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On the validity of the elastic model for the nematic surface anchoring energy†

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The intrinsic uniform and non-uniform contributions to the anisotropic part of the surface energy are considered. Our analysis shows that the uniform part can be separated into an intrinsic and an extrinsic term. The first one is due to the nematic–nematic interaction only, whereas the second one is due to the nematic–substrate interaction. They are found to be of the same order of magnitude ($\approx 1 \text{ erg cm}^2$). The non-uniform part takes its origin from the spatial variation of the elastic constants. By means of a semi-microscopic model it is shown that, in the framework of perfect nematic order, the extrapolation length of the elastic origin is microscopic. On the contrary, if the spatial variation of the scalar order parameter is taken into account, simple calculations indicate that the extrapolation length is of the order of the coherence length in the nematic phase.

1. Introduction

The bulk elastic theory of nematic liquid crystals (NLC) is well established [1]. It was built up by analogy with the elastic theory for solid materials by substituting the usual deformation tensor [2] with the tensor $n_{i,j} = \partial n_i / \partial x_j$. \mathbf{n} is the macroscopic vector field describing the average molecular orientation of the major axis. x_j are the Cartesian coordinates of a small volume $d\tau$ containing a number of molecules so large that the statistical average, by means of which \mathbf{n} is defined, is meaningful. According to the elastic theory, the elastic energy density, F , is a positive defined quadratic form in $n_{i,j}$. This means that

$$F = \frac{1}{2} \beta_{ijkl} n_{i,j} n_{k,l}, \quad (1)$$

where the elastic tensor $\beta_{ijkl} = \beta_{klij}$ is position independent in the bulk. It can be decomposed, as is well known [3], in terms of the elements of symmetry of the NLC phase. This usual procedure leads to

$$F = \frac{1}{2} [k_{11}(\text{div } \mathbf{n})^2 + k_{22}(\mathbf{n} \times \text{rot } \mathbf{n})^2 + k_{33}(\mathbf{n} \times \text{rot } \mathbf{n})^2], \quad (2)$$

which is the well-known Frank expression for the elastic energy density of a NLC [4].

2. Model

By means of semi-microscopic models, it is possible to evaluate the elastic tensor β_{ijkl} when the intermolecular interaction responsible for the nematic phase is known [5–8]. This kind of calculation is relatively simple for the bulk, where the elements of symmetry of the NLC phase reduce to \mathbf{n} . Near the surface, the situation is more complicated for two different reasons. First, the elements of symmetry of the NLC phase are \mathbf{n} and the geometrical normal to the bounding surface, \mathbf{z} . This implies that usually the number of surface elastic constants is larger than the one in the bulk [6–9]. Second, the ‘elastic constants’ are expected to be position dependent. Consequently, in a surface layer whose thickness is of the order of the range of the intermolecular forces giving rise to the NLC phase, the elastic energy density is

$$F = \frac{1}{2} \beta_{ijkl}(z) n_{i,j} n_{k,l} + \delta F(n_{i,j}), \quad (3)$$

where $\beta_{ijkl}(z)$ take into account the incomplete NLC–NLC interaction and δF the new elements of symmetry of the phase. Recently, by means of a Maier–Saupe [10] interaction law, we have analysed the elastic description of a NLC close to a substrate, by supposing an interaction volume of ellipsoidal shape [7]. In that context, the $\beta_{ijkl}(z)$ and δF have been evaluated. Our analysis shows that $\beta_{ijkl}(z)$ and δF exist in a surface layer whose thickness is of the order of 20–30 molecular dimensions. In the same framework, we have also shown that the uniform part [11] of the free energy density is intrinsically anisotropic with an

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easy axis [12] parallel to the geometrical normal (homeotropic orientation). The associated anisotropic anchoring energy is found to be of the order of 1 erg cm^{-2} , using reasonable values for the physical parameters characterizing a normal NLC [13]. Since this anisotropic anchoring energy comes only from the NLC itself, from now on it will be called intrinsic uniform and denoted by W_{iu} [11]. The extrapolation length connected to this energy is defined as $L_{iu} = k_b/W_{iu}$, with k_b being the bulk value of the average Frank elastic constant.

