

This article was downloaded by:

On: 25 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



## Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713926090>

### Elastic model for twisted nematic textures in OOBA layers

S. Frunza; L. Frunza; M. Petrov; G. Barbero

Online publication date: 06 August 2010

**To cite this Article** Frunza, S. , Frunza, L. , Petrov, M. and Barbero, G.(1998) 'Elastic model for twisted nematic textures in OOBA layers', *Liquid Crystals*, 24: 2, 215 – 218

**To link to this Article:** DOI: 10.1080/026782998207389

**URL:** <http://dx.doi.org/10.1080/026782998207389>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

# Elastic model for twisted nematic textures in OOBA layers

by S. FRUNZA†‡, L. FRUNZA†‡, M. PETROV†§ and G. BARBERO\*†

†Dipartimento di Fisica del Politecnico di Torino, Corso Duca degli Abruzzi 24,  
10129 Torino, Italy

‡Institute of Physics and Technology of Materials, PO Box Mg 07,  
76900 Bucharest-Magurele, Romania

§Institute of Solid State Physics, Georgy Nadjakov Blvd.,  
Tzarigradsko Chaussee 72, 1784 Sofia, Bulgaria

(Received 30 June 1997; accepted 31 August 1997)

An elastic model for the twisted nematic texture observed in nematic cells containing octyloxybenzoic acid is proposed. According to the model the twisted textures are due to the presence of cybotactic groups which are responsible for the chirality of the liquid crystal. We show that by assuming for the density of cybotactic groups a critical temperature behaviour close to a special temperature, the experimental data can be well interpreted by our mechanical model.

## 1. Introduction

The study of 4-*n*-alkoxybenzoic acids by conductivity measurements [1], depolarized Rayleigh scattering [2], X-ray diffraction [3], DSC and impedance spectroscopy [4] has produced evidence for a special behaviour at a particular temperature within the nematic range. This behaviour of 4-*n*-alkoxybenzoic acids especially in the nematic range is usually related to the existence of different states of hydrogen bonding leading to monomers and different types of dimers [5] and to the appearance of the skewed cybotactic groups [3]. The way in which these are involved in some of the observed phenomena is still unclear. Furthermore, in *trans*-4-alkylcyclohexanecarboxylic acids, which are mesomorphic due to the formation of dimers via hydrogen bonds [6], chiral structures were also observed in the nematic phase, even if the molecules have no chiral groups. Such domains were found both in a narrow temperature range close to the clearing point [7], and in a large temperature range contiguous to the smectic–nematic transition [8]. In fact the latter was found only for acids exhibiting a hexagonal smectic B phase. The chiral ordering was explained in the first case as being due to the presence of open dimers [9], and in the second case to the presence of cybotactic clusters. As a consequence of the molecular shape, due to steric effects, the open dimers pack themselves in chiral domains, partially right- and partially left-handed, and for the same reason cybotactic clusters organize chiral symmetric structures.

For 4-*n*-octyloxybenzoic acid (OOBA), the appearance of a twisted nematic structure within the nematic range has been recently reported [10]. In these twisted structures the tilt angle  $\theta$  and the surface twist angle  $\phi$  have a specific temperature dependence.

In this paper we propose an elastic model that considers the twisted structures as being related to the cybotactic groups. Assuming the one-constant approximation and finite values for the anchoring energies, a simple analysis is made for the homogeneously oriented liquid crystal layers. We also obtain the temperature dependence for the tilt and twist angles. Agreement between the theoretical predictions and the experimental data reported by Petrov *et al.* [10] is fairly good near the particular temperature.

## 2. Elastic description

Let us consider a liquid crystal layer confined between the two walls of a cell. Let  $z$  be the coordinate perpendicular to the walls. Everywhere in the cell, the local director  $\mathbf{n}$  can be defined by the polar azimuthal angles  $\theta$  and  $\phi$ , called the tilt and twist angles, respectively. The twist angle is measured with respect to the direction of the grooves created by the oblique evaporation of the SiO, as described in [10]. We assume that this layer has an intrinsic twist due to the presence of cybotactic groups. We suppose also that the director orientation depends only on the  $z$ -coordinate.

