this means that liquid crystals are more ordered than liquids. The continuum theory has been successfully applied to conditions where the effect of external fields on the physical properties of liquid crystals has been followed [15]

The ordering and rearrangement of liquid crystal molecules by a magnetic field and wall interaction ([16]) is a particular interest because it forms the basis of a broad class of electro-optical devices. In the presence of magnetic field, the free energy density will contain additional terms [17]. The field influences the liquid crystal molecular director due to magnetic anisotropy. The reorientation changes the optical properties of the sample due to the anisotropy of the liquid crystal refraction. The alignment of the director of a nematic sample will not be influenced by the external magnetic or electric field when its magnitude is less than the critical field strength or Freedericksz threshold, but will be influenced by the external field and will begin to adjust its orientation whenever the field magnitude is greater than the critical field strength. According to the classical Fredericksz transition theory, the decrease of the critical field can be o obtained by increasing the cell's thickness. Yet this procedure has a major inconvenience related to the molecular ordering in the crystal. For very thick sandwich cells, the alignment induces on the cell's surface is lost in the middle of cell leading to a disordered structure that requires more energy to be aligned so the purpose or reducing the critical field is not reached. It is the aim of this paper to provide an alternative solution to decrease the transition threshold. A possible solution is to increase the initial anchoring angle from 0^o0 to at most 10^o so the effort required by the field to reorient the molecules is reduced.

2. **Theoretical modeling**

To present the reorientation phenomena of the liquid crystal under the influence of external fields and wall interaction, we consider a sandwich cell, which consists of two parallel plates previously prepared for a desired alignment. Unlike the classical homogenous aligned cell, we considered a cvariplanar cell in which the orientation is induced by a pretilt angle θ_0 as shown in figure Fig. When the magnetic field is applied, the molecules change their orientation from θ_0 to θ which depends both on the field intensity and the molecule position on Oz axis.

The magnetic field intensity for which the molecular reorientation appears can be calculated using the elastic continuum theory in which the liquid crystal is considered a continuum environment where elastic interaction acts between the molecules. In this model, the stability of the system is obtained by the minimum free energy acquired when the Euler Lagrange equations are fullfiled. The free energy density f in a nematic liquid crystal subjected to a

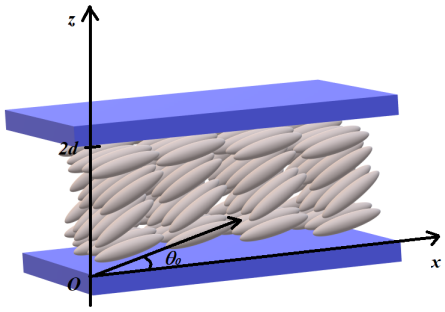


FIGURE 1. Initial orientation of the nematic molecule in the quasi-planar cell

magnetic field can be expressed as:

$$f = \frac{1}{2}\left(K_1 \cos^2\theta + K_3 \sin^2\theta\right)\theta_z^2 - \frac{1}{2}\mu_0^{-1}\chi_a B^2 \sin^2\theta \tag{1}$$

where:

- θ is the angle between the nematic director and the applied field's direction.
- K_1 and K_3 are the splay and bend elastic constants, respectively.
- θ_z represents the spatial derivative of θ along the z-axis, which is an alternative notation for $\frac{d\theta}{dz}$.
- μ_0 is the magnetic permeability of free space.
- χ_a is the magnetic susceptibility anisotropy.
- B is the magnetic field strength.

The total free energy F in a nematic liquid crystal can be calculated by integrating the free energy density $f(z)$ over the thickness of the liquid crystal layer. We choose a planar configuration because, in this case, it is sufficient to study the behavior of the liquid crystal in the case of $z \in [-d, 0]$. This is permissible because the function $\theta(z)$ is symmetric, satisfying $\theta(z) = \theta(-z)$. This symmetry implies that the liquid crystal's properties are mirrored on either side of the center. Additionally, the maximum deviation of the director is obtained in the center of the liquid crystal at $z = 0$, where the spatial derivative of θ with respect to z (denoted as $\frac{d\theta}{dz}$) is zero. This symmetry and central peak in deviation allow us to comprehensively understand the liquid crystal's behavior by examining just half of its thickness.