3. Analysis

In this paper we want to analyse all the possible contributions to the anisotropic part of the surface energy, and to evaluate them in the framework of the Maier–Saupe model. As shown in [11], if the interaction volume is of ellipsoidal shape, the uniform part of the surface energy is anisotropic with a homeotropic easy direction. Let us consider a semi-infinite NLC sample and a Cartesian reference frame whose z axis is normal to the bounding wall, placed at $z = 0$, and $z > 0$ corresponds to the NLC half-space. The NLC distortion is supposed to be planar in the (x, z) plane. The average NLC orientation is described by means of the tilt angle $\phi = \arccos(\mathbf{n} \cdot \mathbf{z})$. For the sake of simplicity, $\phi = \phi(z)$ only. Assuming the Maier–Saupe law for the intermolecular interaction, and considering that both the molecular and the effective interaction volume are ellipsoids of revolution (of similar shape) around \mathbf{n} , it is possible to define the energy of the undistorted configuration, F_0 , as

$$F_0 = -\frac{1}{2} \int_{V_N} J(r) dV_N$$

where $J(r) = -C/r^6$, with C being a positive constant, and V_N the effective interaction volume. In the situation in which the interaction volume is incomplete, i.e. close to the surface, a surface free energy density can be defined as

$$G(e, \phi) = \int_{A_m}^{A_M} \Delta F_0(e, \phi; z) dz \quad (4)$$

where e is the eccentricity of the ellipsoidal interaction volume and it is supposed to be equal to that of the NLC molecule. Furthermore, A_m and A_M are, respectively, the z coordinate of the lowest and highest point of the ellipsoid, and $\Delta F_0 = F_{0b} - F_0(z)$, where F_{0b} is the bulk value of the uniform part of the free energy density.

The physical meaning of equation (4) is that due to NLC–NLC interaction, there exists, in a surface layer whose thickness, σ , is several molecular dimensions, an anisotropic surface field characterized by a well-defined easy direction and anchoring energy. Of course a direct

NLC–substrate interaction can exist. It is delocalized over a surface layer of thickness ρ_s depending on the anisotropic part of the NLC–substrate interaction. This direct interaction, when integrated over this characteristic distance, gives an extrinsic contribution to the anchoring energy. It is characterized by another easy direction which depends on the physical symmetry of the surface and of the NLC. Furthermore, it is also characterized by an anisotropic anchoring strength, W_{eu} . Since $\sigma \simeq \rho_s$ because the NLC–substrate and NLC–NLC interactions are of the same kind, it is possible to introduce a total uniform part of the surface energy, defined as the sum of the above mentioned terms. In principle, the easy axes are different, and the actual easy axis will be in between them. For simplicity, we will suppose that they coincide with the z axis, and hence

$$W_u = W_{iu} + W_{eu} \quad (5)$$

However, since we are mainly interested in the analysis of the intrinsic part of the surface energy coming from the spatial variation of the elastic constants, this hypothesis is not very restrictive.

Some time ago Yokoyama [14] suggested that a spatial variation of the elastic constant is equivalent to a surface energy. This problem has been reconsidered more recently by other authors [15–18]. The main conclusion from these kinds of investigation are the following. If close to a boundary, $k = k(z)$, the associated anisotropic part of the anchoring energy is given by [15]

$$\frac{1}{W_{\text{elast}}} = \int_0^\infty \frac{k_b - k(z)}{k_b k(z)} dz, \quad (6)$$

where, as before, k_b is the bulk value of the elastic constant, whereas $k(z)$ is its actual value at a distance z from the wall. It changes over a surface layer whose thickness will be denoted by σ . Equation (6) holds only when σ is very small with respect to the thickness of the real sample. This implies that long range parts of the surface energy, like those connected with electrical effects, are not considered [19–21].

4. Discussion

We are now in a position to use the results obtained previously in [7] to estimate the order of magnitude of W_{elast} . In our case, in which the surface is supposedly flat and $\phi = \phi(z)$, equation (3) can be rewritten as

$$F(\phi, z) = \frac{1}{2} k(z) \phi^2, \quad (7)$$

where $k(z)$ takes into account the positional dependence of the Frank elastic constants and the new elastic constants connected with the reduction of symmetry introduced by the wall (the terms c_i , for $i = 1, 2, 3, 4$ of [7]). As follows from [7], $k(z)$ is well-approximated by the

function

$$k(z) = k_b - \frac{1}{2}k_b e^{-z/\sigma}. \quad (8)$$

By substituting (8) into (6), straightforward calculations give

$$\frac{1}{W_{\text{elast}}} = \frac{\sigma}{k_b} \ln 2. \quad (9)$$

According to our semi-microscopic calculations, σ is expected to be of the order of 20–30 a_0 , with a_0 being the minor axis of the internal ellipsoid (i.e. the molecular volume). By assuming $a_0 \simeq 5 \text{ \AA}$ and $k_b \simeq 10^{-6} \text{ erg cm}^{-2}$, we find $W_{\text{elast}} \simeq 1 \text{ erg cm}^{-2}$. This situation corresponds to the so-called strong anchoring [22, 23]. From this result it follows that some other mechanism could be responsible for the weak anchoring energy experimentally detected [22, 23].