In the one-elastic constant approximation and by taking into account the surface contribution to the total energy, we can write the total energy per unit area as

\* Author for correspondence.

$$F = \int_{-d/2}^{d/2} \frac{1}{2} k [\theta'^2 + \sin^2 \theta (\phi'^2 - 2q\phi')] dz + G_- + G_+, \quad (1)$$

where  $k$  is the elastic constant,  $q = 2\pi/P$  ( $P$  being the pitch of the structure),  $G_-$  and  $G_+$  are the surface energies corresponding to the boundary surfaces at  $z = -d/2$  and  $z = d/2$  respectively; the prime means the derivative with respect to  $z$ . In equation (1) we have neglected the term  $(1/2)kq^2$  since it does not contribute to further Euler–Lagrange equations. The surface energies are assumed to have the following expressions

$$G_{\pm} = \frac{1}{2} w_{\pm} (\theta_s^{\pm} - \Theta^{\pm})^2 + \frac{1}{2} u_{\pm} (\phi_s^{\pm})^2, \quad (2)$$

where  $w_{\pm}$  and  $u_{\pm}$  are the anchoring energies,  $\Theta^{\pm}$  are the easy axes of tilt and the easy twist axes are assumed to be zero;  $\theta_s^{\pm}$  and  $\phi_s^{\pm}$  are the actual tilt and twist surface angle.  $+$  and  $-$  means  $z = d/2$  and  $z = -d/2$ , respectively. In the following, we limit our analysis to a symmetric sample in which  $w_+ = w_- = w$ ,  $u_+ = u_- = u$ ,  $\Theta^+ = \Theta^- = \Theta$ . In this case the symmetry of the problem suggests that  $\theta(z) = \theta(-z)$  and  $\phi(z) = -\phi(-z)$ . In particular, for the surface angles we have  $\theta_s^+ = \theta_s^- = \theta_s$  and  $\phi_s^+ = -\phi_s^- = \phi_s$ .

The usual variational approach provides the following Euler–Lagrange equations for  $\phi$  and  $\theta$

$$\frac{d}{dz} [\sin^2 \theta (\phi' - q)] = 0, \quad (3)$$

and

$$\theta'' - \sin(2\theta)(\phi'^2 - 2q\phi') = 0, \quad (4)$$

as well as the boundary conditions at  $z = d/2$

$$k \sin^2 \theta_s (\phi_s - q) + u \phi_s = 0, \quad (5)$$

$$k \theta' + w(\theta_s - \Theta) = 0. \quad (6)$$

Equation (3) has the solution

$$\phi' = q + \frac{C}{\sin^2 \theta}, \quad (7)$$

where  $C$  is an integration constant. By substituting  $\phi'$  given by equation (7) into (4) and integrating once, one obtains

$$\theta'^2 = b - \left( \frac{C}{\sin^2 \theta} + q^2 \sin^2 \theta \right), \quad (8)$$

where  $b$  is an integration constant. By using equations (7) and (8), simple calculations give

$$C = -\frac{u}{k} \phi_s, \quad (9)$$

and

$$b = \left( \frac{u}{k} \frac{\phi_s}{\sin \theta_s} \right)^2 + q^2 \sin^2 \theta_s + \left( \frac{w}{k} \right)^2 (\theta_s - \Theta)^2. \quad (10)$$

The last two equations relate the integration constants  $C$  and  $b$  with  $\theta_s$  and  $\phi_s$ . Taking into account that  $\theta(z)$  is an even function and  $\phi(z)$  is an odd function of  $z$ , from equations (7) and (8) we obtain

$$2\phi_s = qd + 2C \int_{\theta_s}^{\theta_0} \frac{d\theta}{\theta' \sin^2 \theta}, \quad (11)$$

and

$$2 \int_{\theta_s}^{\theta_0} \frac{d\theta}{\theta'} = d, \quad (12)$$

where  $\theta_0 = \theta(0)$  and  $\theta'(0) = 0$  for symmetry. The value of  $\theta_0$  is related to  $b$  by the equation

$$b = \frac{C^2}{\sin^2 \theta_0} + q^2 \sin^2 \theta_0. \quad (13)$$

Equations (9)–(12) give the thickness dependence of  $\theta_s$ ,  $\phi_s$  and  $\theta_0$ . The actual values are the ones minimizing the total energy per unit surface given by equation (1).

