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Influence of spatial inhomogeneities on the Fréedericksz threshold

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By analyzing the Fréedericksz transition induced by an external magnetic field on a nematic liquid crystal, we determine the elastic contribution to the anisotropic part of the anchoring energy. Our result is in good agreement with the one obtained by other groups for the same problem. In the simple case in which the elastic constants change in a surface layer whose thickness is very small with respect to the thickness of the sample, our analysis shows that the extrapolation length of elastic origin is of the order of the thickness of the surface layer. The influence of the spatial variation of the diamagnetic anisotropy is also analyzed. It is shown that the contribution to the surface energy, arising from this spatial variation, is negligible.

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Let us consider a nematic liquid crystal (NLC) slab of thickness d. The surface anchoring energy is supposed strong and the easy direction homeotropic [1]. In the presence of an external field $\vec{H}$ parallel to the bounding walls, the bulk free energy density is [1]

$$f_b = \frac{1}{2}k\,\phi'^2 - \frac{1}{2}\chi_a H^2 \sin^2\phi, \qquad (1)$$

where the first term on the right-hand side is the elastic contribution and the second one is connected with the magnetic anisotropy. ϕ is the tilt angle defined by $\phi = \arccos(\vec{n}\cdot\vec{z})$, where $\vec{n}$ is the NLC director and the z axis is normal to the boundaries. k and χ_a are the Frank elastic constant and the diamagnetic anisotropy, respectively, and $\phi' = d\phi/dz$. The total free energy, per unit surface, of the sample under consideration is given by [1]

$$F = \int_{-d/2}^{d/2} \left[\tfrac{1}{2}k\,\phi'^2 - \tfrac{1}{2}\chi_a H^2 \sin^2\phi\right] dz. \qquad (2)$$

By minimizing (2) it is possible to obtain the profile $\phi = \phi(z;H)$ and the critical field for the Fréedericksz transition H_C [2]. This critical field is defined by the condition that for $H < H_C$, $\phi \equiv 0$, $\forall z \in (-d/2, d/2)$, minimizes F given by (2). This effect has been important in the past because the first experimental determinations of the Frank elastic constants have been done by analyzing the threshold field in different geometries. A simple calculation shows that if k and χ_a are position independent, H_C is given by [1]

$$H_{C\infty} = \frac{\pi}{d}\sqrt{\frac{k}{\chi_a}}. \qquad (3)$$

In the case in which the surface anchoring energy is finite, instead of (2) it is necessary to minimize the quantity [3]

$$G = \int_{-d/2}^{d/2} [\tfrac{1}{2}k\,\phi'^2 - \tfrac{1}{2}\chi_a H^2 \sin^2\phi]\, dz + f_S(-d/2) + f_S(d/2), \qquad (4)$$

where $f_S(\pm d/2)$ takes into account the anisotropic part of the surface energy. In the Rapini-Papoular approximation, $f_S(\pm d/2) = W_\pm/2\ \sin^2\phi(\pm d/2)$, where $W_\pm$ are the surface anchoring strengths [3]. In the framework of a symmetric sample, $W_+ = W_- = W$ and (4) writes, taking into account that $\phi(z) = \phi(-z)$, as

$$G = \int_{-d/2}^{d/2} \left[\tfrac{1}{2}k\,\phi'^2 - \tfrac{1}{2}\chi_a H^2 \sin^2\phi\right] dz + W\sin^2\phi_S, \qquad (5)$$

where $\phi_S = \phi(\pm d/2)$. In this situation the analysis of the stability of the undeformed state shows that the critical field is given by [3]

$$\frac{H_C}{H_{C\infty}}\frac{d}{\pi L} = \tan\left(\frac{\pi H_C}{2H_{C\infty}}\right), \qquad (6)$$

known as Rapini-Papoular equation. In (6) $L = k/W$ is the extrapolation length and $H_{C\infty}$ is still given by (3). In the limit of relatively strong anchoring ($L \ll d$), (6) is well approximated by [3]

$$H_C = H_{C\infty}\left(1 - \frac{2L}{d}\right). \qquad (7)$$

Equation (6) holds in the hypothesis in which k and χ_a are position independent.

