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MACROSCOPIC MODEL FORMULAE DESCRIBING ANISOTROPIC ANCHORING OF NEMATIC LIQUID CRYSTALS ON SOLID SUBSTRATES

Formulae used for description of anchoring energy of nematic liquid crystal aligned on solid substrates are reviewed. They are based on macroscopic approach considering the concepts of the easy axis and of the anchoring strength parameters. Properties of the modified formula proposed in our earlier article are illustrated by exemplary plots which allows for comparison with other formulae. The modified formula describes the dependence of energy on the azimuthal and polar deviation of director from the easy axis and is valid qualitatively for deviation of any magnitude.

Keywords: nematics, anchoring strength, director alignment.

1. INTRODUCTION

Orienting influence of solid surfaces exerted on director is crucial for all applications of liquid crystals, e.g. in liquid crystal displays. Properties of liquid crystalline systems are usually studied in terms of continuum theory. In this approach, the anchoring is determined by the easy axis **e** and by the anchoring strength parameters. The easy axis indicates the preferable director orientation, i.e. the orientation adopted in the absence of any external torques. The anchoring strength parameters determine the surface energy density i.e. the anchoring energy per unit area of the surface, g_s. They represent the work necessary to deviate the director from the easy axis. Experiments indicate that the anchoring is anisotropic, which means that the work needed to rotate the director by an angle α around the normal to the substrate is smaller than the work necessary to deviate it from the surface by the same angle. The anchoring energy gives

important contribution to the free energy of a liquid crystal system and should be taken into account during calculations concerning elastic deformations of such systems. For this reasons, the macroscopic models describing the anisotropic dependence of anchoring energy on the director deviation from the easy axis are required. The most popular are the approaches which stem from the famous paper by Rapini and Papoular [1] in which the formula for the energy due to director deviation from the planar orientation was proposed. Various forms of this formula are used [2-11], for example

$$g_s = -\frac{1}{2} W_\theta \cos^2 \theta \tag{1}$$

where W_θ is the anchoring strength parameter and θ is the angle between the director $\mathbf{n}$ and the easy axis lying on the surface. (The anchoring energy is determined with accuracy to arbitrary constant. Here and in the following the formulae predict the negative anchoring energy with maximum equal to zero.) This formula is suitable for deformation in which the director remains in the plane perpendicular to the surface. Analogous formula

$$g_s = -\frac{1}{2} W_\phi \cos^2 \phi \tag{2}$$

corresponds to director lying in the plane of the surface and rotated around the normal to the surface by an angle ϕ from the easy axis. Both formulae can be written in a more general form suitable if the orientation of the easy axis is determined by the angle θ_s (between the plane of the surface, *xy*, and the easy axis $\mathbf{e}$)

$$g_s = -\frac{1}{2} W_\theta \cos^2 (\theta - \theta_s) \tag{3}$$

or by the angle ϕ_s (between the axis *x* and the projection of $\mathbf{e}$ on the plane *xy*)

$$g_s = -\frac{1}{2} W_\phi \cos^2 (\phi - \phi_s). \tag{4}$$

The angles which describe the director orientation are defined in analogous way. The angle θ is measured between the *xy* plane and the director $\mathbf{n}$ while the angle ϕ is between the *x* axis and the projection of $\mathbf{n}$ on the plane *xy*.

There are situations in which the director adopts orientation determined by $\theta \neq \theta_s$ and simultaneously by $\phi \neq \phi_s$. Then the anchoring energy can be expressed by the formula

$$g_s = -\frac{1}{2} W (\mathbf{n} \cdot \mathbf{e})^2. \tag{5}$$

However, this formula does not take into account anchoring anisotropy i.e. all the directions of deviation are equivalent.

