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Azimuthal anchoring energy of a nematic liquid crystal at a grooved interface

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The azimuthal anchoring of a nematic liquid crystal at a grooved interface is usually explained in terms of the well-known Berreman model. Recent experimental results, however, suggest that the original Berreman model must be modified in order to account for the presence of a reduced (or increased) order at the surface. A further important parameter, assumed to be infinite in the Berreman model, is the polar anchoring energy. In this paper we investigate how finite polar anchoring and the reduced (or increased) surface order affect the azimuthal anchoring, and we propose a more general expression for the azimuthal anchoring energy at a grooved interface. The main result of this paper is that the finite polar anchoring can lead to an important contribution to the azimuthal anchoring, while the effect of surface order can be usually neglected except in the case where the isotropic phase wets the substrate.

In recent years there has been a growing interest in the interfacial properties of liquid crystals (LC).[1,2] The interface is characterized by an excess of free energy per unit surface area γ which depends on the surface orientation of the director $\mathbf{n}$. γ is minimized when the director is aligned along an easy axis defined by the two angles θ_0 and ϕ_0 (see Fig. 1) and it can be written as

$$\gamma \equiv \gamma(\theta_0,\phi_0) + W(\theta-\theta_0,\phi-\phi_0) , \tag{1}$$

where θ and ϕ are the director polar and azimuthal angles shown in Fig. 1 and $W(\theta-\theta_0,\phi-\phi_0)$ is a positive function termed the "anchoring energy." If θ is kept equal to θ_0, the anchoring energy becomes a function of ϕ only:

$$W \equiv W_a(\phi-\phi_0) . \tag{2}$$

In this case W is named "*azimuthal*" anchoring energy. On the other hand, if $\phi=\phi_0$, one obtains

$$W \equiv W_p(\theta-\theta_0) \tag{3}$$

which is the "*polar*" anchoring energy.

At the interface between a nematic LC and a planar isotropic medium, the symmetry of the system requires the azimuthal anchoring energy to vanish $[W_a(\phi-\phi_0)=0]$. This is not the case when the interface exhibits a grooved structure as schematically shown in Fig. 2. This kind of interface can be obtained by "rubbing" of the surface[3] or by oblique evaporation of a thin SiO film.[4] Some years ago Berreman[5] proposed a simple model to explain the azimuthal anchoring of a nematic LC at a grooved interface. The basic assumptions of this model are the following.

(i) The director at the surface is strongly forced to lie parallel to the surface (infinite polar anchoring energy).

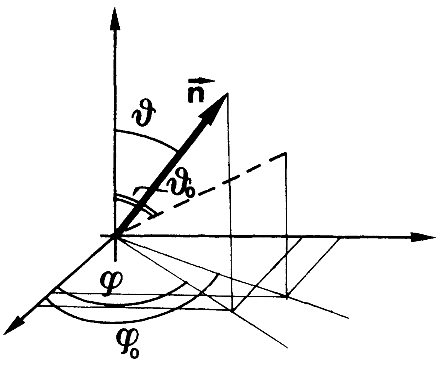
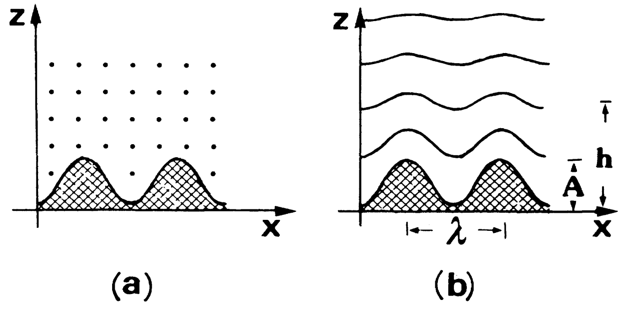


FIG. 1. Geometrical parameters defining the director orientation at the interface between a nematic LC and a different isotropic medium. The interface is assumed to coincide with the x-y plane. θ and φ are the polar and azimuthal angles of the director $\mathbf{n}$, respectively. θ_0 and φ_0 are the polar and azimuthal angles corresponding to the easy axis (dashed line).



(a) (b)

FIG. 2. Schematic geometry of a grooved nematic-solid interface. The grooves are assumed to be parallel to the y axis and to have a sine profile. A and λ are the amplitude and the wavelength of the grooves, respectively. h is the characteristic length of the director distortion. (a) Equilibrium director orientation near the interface when the surface director orientation is parallel to the y axis. Points indicate that the director is everywhere parallel to the y axis. (b) Equilibrium director arrangement when the surface director orientation lies in the x-z plane.