The semi-microscopic calculations have been performed by assuming perfect nematic order (i.e. the scalar order parameter $S = 1$). Thus, we need to reconsider this hypothesis. As is well known, in the framework of the Landau–Ginzburg theory, the actual scalar order parameter profile has to be deduced by minimizing the functional written in terms of S . This functional is of the kind

$$G = \int_0^\infty \left[\frac{1}{2}LS'^2 + f(S) \right] dz, \quad (10)$$

where L is an elastic constant parameter, $S' = dS/dz$ and $f(S)$ is the free energy density of the uniform nematic phase [24]. Standard calculations show that near the boundary, S is given by

$$S(z) = S_b + (S_0 - S_b) e^{-z/\xi}, \quad (11)$$

where the bulk value of the order parameter, S_b , is fixed by the temperature, and the surface value of the order parameter, S_0 , is fixed by the temperature and the surface NLC–substrate interaction. In equation (11), ξ is the coherence length of the medium in the NLC phase [24]. The Frank elastic constants are expected to be proportional to S according to the law

$$k(z) = LS^2(z), \quad (12)$$

as is shown in [5, 24]. It follows that a spatial variation of k is expected in a surface layer whose thickness is of the order of ξ . This is a new contribution which is usually neglected in the semi-microscopic approach. However, equation (6) remains valid because it was obtained without any assumptions about the source of the $k(z)$ term [15]. Hence, instead of equation (8) we have to consider the $k(z)$ behaviour given by

$$k(z) = \left[k_b - \frac{1}{2}k_b e^{-z/\sigma} \right] \left[1 + \Delta e^{-z/\xi} \right]^2 \quad (13)$$

obtained using equation (12), taking into account equa-

tion (8), and introducing $\Delta = (S_0 - S_b)/S_b$. Notice that in the hypothesis of perfect nematic order, the elastic constant parameter, L , is nothing other than equation (8). Since for T close to T_c , $\sigma \ll \xi$, equation (13) is equivalent to

$$k(z) = k_b(1 + \Delta e^{-z/\xi})^2. \quad (14)$$

It follows that the elastic contribution to the anisotropic part of the anchoring energy is given by

$$\frac{1}{W_{\text{elast}}} = \frac{1}{k_b} \int_0^\infty \frac{(1 + \Delta e^{-z/\xi})^2 - 1}{(1 + \Delta e^{-z/\xi})^2} dz. \quad (15)$$

In the limit of $\Delta \ll 1$, which implies S_0 not very different from S_b , from (15) we obtain

$$\frac{1}{W_{\text{elast}}} = 2\Delta \frac{\xi}{k_b}. \quad (16)$$

By assuming $\Delta = 0.3$, and $S_b = 0.5$, which implies $S_0 - S_b = 0.15$, one obtains for the extrapolation length associated with this elastic term, $L_{\text{elast}} \simeq \xi$, i.e. in the macroscopic range, as experimentally observed [22, 23].

The total extrapolation length is the sum of the different contributions analysed above. Hence, it is given by

$$L_T = L_u + L_{\text{elast}}, \quad (17)$$

where

$$L_u = \frac{k_b}{W_u} = \frac{k_b}{W_{eu} + W_{iu}}, \quad (18)$$

and

$$L_{\text{elast}} = \frac{k_b}{W_\sigma} + \frac{k_b}{W_\xi}. \quad (19)$$

Consequently, the total extrapolation length can be rewritten as

$$L_T = \frac{k_b}{W_{eu} + W_{iu}} + \frac{k_b}{W_\sigma} + \frac{k_b}{W_\xi} \simeq \frac{k_b}{W_\xi}. \quad (20)$$

This simple result shows that the weak anchoring is mainly due to the spatial variation of the scalar order parameter.

5. Conclusions

We have considered a semi-microscopic approach based on the Maier–Saupe approximation to analyse the contributions to the intrinsic part of the anisotropic surface energy. Particular attention has been devoted to the effect of the spatial variation of the elastic constants on the surface energy. The main conclusions of our analysis can be summarized as follows:

- (1) Due to the spatial variation of the elastic constants, there is an intrinsic contribution to the

anisotropic surface energy. The extrapolation length connected to this surface energy is found to be of the order of the thickness of the surface layer over which the elastic constants change, when perfect nematic order is supposed. It is of the order of 70 Å for normal nematics;

- (2) When the spatial variation of the scalar order parameter is taken into account, there is an intrinsic elastic contribution whose extrapolation length is found to be of the order of the coherence length in the NLC phase. It is in the macroscopic range and it is of the same order as the extrapolation length experimentally detected ($\approx 0.1-0.5 \mu\text{m}$).

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