    Anchoring anisotropy manifests itself by the difference between W_θ and W_ϕ. Experiments show that W_θ is even ten times larger than W_ϕ. In order to describe the anisotropy, the sum of formulae (3) and (4) is often used, [12]

$$g_s = -\frac{1}{2} W_\theta \cos^2(\theta - \theta_s) - \frac{1}{2} W_\phi \cos^2(\phi - \phi_s). \qquad (6)$$

    Formula (6) is qualitatively suitable for small deviations from planar alignment, however it is inappropriate if the director is oriented homeotropically ($\theta = \pi/2$), since it involves unreasonable dependence on the azimuthal angle ϕ. An example is shown in Fig. 1 where the energy needed for director deviation from the planarly aligned easy axis $\mathbf{e} = [1,0,0]$ is plotted as a function of the azimuthal angle ϕ for several values of the polar angle θ. The anisotropy is determined by adoption that $W_\theta = 5 W_\phi$. It is evident that for homeotropic director orientation, $\theta = \pi/2$, the anchoring energy density g_s depends on ϕ.
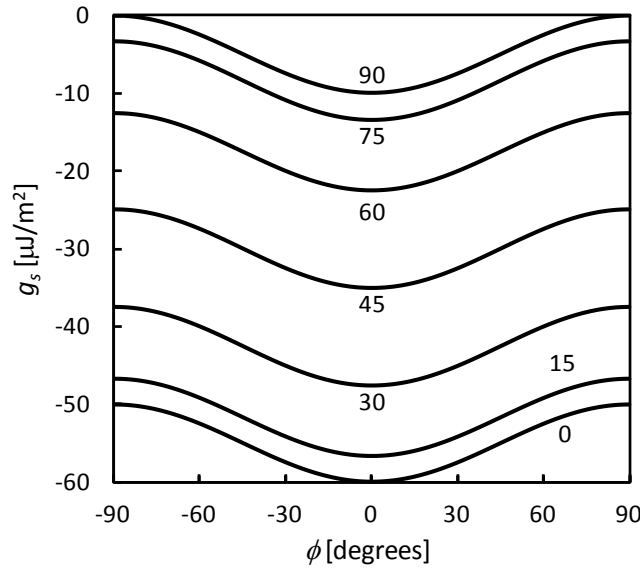

Fig. 1. Anchoring energy density g_s calculated by use of Eq. (6) as a function of the azimuthal angle ϕ for several values of the angle θ (in degrees) indicated at the curves. Planar alignment; $\mathbf{e} = [1,0,0]$, $W_\theta = 10^{-4}$ J/m^2, $W_\phi = 2 \cdot 10^{-5}$ J/m^2

    The formulae of Rapini-Papoular type were proposed to be replaced by other expressions.
    The elliptic sine was adopted for the case of homeotropic alignment [13]. According to the convention adopted here, the anchoring energy can be

expressed as

$$g_s = -\frac{1}{2}W_\theta \text{sn}^2(\theta - \theta_s, k) \qquad (7)$$

This function predicts a very sharp minimum of the surface anchoring for small deviations from the easy axis. The width of the corresponding potential energy well can be controlled by the choice of parameter k.

A generalized anchoring energy formula based on a spherical harmonic expansion was proposed in in the form

$$g_s = W_\xi(\mathbf{n}\cdot\boldsymbol{\xi})^2 + W_\eta(\mathbf{n}\cdot\boldsymbol{\eta})^2 \qquad (8)$$

where versors $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ and $\mathbf{e}$ create an orthonormal vector triplet [14]. Its orientation with respect to the surface determines the anisotropy of the aligning properties of the substrate. Equation (8) implies the presence of surface-induced nematic biaxiality. The parameter W_ξ concerns the deviation of director from the easy axis in the $\mathbf{e},\boldsymbol{\xi}$ plane, whereas W_η describes the deviation in the $\mathbf{e},\boldsymbol{\eta}$ plane. This formula is suitable for the homeotropic surface with in-plane anisotropy.

2. MODIFIED FORMULA FOR ANCHORING ENERGY

In order to avoid the disadvantage of Eq. (6) and to retain simultaneously the possibility of description of arbitrary deviations, a modified macroscopic model of anisotropic anchoring was proposed in our previous article [15]. It is expressed by the formula

$$g_s = \frac{1}{2}\left[W_\varphi \cos^2(\theta - \theta_s) + W_\theta \sin^2(\theta - \theta_s)\right]\left[1 - (\mathbf{ne})^2\right] - \frac{1}{2}W_\theta. \qquad (9)$$

Here, the last term was added for convenience in order to obtain the range of energy comparable with the ranges obtained by previous formulae. The proposed model has proper qualitative features and can be used for all kinds of deformations of director adjacent to the solid substrate, e.g. for the twisted nematic cells. In the present paper we give examples which allow to compare it with other formulae.