(ii) The elastic constants of the nematic LC near the surface have the same value as in the bulk.

Both these assumptions might not be satisfied in many practical cases. For example, there is strong circumstantial evidence that the surface order parameter Q_S is lower (or higher) than the bulk value Q_B.[6–10] Therefore, the surface elastic constants, too, are different from the bulk ones because they scale approximately as the square power of the scalar order parameter. Dramatic consequences of the breakdown of assumption (ii) are expected when wetting of the surface by isotropic phase occurs.[11,12] Also assumption (i) turns out to be unvalidated in some important cases.[13]

In this paper we investigate how the Berreman expression for the azimuthal anchoring energy at a grooved interface must be modified if assumptions (i) and (ii) are released. According to Berreman,[5] we assume that the surface profile is given the simple form (see Fig. 2)

$$\xi(x)=A\sin\left[\frac{2\pi}{\lambda}x\right], \tag{4}$$

where A and λ are the amplitude and the wavelength of grooves, respectively.

The physical mechanism responsible for the azimuthal anchoring is schematically shown in Figs. 2(a) and 2(b). The polar anchoring is assumed to align the director parallel to the interface [$\theta_0=\pi/2$ in Eq. (3)]. If the director lies in the y-z plane ($\phi=\pi/2$), no director distortion occurs and thus the total free energy per unit surface area vanishes. On the contrary, if the director lies in the x-z plane ($\phi=0$), a director distortion occurs and the elastic free energy per unit surface area does not vanish. By making assumptions (i) and (ii) and by setting in Eq. (4) the elastic constants to be isotropic ($K_{ii}=K$, for $i=1,\ldots,3$) and $A/\lambda \ll 1$, Berreman obtained[5]

$$W_a(\phi)=W_a\sin^2\left[\phi-\frac{\pi}{2}\right], \tag{5}$$

where

$$W_a=\frac{2\pi^3A^2K}{\lambda^3} \tag{6}$$

is the azimuthal anchoring energy coefficient. Note that the major contribution to W_a comes from the thin distorted layer of thickness $h\sim\lambda/2\pi$ near the surface.

We now investigate how Eqs. (5) and (6) must be modified to take into account the finite value of the polar anchoring energy

$$W_p(\epsilon)=W_p\sin^2\epsilon, \tag{7}$$

where W_p is the polar anchoring energy coefficient and $\epsilon=\pi/2-\theta$ is the angle which the director makes with the surface [see Fig. 2(a)]. Let us name $\alpha(x,z)$ the angle between the director and the x axis. Therefore, the angle ϵ of Eq. (7) is given by

$$\epsilon(x)=\alpha\left[x,z=A\sin\left[\frac{2\pi x}{\lambda}\right]\right]-\arctan\left[\frac{2\pi}{\lambda}A\cos\left[\frac{2\pi}{\lambda}x\right]\right]. \tag{8}$$

In the same spirit of the Berreman calculation we assume $A\ll\lambda$ and we replace Eq. (8) with

$$\epsilon(x)\simeq\alpha(x,z=0)-\frac{2\pi}{\lambda}A\cos\left[\frac{2\pi}{\lambda}x\right]. \tag{9}$$

It is evident that $\epsilon(x)$ will never exceed the value $(2\pi/\lambda)A$ and thus $\epsilon(x)\ll 1$. At equilibrium the director orientation minimizes the total free energy

$$F\equiv\int_v\tfrac{1}{2}K\left[\left[\frac{\partial\alpha}{\partial x}\right]^2+\left[\frac{\partial\alpha}{\partial z}\right]^2\right]dV+\int_S W_p\sin^2\epsilon\,dS, \tag{10}$$

where the first term in the right-hand side of Eq. (10) corresponds to the bulk elastic free energy, while the second term corresponds to the surface free energy and differences among the three elastic constants are ignored. Minimization of Eq. (10) gives the Euler-Lagrange equation

$$\frac{\partial^2\alpha}{\partial x^2}+\frac{\partial^2\alpha}{\partial z^2}=0 \tag{11}$$

with the boundary condition (valid for $A\ll\lambda$)

$$K\left.\frac{\partial\alpha}{\partial z}\right|_{z=0}=W_p\sin(2\epsilon)\simeq 2W_p\epsilon. \tag{12}$$

Equations (11) and (12) admit the simple solution

$$\alpha(x,z)=\alpha_0\exp\left[-\frac{2\pi}{\lambda}z\right]\cos\left[\frac{2\pi}{\lambda}x\right], \tag{13}$$

where

$$\alpha_0=\frac{\dfrac{2\pi}{\lambda}A}{1+\dfrac{\pi K}{W_p\lambda}}. \tag{14}$$