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Recent papers devoted to the evaluation of the elastic constants by means of semimicroscopic models show that, actually, the elastic constants near the bounding walls are expected to be position dependent [4–7]. The surface layer over which the elastic constants are position dependent has a thickness of the order of several molecular dimensions. Long ago, Mada [8] suggested that the $k(z)$ dependence may be macroscopically interpreted as a weak anchoring, even if actually the surface energy is very large, i.e., the anchoring is strong. Despite the fact that the analysis performed by Mada was not completely correct, the idea was physically sound [9]. More recently, Yokoyama *et al.* [10], Faetti [11], Barbero and Durand [12], and Alexe-Ionescu *et al.* [13] have analyzed in what manner it is possible to define an effective anchoring energy connected to the spatial variation of the elastic constants. By means of a rather complex analysis they show that the effective anchoring energy is connected to the $k(z)$ dependence by [10–13]

$$\frac{1}{W} = \rho \left\langle \frac{k_b - k(z)}{k_b k(z)} \right\rangle = \int_0^\infty \frac{k_b - k(z)}{k_b k(z)}\, dz, \tag{8}$$

where ρ is the thickness of the surface layer in which $k(z)$ changes and k_b is the bulk value of the elastic constant. The spatial variation of the elastic constant has two origins. The first one is due to the fact that the interaction volume is incomplete near the surface, in a layer whose thickness is of the order of the range of the intermolecular forces responsible for the nematic phase [4,5]. The second origin is connected with the fact that near a bounding wall there is a profile of scalar order parameter $S = S(z)$ [1]. The spatial variation of S takes place over a few coherence lengths ξ and S passes from the surface value, which depends on the NLC-substrate interaction and on the temperature, to the bulk value, which depends only on the temperature [1]. Since the elastic constants are, in a first approximation, proportional to S^2 [14], it follows that $S = S(z)$ implies $k = k(z)$. Of course if $S = S(z)$ not only the elastic constants are expected to be position dependent, but also the diamagnetic or dielectric anisotropy, which are proportional to S.

Now we want to rederive the effective anchoring energy (8) in a simple way by considering the Fréedericksz effect. We will suppose that the NLC is characterized by strong homeotropic anchoring, but $k = k(z)$ and $\chi_a = \chi_a(z)$. In this framework (2) needs to be rewritten as

$$F = \int_{-d/2}^{d/2} \left[\tfrac{1}{2}k(z)\,\phi'^2 - \tfrac{1}{2}\chi_a(z)H^2\sin^2\phi\right] dz, \tag{9}$$

where

$$k(z) = k_b - \delta k(z)\,, \quad \chi_a = \chi_{ab} - \delta\chi_a(z). \tag{10}$$

In (10) k_b and χ_{ab} are, respectively, the bulk values of the elastic constant and of the diamagnetic anisotropy. Both $\delta k(z)$ and $\delta\chi_a(z)$ take into account the spatial variations of $k(z)$ and $\chi_a(z)$. They are localized in two surface layers of thickness σ. This thickness coincides with ρ or ξ according to the fact that the incomplete interaction or the spatial variation of the scalar order parameter is the most important source for the $k(z)$ and $\chi_a(z)$ variations. Hence $\delta k(z) \neq 0$ and $\delta\chi_a(z) \neq 0$ for $z \in (-d/2, -d/2+\sigma)$ and $z \in (d/2-\sigma, d/2)$. For H close to H_C, $\phi \ll 1$, $\forall z \in (-d/2, d/2)$. By expanding $\phi(z)$ in Fourier series and retaining only the first harmonic we have

$$\phi(z) = \phi_0 \cos\left(\frac{\pi}{d}\,z\right), \tag{11}$$

since $\phi(\pm d/2)$=0 for the strong anchoring hypothesis. By substituting (11) into (9) one obtains

$$F = \frac{1}{2}{\phi_0}^2\left[\left(\frac{\pi}{d}\right)^2\int_{-d/2}^{d/2} k(z)\,\sin^2\left(\frac{\pi}{d}\,z\right)dz - H^2\int_{-d/2}^{d/2}\chi_a(z)\cos^2\left(\frac{\pi}{d}\,z\right)dz\right]. \tag{12}$$

From (12) in the case in which $k(z) = k_b$ and $\chi_a(z) = \chi_{ab}$ simple calculations give $F < 0$ for $H > H_{C\infty}$ defined by (3). In the present case the above-mentioned condition $F < 0$ gives

$$H_C = \frac{\pi}{d}\left[\frac{\int_{-d/2}^{d/2} k(z)\sin^2(\frac{\pi}{d}\,z)dz}{\int_{-d/2}^{d/2}\chi_a(z)\cos^2(\frac{\pi}{d}\,z)dz}\right]^{1/2}, \tag{13}$$

for the threshold field. If we now consider (10), Eq. (13) can be rewritten as

$$H_C = H_{C\infty}\left[\frac{1 - \frac{2}{d}\int_{-d/2}^{d/2}\frac{\delta k(z)}{k_b}\sin^2(\frac{\pi}{d}\,z)dz}{1 - \frac{2}{d}\int_{-d/2}^{d/2}\frac{\delta\chi_a(z)}{\chi_{ab}}\cos^2(\frac{\pi}{d}\,z)dz}\right]^{1/2}. \tag{14}$$