Figure 2 presents the predictions of Eq. (9) for the same planar alignment of the easy axis, $\mathbf{e} = [1,0,0]$, and for the same anchoring strengths as those used in Eq. (6) and shown in Fig. 1. For homeotropic director orientation, $\theta = \pi/2$, the energy density g_s is independent of ϕ. Figures 3-5 illustrate the $g_s(\theta,\phi)$ function for planar, oblique and homeotropic orientations of the easy axis. In the case of planar alignment, (Fig. 3) the stable equilibrium orientation due to global minimum equal to $-W_\theta/2$ occurs for $\theta_s = 0°$ and $\phi_s = 0°$. The work necessary to rotate director by 90° around the normal to the surface is $W_\phi/2$ and the work
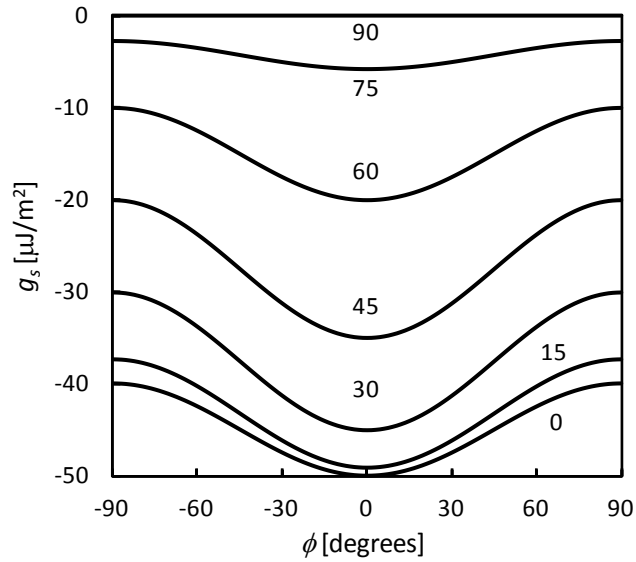
Fig. 2. Anchoring energy density g_s calculated by use of Eq. (9) as a function of the azimuthal angle ϕ for several values of the angles θ (in degrees) indicated at the curves. Planar alignment; $\mathbf{e} = [1,0,0]$, $W_\theta = 10^{-4}$ J/m^2, $W_\phi = 2 \cdot 10^{-5}$ J/m^2
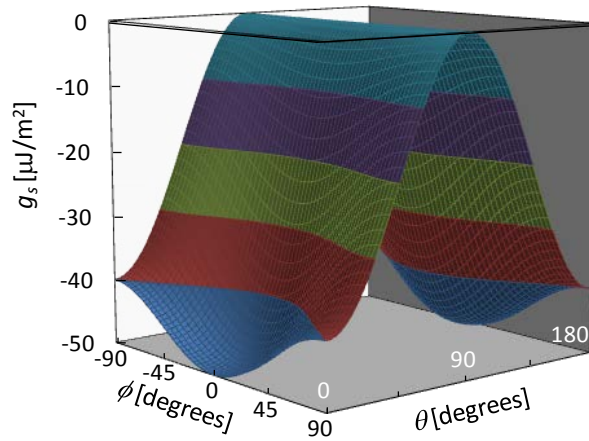