The Lagrange equation is used to ensure that the free energy F attains a minimum value. At thermodynamic equilibrium, the free energy is minimized. This principle is particularly relevant for a liquid crystal that is confined within a cell of fixed volume. In such a system, variations in free energy rather than total energy are critical for understanding the equilibrium state, as the liquid crystal's configuration is constrained by the cell's boundaries. Therefore,

the minimization of free energy, rather than total energy, becomes the key condition for achieving equilibrium.

$$\frac{\partial}{\partial z}\left(\frac{\partial f}{\partial \theta_z}\right) - \frac{\partial f}{\partial \theta} = 0 \tag{2}$$

where:

$$\frac{\partial f}{\partial \theta} = (-K_1 \sin(\theta)\cos(\theta) + K_3 \sin(\theta)\cos(\theta))\theta_z^2 - \\ -\mu_0^{-1}\chi_a B^2 \sin(\theta)\cos(\theta) \tag{3}$$

$$\frac{\partial f}{\partial \theta_z} = \left(K_1 \cos^2(\theta) + K_3 \sin^2(\theta)\right)\theta_z \tag{4}$$

$$\frac{\partial}{\partial z}\left(\frac{\partial f}{\partial \theta_z}\right) = 2(-K_1 \sin(\theta)\cos(\theta) + \\ +K_3 \sin(\theta)\cos(\theta))\theta_z^2 + (K_1 \cos^2(\theta) + K_3 \sin^2(\theta))\theta_{zz} \tag{5}$$

$$\theta_{zz} = \frac{d^2\theta}{dz^2} \tag{6}$$

Equation (2) leads to:

$$(K_1 \cos^2(\theta) + K_3 \sin^2(\theta))\theta_{zz} + (K_3 - K_1)\sin(\theta)\cos(\theta)\theta_z^2 + \\ +\mu_0^{-1}\chi_a B^2 \sin(\theta)\cos(\theta) = 0 \tag{7}$$

We multiply Eq.7 with $2\theta_z$:

$$2(K_1 \cos^2(\theta) + K_3 \sin^2(\theta))\theta_z\theta_{zz} + 2(K_3 - K_1)\sin(\theta)\cos(\theta)\theta_z^3 + \\ +2\mu_0^{-1}\chi_a B^2 \sin(\theta)\cos(\theta)\theta_z = 0 \tag{8}$$

We observe that:

$$\frac{d}{dz}\left(K_1 \cos^2(\theta)\theta_z^2\right) = -2K_1 \sin(\theta)\cos(\theta)\theta_z\theta_z^2 + \\ +2K_1 \cos^2(\theta)\theta_z\theta_{zz} \tag{9}$$

$$\frac{d}{dz}\left(K_3 \sin^2(\theta)\theta_z^2\right) = 2K_3 \sin(\theta)\cos(\theta)\theta_z\theta_z^2 + 2K_3 \sin^2(\theta)\theta_z\theta_{zz} \tag{10}$$

We integrate Eq. 8:

$$\int_0^{2d} [2(K_1 \cos^2(\theta) + K_3 \sin^2(\theta))\theta_z\theta_{zz} + 2(K_3 - K_1)\sin(\theta)\cos(\theta)\theta_z^3 + \\ +2\mu_0^{-1}\chi_a B^2 \sin(\theta)\cos(\theta)\theta_z]dz = C \tag{11}$$

And the solution is:

$$(K_1 \cos^2\theta + K_3 \sin^2\theta)\theta_z^2 + (\mu_0^{-1}\chi_a B^2)\sin^2\theta = C \tag{12}$$

To determine the constant C, we must take into account that the relationship is valid for any z, including for z = d. At this value of z, the first derivative of theta is zero (The angle for the minimum deviation is maxim in the center of the cell) Then:

$$\frac{d\theta}{dz} = 0 \tag{13}$$

So the constant is:

$$\mu_0^{-1}\chi_a B^2 \sin^2\theta_m = C \tag{14}$$

Eq.7 becomes :

$$(K_1 \cos^2\theta + K_3 \sin^2\theta)\theta_z^2 = (\mu_0^{-1}\chi_a B^2)(\sin^2\theta_m - \sin^2\theta) \tag{15}$$