For $W_p\gg\pi(K/\lambda)$ (strong polar anchoring), Eqs. (13) and (14) coincide with the Berreman result, i.e., $\alpha_0\sim 2\pi A/\lambda$. In the opposite case [$W_p\ll\pi(K/\lambda)$], $\alpha_0\sim 0$ and the director is almost uniformly oriented along the x axis. Note that the angle ϵ of Eq. (9) is always lower than $2\pi A/\lambda$ and thus the integrand in the second term of the right-hand side of Eq. (10) can be replaced by $W_p\epsilon^2$. The azimuthal anchoring coefficient corresponds to the excess of free energy per unit surface area

$$W_a=\int_0^\infty\tfrac{1}{2}K\left[\left[\frac{\partial\alpha}{\partial x}\right]^2+\left[\frac{\partial\alpha}{\partial z}\right]^2\right]dx+\frac{1}{\lambda}\int_0^\lambda W_p\epsilon^2dx. \tag{15}$$

By substituting $\alpha(x,z)$ and $\epsilon(x)$ of Eqs. (13) and (9) into Eq. (15) we obtain

$$W_a=\frac{2\pi^3A^2K}{\lambda^3}\left[\frac{1}{1+\frac{\pi K}{\lambda W_p}}\right] . \qquad (16)$$

Note that, for $W_p \gg (\pi/\lambda)K$, the major contribution to W_a comes from the elastic Berreman mechanism [first term in the right-hand side of Eq. (15)] and thus W_a coincides with the Berreman result of Eq. (6). On the contrary, for $W_p \ll \pi K/\lambda$, W_a is almost entirely due to the polar anchoring contribution and assumes the limiting value

$$W_a=\frac{2\pi^2A^2W_p}{\lambda^2} . \qquad (17)$$

In order to estimate the possible relevance of the polar anchoring contribution, we consider, for instance, the obliquely evaporated SiO-nematic interface which is known to exhibit a grooved structure [$A\sim 100$ Å and $\lambda\sim 300$ Å (Ref. 2)]. The polar anchoring coefficient at this interface for the nematic LC 5CB has been recently measured by Yokoyama *et al.*[13,14] They found $W_p\sim 0.05$ erg/cm^2 at 5° below the clearing temperature T_{Ni}, while $W_p\sim 0.005$ erg/cm^2 at the clearing point. By assuming $K\sim 4.10^{-7}$ dyn,[15] we found $\pi K/\lambda \sim 0.4$ erg/cm^2 and thus the condition $W_p \gg \pi K/\lambda$ is never fulfilled.

Now we briefly discuss the contribution of the surface order to the azimuthal anchoring energy. As already remarked, the elastic constant K scales approximately as the square power of the local scalar order parameter Q. On the other hand, the scalar order parameter changes within a thin layer of thickness δ near the interface ranging from the surface value Q_S to the bulk one Q_B. Therefore, the elastic constant, too, must change near the interface. A complete theory of the azimuthal anchoring should start from the minimization of the Landau–de Gennes free-energy density[16] and of the surface free energy.[11] This procedure, however, furnishes a set of differential equations which do not admit simple analytical solutions.

In most of the practical cases, however, the characteristic length δ is much lower than that of the orientational distortion $(h\sim\lambda/2\pi)$. Therefore, the elastic constant within the distorted layer assumes almost everywhere the bulk value K and thus Eq. (16) is substantially correct. This case $(\delta \ll h)$ is no doubt the most general one; in fact, the δ parameter is usually expected to be of the order of 10 Å.[11]

The only special case where the characteristic length δ becomes very large is when the isotropic phase wets the solid surface.[11] In this case, indeed, the δ length is known to diverge with a logarithmic law as the temperature approaches the clearing value T_{Ni}. Therefore there will exist a temperature range near T_{Ni} where Eq. (16) completely fails. Also in this case, however, a simple analytic expression for the azimuthal anchoring energy can be obtained if the temperature T is very close to the clearing value. In this regime, in fact, δ is much larger than h and the elastic constant within the distorted layer is almost coincident with the surface value K_S. Therefore, Eq. (16) still holds provided that the bulk elastic constant K is replaced by K_S. The surface elastic constant, in turn, is proportional to the square power of the surface order parameter which is known to vanish at the wetting transition.[11] Therefore, the azimuthal anchoring energy, too, is expected to vanish [see Eq. (16) where K is replaced by K_S]. A more detailed discussion of this effect was already given in Ref. 12 where experimental measurements of the azimuthal anchoring energy coefficient at the SiO-nematic interface of 5CB were reported.

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