Fig. 3. Anchoring energy density g_s calculated by use of Eq. (9) as a function of the angles θ and ϕ. Planar alignment, $\theta_s = 0°$, $\phi_s = 0°$, $\mathbf{e} = [1,0,0]$, $W_\theta = 10^{-4}$ J/m^2, $W_\phi = 2 \cdot 10^{-5}$ J/m^2
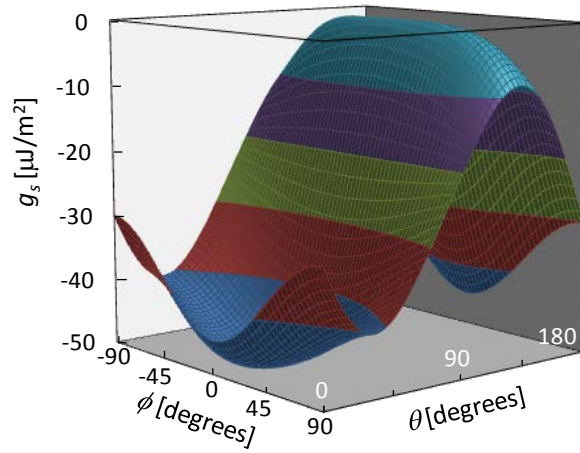
Fig. 4. Anchoring energy density g_s calculated by use of Eq. (9) as a function of the angles θ and ϕ. Oblique alignment, $\theta_s = 30°$, $\phi_s = 0°$; $W_\theta = 10^{-4}$ J/m^2, $W_\phi = 2\cdot10^{-5}$ J/m^2
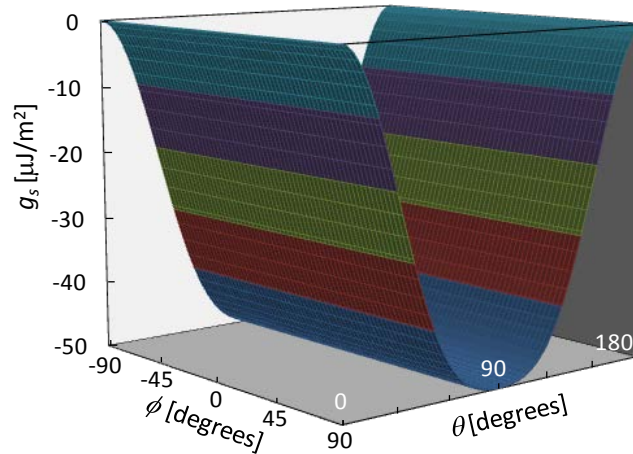

Fig. 5. Anchoring energy density g_s calculated by use of Eq. (9) as a function of the angles θ and ϕ. Homeotropic alignment, $\theta_s = 90°$, $\phi_s = 0°$; $\mathbf{e} = [0,0,1]$, $W_\theta = 10^{-4}$ J/m^2, $W_\phi = 2\cdot10^{-5}$ J/m^2

needed to deviate director by 90° from the plane *xy* is $W_\theta/2$. The unstable equilibrium corresponds to the homeotropic director orientation.

In the example of oblique alignment, (Fig. 4), determined by $\theta_s = 30°$ and $\phi_s = 0°$, the stable equilibrium due to global minimum $-W_\theta/2$ occurs. The homeotropic orientation is not due to any equilibrium. Maximum corresponds to orientation perpendicular to the easy axis. The work necessary to achieve the planar orientation depends on the angle ϕ.

In the case of homeotropic orientation of the easy axis, (Fig. 5), only the angle θ is of importance. Deviation by some angle from **e** requires the work which does not depend on direction of deviation i.e. is independent of the angle ϕ. The planar director orientation, $\theta = 0°$, corresponds to an unstable equilibrium.

To summarize, we considered the formula (Eq. (9)), proposed in our previous article [15] which describes the model of anisotropic anchoring of nematic liquid crystal on solid substrates. The formula allows to avoid the disadvantage of Eq. (6) and yields qualitatively valid description of polar and azimuthal anchoring. Properties of the proposed model were illustrated by plots presented for three particular orientations of easy axis.

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MAKROSKOPOWE MODELE ANIZOTROPOWEGO KOTWICZENIA NEMATYCZNYCH CIEKŁYCH KRYSZTAŁÓW NA POWIERZCHNIACH CIAŁ STAŁYCH

Streszczenie

Artykuł zawiera przegląd wzorów stosowanych do opisu energii kotwiczenia ciekłych kryształów nematycznych na powierzchniach ciał stałych. Wywodzą się one z makroskopowego podejścia wykorzystującego pojęcie osi łatwej i energetyczne parametry opisujące oddziaływanie ciekłego kryształu z podłożem. Opisano właściwości zaproponowanego we wcześniejszym artykule zmodyfikowanego wzoru, uwzględniającego anizotropię oddziaływania powierzchniowego, który ujmuje zależność energii kotwiczenia od odchylenia direktora od osi łatwej i jest słuszny jakościowo dla odchylenia o dowolnej wielkości. Zilustrowano go przykładowymi wykresami pozwalającymi na porównanie z innymi wzorami.