Since usually $\sigma \ll d$ and max $\mid \delta k(z) \mid$ is of the order of k_b and max $\mid \delta\chi_a(z) \mid$ is of the order of χ_{ab}, (14) is equivalent to

$$H_C = H_{C\infty}\left\{1 - \frac{1}{d}\int_{-d/2}^{d/2}\left[\frac{\delta k(z)}{k_b}\sin^2\left(\frac{\pi}{d}\,z\right) - \frac{\delta\chi_a(z)}{\chi_{ab}}\cos^2\left(\frac{\pi}{d}\,z\right)\right]dz\right\}. \tag{15}$$

By comparing (15) with (7) we derive that to a $k(z)$ and $\chi_a(z)$ dependence it is possible to associate an effective anchoring energy whose extrapolation length is given by

$$L = \frac{1}{2}\int_{-d/2}^{d/2}\left[\frac{\delta k(z)}{k_b}\sin^2\left(\frac{\pi}{d}\,z\right) - \frac{\delta\chi_a(z)}{\chi_{ab}}\cos^2\left(\frac{\pi}{d}\,z\right)\right]dz. \tag{16}$$

Since $\delta k(z)$ is different from zero only in the two layers $(-d/2, -d/2+\sigma)$ and $(d/2-\sigma, d/2)$, $\cos^2(\frac{\pi}{d}z)$ is practically zero in the case in which $\sigma \ll d$. Consequently, from (16) one derives that

$$L \simeq \frac{1}{2}\int_{-d/2}^{d/2}\frac{\delta k(z)}{k_b}\sin^2\left(\frac{\pi}{d}\,z\right)dz. \tag{17}$$

This means that $\chi_a(z)$ does not contribute in a significant manner to the effective extrapolation length, or to the effective anchoring energy. From (17) the effective anchoring energy is found to be

$$\frac{1}{W} = \int_{-d/2}^{d/2} \frac{\delta k(z)}{{k_b}^2} \sin^2\left(\frac{\pi}{d} z\right) dz. \tag{18}$$

Since $\sigma \ll d$, (17) is equivalent to

$$L \simeq \sigma \left\langle \frac{\delta k}{k_b} \right\rangle_\sigma = \int_{-d/2}^{-d/2+\sigma} \frac{\delta k(z)}{k_b} dz. \tag{19}$$

In the limit $\sigma \ll d$, L is an intrinsic property of the NLC, independent of the thickness of the sample. For a rough estimation of (19) we can assume for $\delta k(z)$ an exponential behavior of amplitude $k_b/2$ [4–6] and relaxation length σ. In this case, from (19) we obtain

$$L \simeq \sigma, \tag{20}$$

which is consistent with the estimation of the same parameter obtained in [10–13] in a different manner.

However, there is a difference between the result obtained by us and the previous one reported in [10–13]. Formula (19) is approximated in the sense that k_b appears in the denominator. On the contrary, in the one obtained by means of (8), which is

$$L = \int_{-d/2}^{-d/2+\sigma} \frac{\delta k(z)}{k(z)} dz, \tag{21}$$

$k(z)$ is present. This implies that (19) is a good approximation of (21) only if $\delta k(z)$ is small with respect to k_b. In the opposite case in which $\delta k/k_b \sim 1$ the difference between (19) and (21) could be important. In this situation the equivalent anchoring energy, which is possible to define by means of the Fréederickz transition, no longer corresponds to the one usually defined according to Gibbs theory of interfaces [10–13].

However, if $k = k(z)$ due to the spatial dependence of the scalar order parameter S, a simple calculation shows that

$$\frac{\delta k(z)}{k_b} = 1 - \left(\frac{S(z)}{S_b}\right)^2 \simeq 1 - \left(\frac{S_s}{S_b}\right)^2, \tag{22}$$

where S_s and S_b are the surface and bulk values of the scalar order parameter. Usually S_s is not very different from S_b [15], and hence $\delta k/k_b \ll 1$. This means that, at least in this case our model works well.

In conclusion we can stress the main results of our paper. By considering the well known Fréedericksz effect we have shown that to a spatial variation of the elastic constants it is possible to associate an effective anchoring energy, even if the true anchoring energy is strong. The result obtained by us is in agreement with the one obtained by other authors in a more complicated manner. We have shown, furthermore, that in the case in which the thickness of the surface layer σ is very small with respect to d, the spatial variation of the diamagnetic anisotropy does not play an important role in the effective surface energy.

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