If we highlight the second derivative of theta with respect to z, we obtain:

$$(\frac{d\theta}{dz})^2 = \frac{(\mu_0^{-1}\chi_a B^2)}{K_1}\frac{(\sin^2\theta_m - \sin^2\theta)}{\cos^2\theta + \frac{K_3}{K_1}\sin^2\theta} \tag{16}$$

We multiply the equation by $(\frac{2d}{\pi})^2$ because 2d is the width of the liquid crystal cell and get:

$$(\frac{d\theta}{dz})^2(\frac{2d}{\pi})^2 = (\frac{2d}{\pi})^2\frac{\chi_a}{\mu_0 K_1}B^2\frac{(\sin^2\theta_m - \sin^2\theta)}{\cos^2\theta + \frac{K_3}{K_1}\sin^2\theta} \tag{17}$$

Considering the critical magnetic field strength as :

$$B_c = \frac{\pi}{2d}\sqrt{\frac{K_1\mu_0}{\chi_a}}, \tag{18}$$

the new equation is :

$$(\frac{d\theta}{dz})^2(\frac{2d}{\pi})^2 = \frac{B^2}{B_c^2}\frac{(\sin^2\theta_m - \sin^2\theta)}{\cos^2\theta + \frac{K_3}{K_1}\sin^2\theta} \tag{19}$$

or:

$$\frac{d\theta}{dz}\frac{2d}{\pi} = \frac{B}{B_c}(\frac{\sin^2\theta_m - \sin^2\theta}{\cos^2\theta + \frac{K_3}{K_1}\sin^2\theta})^{1/2} \tag{20}$$

This yields to:

$$\frac{\pi}{2d}\frac{B}{B_c}dz = (\frac{\cos^2\theta + \frac{K_3}{K_1}\sin^2\theta}{\sin^2\theta_m - \sin^2\theta})^{1/2}d\theta \tag{21}$$

We change the notation : $\theta -> \alpha$, $z -> y$

$$\frac{\pi}{2d}\frac{B}{B_c}dy = (\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha \tag{22}$$

We integrate the above equation, consider y = z and $\alpha = \theta$ and obtain:

$$\frac{\pi}{2d}\frac{B}{B_c}\int_{-d}^{z} dy = \int_{\theta_0}^{\theta}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha \tag{23}$$

whih leads to

$$\frac{\pi}{2d}\frac{B}{B_c}(z+d) = \int_{\theta_0}^{\theta}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha \tag{24}$$

$$\begin{gathered}\int_{\theta_0}^{\theta}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha = \\ \int_0^{\theta_m}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha - \int_0^{\theta_0}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha\end{gathered} \tag{25}$$

To estimate the first integral, we change the variables:

$$\sin\psi = \frac{\sin\alpha}{\sin\theta_m}$$

$$\cos\psi\, d\psi = \frac{\cos\alpha\, d\alpha}{\sin\theta_m}$$

$$d\alpha = \frac{\cos\psi\ \sin\theta_m}{\cos\alpha}\, d\psi = \frac{\cos\psi\ \sin\theta_m}{\sqrt{1-\sin^2\alpha}}\, d\psi$$

When $\alpha = \theta_m, \sin\psi = 1, \psi = \pi/2$

$$I = \int_0^{\theta_z}(\frac{\cos^2\alpha + \frac{K_3}{K_1}\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha = \int_0^{\theta}(\frac{1 + (\frac{K_3}{K_1}-1)\sin^2\alpha}{\sin^2\theta_m - \sin^2\alpha})^{1/2}d\alpha \tag{26}$$

For:

$$\alpha = \theta, \psi = \Phi \tag{27}$$

$$\alpha = 0, \psi = 0 \tag{28}$$

$$I = \int_0^{\theta}\frac{(1 + (\frac{K_3}{K_1}-1)\sin^2\alpha)^{1/2}}{(\sin^2\theta_m - \sin^2\alpha)^{1/2}}\frac{\cos\psi\ \sin\theta_m}{\sqrt{1-\sin^2\alpha}}\, d\psi \tag{29}$$