### 3. Temperature dependence of the tilt and twist angles

We now look for the temperature dependence of  $\theta$  and  $\phi$ . It emerges from equations (3)–(6) that if  $q = 0$ , then  $\phi' = 0$  and hence  $\theta' = 0$ . This means that  $\phi$  and  $\theta$  are  $z$ -independent. On the contrary, when  $q \neq 0$ , then  $\phi' \neq 0$  and further  $\theta' \neq 0$ .

Let us suppose that  $q$  is very small. In this case we can expand  $\theta$  and  $\phi$  in a power series of  $q$  as follows [11]

$$\theta(z) = \Theta + q^2 \varepsilon(z), \quad (14)$$

and

$$\phi(z) = q\varphi(z), \quad (15)$$

because, as follows from equation (3),  $\phi(z)$  is expected to be linear in  $q$ , whereas from (4) we deduce that  $\theta(z)$  has to be quadratic in the same parameter. In equations (14) and (15)  $\varepsilon(z)$  and  $\varphi(z)$  are two new functions to be determined. By substituting equation (15) into (3), at the first order in  $q$ , we obtain

$$\varphi(z) = 2 \frac{\varphi_s}{d} z, \quad (16)$$

where  $\varphi_s$  is an integration constant. In this approximation  $\varepsilon(z)$  is a solution of the differential equation

$$\varepsilon''(z) - \frac{1}{2} \sin(2\Theta)(\varphi'^2 - 2\varphi') = 0. \quad (17)$$

The boundary conditions at  $z = d/2$ , represented by

equations (5) and (6), become in this perturbative approach

$$k \sin^2 \Theta (\varphi' - 1) + w \varphi_s = 0, \quad (18)$$

and

$$k \varepsilon' + w \varepsilon_s = 0. \quad (19)$$

By means of equation (18), the integration constant  $\varphi_s$  entering in equation (16) is found to be

$$\varphi_s = \frac{1}{(2/d) + [ul/(k \sin^2 \Theta)]}. \quad (20)$$

The solution of equation (17), with the boundary condition (19), even in  $z$  when  $\varphi(z)$  is given by (16) and (20) is

$$\varepsilon(z) = \frac{\alpha}{4} z^2 + \mu, \quad (21)$$

where

$$\alpha = - \frac{1 + ul/(k \sin^2 \Theta)}{[1 + ul/(2k \sin^2 \Theta)]^2} \quad (22)$$

and

$$\mu = - \frac{1}{16} d^2 \alpha \sin(2\Theta) \left( 1 + 4 \frac{1}{d} \frac{k}{w} \right). \quad (23)$$

When the perturbative expansion is valid, the surface twist angle is given by

$$\phi_s = q \varphi_s, \quad (24)$$

and the tilt angle changes according to the law

$$\theta(z) - \Theta = q^2 \varepsilon(z), \quad (25)$$

where  $\varphi_s$  and  $\varepsilon(z)$  are defined by equations (20)–(23). It is important to notice that  $\phi_s$  is proportional to  $q$ ; that in turn is proportional to the density of cybotactic groups  $\rho$ . By assuming [7, 8] that  $\rho \propto (T^* - T)^{1/2}$  where  $T^*$  is the temperature at which the cybotactic groups appear, the temperature dependence of the surface twist angle is expected to be

$$\phi_s \propto (T^* - T)^{1/2}. \quad (26)$$

In the same approximation, from equation (25), we have

$$\langle \theta(z) - \Theta \rangle \propto (T^* - T), \quad (27)$$

where  $\langle \rangle$  means the average over the thickness of the sample. Taking into account that  $q$  depends on the concentration of cybotactic groups which in turn depends on the temperature in a critical manner, we can assume  $\rho(T > T^*) = 0$ ; that implies  $q(T > T^*) = 0$ . It follows that

$$\langle \theta(z) \rangle = \Theta, \quad \text{and} \quad \phi_s = 0, \quad \text{for} \quad T > T^*. \quad (28)$$

Then, equations (26)–(28), which are shown in figures

1 and 2, are in good agreement with the temperature dependence for the surface twist angle and for the average tilt angle as experimentally found by Petrov *et al.* [10], where these parameters were the only ones detectable. The trends of  $\phi_s(T)$  and  $\langle \theta(z) \rangle$ , experimentally detected, are reported also in figures 1 and 2.

In real cases, the concentration of cybotactic groups is position dependent, since the monomers and dimers usually have different adsorption energies with respect to the substrate [12]. This implies that  $q = q(z)$ . However, since we are interested in the trend close to  $T^*$ , where  $q$  passes from zero to a finite value, this effect may be neglected. In fact, near  $T^*$ ,  $P = 2\pi/q$  is much

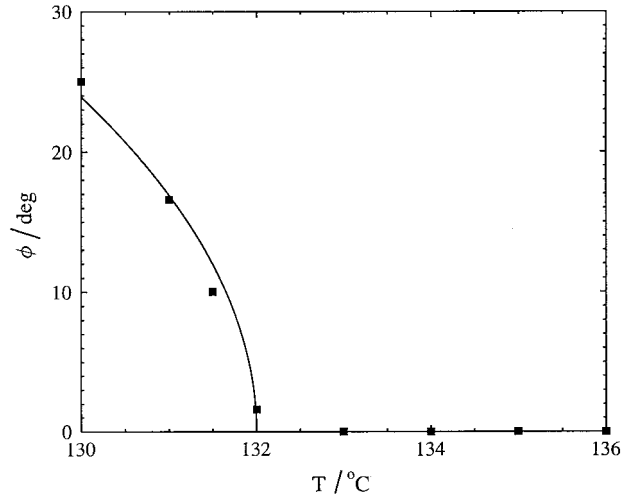


Figure 1. Trend of the temperature dependence of the surface twist angle  $\phi_s$ . Continuous curve: best fit of the theoretical prediction. Squares: experimental points.

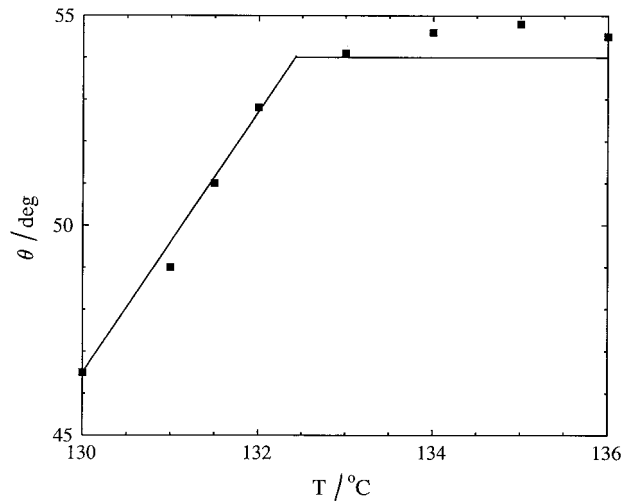


Figure 2. Trend of the temperature dependence of the average tilt angle  $\langle \theta(z) \rangle$ . Continuous curve: best fit of the theoretical prediction resulting from the elastic model. Squares: experimental points.

larger than the extrapolation length connected with the adsorption effects.