We substitute $\sin\alpha = \sin\theta_m \sin\psi$ and we simplify:

$$I = \int_0^{\theta}\frac{(1 + (\frac{K_3}{K_1}-1)\sin^2\theta_m\sin^2\psi)^{1/2}}{\sqrt{1-\sin^2\theta_m\sin^2\psi}}d\psi \tag{30}$$

We substitute $\beta = \frac{K_3}{K_1} - 1$:

$$I = \int_0^{\theta}\frac{(1 + \beta\sin^2\theta_m\sin^2\psi)^{1/2}}{\sqrt{1-\sin^2\theta_m\sin^2\psi}}d\psi \tag{31}$$

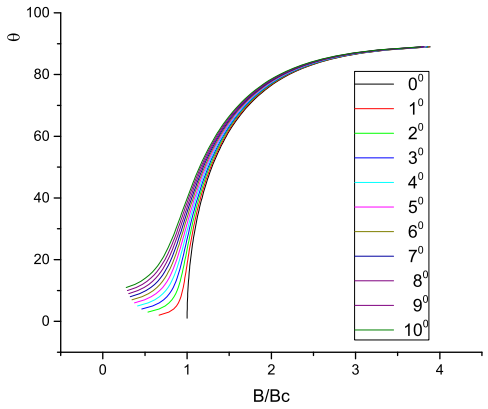
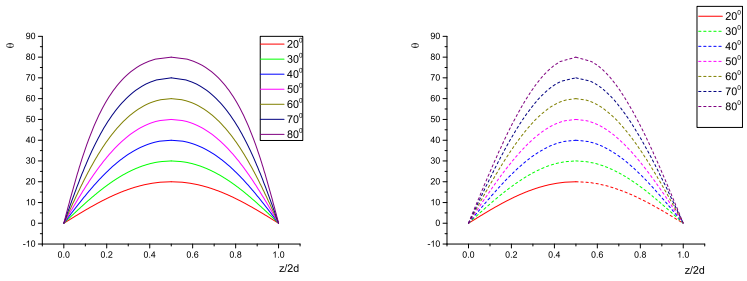


FIGURE 2. Distortion versus the applied magnetic field for different anchtoring angles



(a) (b)

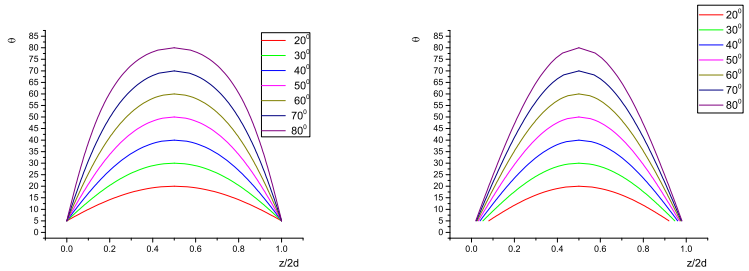
FIGURE 3. Distortion angle θ versus molecule's position z *a)* the model consider the initial anchoring angle $\theta = 0^o$

b) the model doesn't take into account initial anchoring,

At $z = 0$ and $\theta = \theta_m$: $\sin\psi = 1$ and $\psi = \frac{\pi}{2}$
So the the ratio between B and Bc becomes:

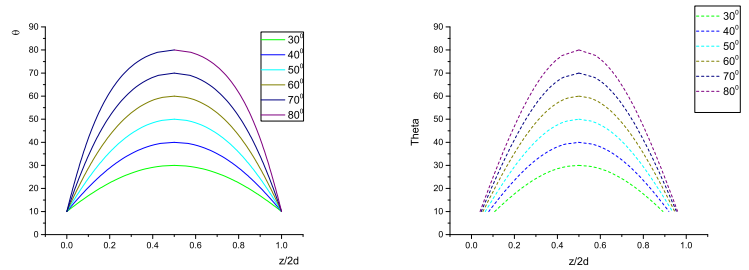
$$\frac{B}{B_c} = \frac{2}{\pi}\left[\int_0^{\pi/2} \sqrt{\frac{1+\beta\sin^2\theta_m\sin^2\psi}{1-\sin^2\theta_m\sin^2\psi}}d\psi - \int_0^{\theta_0} \sqrt{\frac{1+\beta\sin^2\alpha}{\sin^2\theta_m-\sin^2\alpha}}d\alpha\right] \quad (32)$$

Numerical simulation of Eq. 32 provides the dependence of the critical field for the magnetic Freedericksz transition on the anchoring angle θ_0 and also the variation of the distortion angle with the magnitude of the applied field B.



(a) (b)

FIGURE 4. Distortion angle θ versus molecule's position z *a)* the model consider the initial anchoring angle $\theta = 5^o$
b) the model doesn't take into account initial anchoring.



(a) (b)

FIGURE 5. Distortion angle θ versus molecule's position z *a)* the model doesn't take into account initial anchoring. *b)* the model consider the initial anchoring angle $\theta = 10^o$

3. **Results and discussions**

A numerical simulation of Eq.32 was done for a commonly used liquid crystal known as 5CB at room temperature using the elastic parameters given in [18] i.e. $K_1 = 1.407$ pN and $K_1 = 1.9632$ pN.The anchoring angle was set to different values from $\theta_0 = 0$ to $\theta - 10^o$ and the deviation angle θ was calculated for different values of the ratio B/B_c. The results are presented in Fig.2 and it can be observed a clear advantage of using a higher anchoring angle on the glass support. First of all, the threshold value decreases with more than 60% from the reference value. The B/B_c ratio decrease from $B/B_c = 1$ for an anchoring angle $\theta = 0$ to $B/B_c = 0.3$ for an anghoring angle of 10^o. Besides, the dependence of $\theta = f(B/B_c)$ is smoother for higher values of θ_0 indicating a slower variation of the distortion angle and a reduced backflow effect. This behavior is benefic for photonic devices as it can be used to controll the refractive index of the system by the magnetic field.

From Eq.24 several simulations were performed for the distortion angle versus $z/2d$. They were compared with the results obtained in other models where the influence of the anchoring angle was not considered. The detailed model without the anchoring angle is described in [19]. As it can be observed from Fig.3, Fig.4 and Fig.5, the plot using the model described in this manuscript indicates a slower increase of the deviation angle with z coordinate and a less sharp peak to the maximum value is obtained in the middle of the cell at z=d. In Fig.3 we observe that in both cases a) and b) the starting point is the same for each value of the maximum deviation angle but the curve tends to maximum with a lower slope and the range of z parameter for which θ reaches its maximum value is larger indicating an incrased stability on that value. This idea is plausible since thre relaxation times in magnetic field are even 10 times larger that those of the systems subjected to electric field, as it is presented in [18] and [19] In the simulation for higher anchoring angle (Fig.4 and Fig.5), the same slope decrease is observed but, initial anchoring come with an advantage of an initial orientation of the molecular direction with the applied field from the beginning. The starting angle value from

4. **Conclusions**

A new mathematical model for the behavior of the molecular director in nematic liquid crystals subjected to magnetic field is proposed based on elastic continuum theory. Unlike other models already present in the literature, this model point the importance of an initial anchoring angle for the decrease of the critical field for the Freedericksz transition. In liquid crystal cells subjected to magnetic field, the thickness of the cell must be increased in order to obtain lower transition threshold. This model indicates that, by using an anchoring angle of maximum 10^o, the critical field may be decreased by 50% without the loss of the molecular ordering that usually appear in very thick cells.

5. **Acknowledgements**

The research was funded by the grant Advanced Infrastructure for Nuclear Photonics research experiments at ELI-NP / ELI-INFRA through the national research and development program PNCDI IV / 5.9.1 ELI-RO: ELI-NP infrastructure development projects

REFERENCES

[1] *Petrescu E., Motoc C., Manaila D.*, A dynamical method for determining the elastic constants and relaxation parameters in nematic liquid crystals. Modern Physics Letters B, 14(04), pp.139-146.**(2000).**

[2] *Vertogen G. and de De Jeu W.H.,* Thermotropic Liquid Crystals, Fudamental, Springer Verlag Berlin Heidelberg, New York, London, Paris, Tokio **(1988)**