Figures 1 and 2 show the best fits obtained for the data relating to a homogeneous cell of thickness  $d = 20 \mu\text{m}$ , having a SiO alignment layer deposited by evaporation at an incidence angle of  $86^\circ$ . The theoretical fit has been made, near  $T^*$ , by means of the equations

$$\left. \begin{aligned} \phi(T) &= A(T^* - T)^{1/2}, \\ \text{and} \\ \theta(T) &= \langle \theta(z) \rangle = \Theta - B(T^* - T), \end{aligned} \right\} \quad (29)$$

deduced from equations (26) and (27). The parameters for the best fits are  $A = (16.9 \pm 0.8)^\circ\text{C}^{1/2}$ ,  $B = (3.1 \pm 0.25)^\circ\text{C}^{-1}$  and  $T^* = 132^\circ\text{C}$ . The value of  $T^*$  is close to the temperature at which  $\theta$  and  $\phi$  begin to vary during the cooling of the liquid crystal from the isotropic state. On the other hand,  $T^*$  is close to the special temperature of OOBA [4]. Therefore, the type of temperature dependence found in the model proposed by us describes rather well the experimental results.

#### 4. Conclusions

In this paper an elastic model for the twisted nematic texture appearing in cells containing OOBA-like liquid crystals has been proposed. The texture and the specific temperature dependence within the nematic range observed by Petrov *et al.* [10] have, according to the model presented, a bulk origin in relationship to the presence of cybotactic groups responsible for the chirality of the structure. The surface enters into the phenomenon due to the fact that  $\phi_s(T) \neq 0$  is connected with a weak anchoring energy. The dependence of  $\theta(T)$  is also expected to be detectable since the optical path difference depends on the whole  $\theta(z)$ -profile. The proposed model

leads to a temperature dependence of the tilt  $\theta$  and twist  $\phi$  angles in good agreement with the experimental data.

We thank Prof. A. Strigazzi for stimulating discussions. This work has been partially supported by Inco-Copernicus ERBCIC15CT960744 Novel Techniques and Models for the Surface Treatments of Liquid Crystals with Optical Applications.

#### References

- [1] SIMOVA, P. D., and PETROV, M. P., 1983, *Phys. Status Solidi A*, **80**, K153.
- [2] PETROV, M. P., and SIMOVA, P. D., 1985, *J. Phys. D Appl. Phys.*, **18**, 239.
- [3] NEUBERT, M. E., and DE VRIES, A., 1987, *Mol. Cryst. liq. Cryst.*, **145**, 1.
- [4] FRUNZA, S., FRUNZA, L., SPARAVIGNA, A., PETROV, M. P., and TORGOVA, S. I., 1996, *Mol. Mat.*, **6**, 215.
- [5] DELOCHE, B., and CABANE, B., 1972, *Mol. Cryst. liq. Cryst.*, **19**, 25.
- [6] MOLOCHKO, V. A., IRASHCHENKO, A., LIDIN, P. A., and TORGOVA, S. I., 1989, *Zh. Prirodnoi khimii*, **62**; 1605; MOLOCHKO, V. A., IRASHCHENKO, V., LIDIN, P. A., and TORGOVA, S. I., 1990, *J. appl. Chem.*, **62**, 1486.
- [7] TORGOVA, S. I., KOMITOV, L., and STRIGAZZI, A., 1998, *Liq. Cryst.*, **24**, 131.
- [8] TORGOVA, S. I., SPARAVIGNA, A., and STRIGAZZI, A., Azimuthal transition in unidirectional planar nematic layers, Samara Conference on Liquid Crystals, May 1996 (submitted).
- [9] TORGOVA, S. I., ABRAMIC, D., STRIGAZZI, A., and ZUMER, S., Dimerization in *trans*-4-butylcyclohexanecarboxylic acid and its mixture with 12% *cis*-isomer observed via H- and D-NMR, Zakopane E.C.O.C., March 1997 (to be published).
- [10] PETROV, M. P., BRASLAU, A., LEVELUT, A. M., and DURAND, G., 1992, *J. Phys. II (Fr.)*, **2**, 1159.
- [11] ELSGOLTS, L., 1970, *Variational Calculus* (Moscow: MIR).
- [12] BARBERO, G., and DURAND, G., 1990, *J. Phys. (Paris)*, **51**, 281.