[3] *Ilinca T.A., Chiriac L.F., Ilis M., Manaila-Maximean D., Ganea P.C., Pasuk, I. and Circu V.*, Effect of disubstitution pattern of the terminal alkyl chains on the mesophase

of liquid crystals based on lanthanide (III) complexes: A study of the thermal, emission and dielectric behavior. Journal of Molecular Liquids, 360, p.119425. **(2022)**

[4] *Chiriac L.F., Ganea P.C., Maximean D.M., Pasuk I. and Circu V.*, Synthesis and thermal, emission and dielectric properties of liquid crystalline Eu (III), Sm (III) and Tb (III) complexes based on mesogenic 4-pyridone ligands functionalized with cyanobiphenyl groups. Journal of Molecular Liquids, 290, p.111184. **(2019)**

[5] *Rosu C., Manaila-Maximean D., Carcu V., Molard Y. and Roisnel T.*,. Differential negative resistance in the currentâ€'voltage characteristics of a new palladium (II) metallomesogen. Liquid Crystals, 38(6), pp.757-765 **(2011)**

[6] *Cirtoaje C., Petrescu E., Stan C., Creanga D.* Ferromagnetic nanoparticles suspensions in twisted nematic PHYSICA E-Low-dimensional systems & nanostructures, Volume79 Page38-43 **(2015)**

[7] *Ganea C.P., Manaila-Maximean D., Cîrcu V.* Dielectric investigations on carbon nanotubes doped polymer dispersed liquid crystal films EUROPEAN PHYSICAL JOURNAL PLUS Volume135, Issue10 **(2020)**

[8] *Petrov D. A., Zakhlevnykh, AN, Skokov, PK* Influence of Ferromagnetic Carbon Nanotubes on Magnetic Transitions in Liquid Crystals Journal of experimental and theoretical physics Volume127, Issue4 Page 767-777 **(2018)**

[9] *Petrescu E., Cirtoaje C., Stan C.* Dynamic behavior of a nematic liquid crystal mixed with CoFe2O4 ferromagnetic nanoparticles in a magnetic field BJNANO **Volume 8** Page2467-2473 **(2017)**

[10] *Petrescu E., Cirtoaje C., Danila O.* Dynamic behavior of nematic liquid crystal mixtures with quantum dots in electric fields BJNANO **Volume 9** Page399-406 **(2018)**

[11] *Peter J Collings, Michael Hird* Introduction to Liquid Crystals: Chemistry and Physics. Taylor and Francis Ltd.,, ISBN 0-7484-0643-3, pp. 53, 151–15, 2**(1997)**

[12] *Petrescu E., Cirtoaje C. and Postelnicu S.*, Freedericksz transition in nematic liquid crystals with carbon nanomaterials UPB- SCI BULL 84 (1), 201-208 **(2022)**

[13] *Palarie I., Dascalu C., Iacobescu G.E. MC Varut,* "Surface morphology of doped nematic liquid crystals: role of dye concentration" Liquid Crystals VOL 39(7), pg 833-837 (2012)

[14] *Motoc C., Iacobescu G.,* Magnetic field effects on the optical properties of an azo-dye doped liquid crystal. J. Magn. Magn. Mater. Vol 306 **(2006)**

[15] *Frank F. C.,*On the theory of liquid crystals, Discuss. Faraday Soc. , vol (25) pp. 19–28, bf (1958)

[16] *Rapini A., Papoular M.*,DISTORSION D'UNE LAMELLE NÉMATIQUE SOUS CHAMP MAGNÉTIQUE CONDITIONS D'ANCRAGE AUX PAROIS J. Phys. (Paris) Colloq.30, C4 (1969)

[17] *Petrov D.A., Zakhlevnykh N.*, Magnetic field induced orientational transitions in liquid crystals doped with carbon nanotubes Beilstein J. Nanotechnol. 8, 2807–2817, **(2017)**

[18] *Bogi A., Faetti S.*, Liquid Crystals, 28(5), 729–739. **(2001)**.

[19] *Iacobescu G., Paun A. L., Cartoaje C.*, Magnetically induced Freedericksz transition and relaxation phenomena in nematic liquid crystals doped with azo-dyes JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **volume 320** Issue: 17 Pages: 2180-2184 , **(2008)**.