

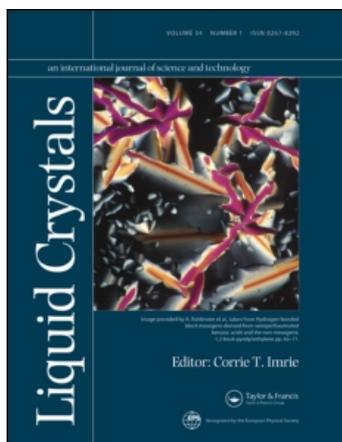
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## Liquid Crystals

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## Surface disclination cores in the $B_2$ phase of bent-shaped molecules described by the Peierls–Nabarro model

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The Peierls–Nabarro model, originally proposed to describe dislocation core in solids, is used to model core structures of  $2\pi$ - and  $\pi$ -surface disclinations in the  $B_2$  phase of bent-shaped molecules. Structures of disclination cores are determined by surface anchoring. Core parameters as core widths (and positions of two partial  $\pi$ -disclinations as parts comprising  $2\pi$ -disclination) are estimated using surface anchoring energy. Disclination core widths are usually narrow for strong anchoring. In such a case they are barely observable; nevertheless, they can exist.

**Keywords:**  $B_2$  phase; bent-shaped molecules; surface disclinations; Peierls–Nabarro model

### 1. Introduction

In liquid crystals composed of bent-shaped molecules, rich varieties of textures are observed. The phase called  $B_2$  has been extensively investigated. Basically, four possible polar structures in the  $B_2$  phase, i.e. two racemic and two homochiral structures, have been identified (1). In the following we will be interested in homochiral phases only.

Observations of textures under an external electric field revealed that the  $B_2$  phase occurs in chiral phases either as an anticlinic antiferroelectric smectic structure (denoted as  $SmC_A P_A$ ) or as a synclinic ferroelectric smectic ( $SmC_S P_F$ ) structure (see e.g. (1–3)). The ( $SmC_S P_F$ ) structure can occur in domains near surfaces with strong polar anchoring.

When a sample is subjected to an external electric field,  $2\pi$  or  $\pi$ -walls can be created in the sample bulk (4). Note that  $2\pi$ -walls do not lead to a change of chirality, while  $\pi$ -walls do change it. When the field is switched off, walls are destabilised and eventually collapse to surface lines, surface disclinations, stabilised by surface anchoring. One may expect that these surface lines are either  $2\pi$ - or  $\pi$ -disclinations. In both cases, far from the dislocation line, molecules of liquid crystal keep their orientations by polar surface anchoring. For  $2\pi$ - disclinations the director rotates by  $2\pi$  with the director changes being localised just near the surface. Surface  $2\pi$ -disclinations are very frequently observed in the chiral smectic C liquid crystal with elongated molecules (5).

The other possibility of surface defects in  $B_2$  phases is  $\pi$ -surface disclination, which mediates synclinic structures of opposite chirality rotated by an angle  $\pi$ . These synclinic structures have the same optical contrast for the  $\pi/4$ -tilt angle (4).

In the present work, inspired by observations in (4, 6), we will propose:

- (i) models of  $2\pi$ - and  $\pi$ - surface disclinations using the Peierls–Nabarro (PN) model originally developed for dislocations in solids;
- (ii) an estimation of model parameters of surface disclination cores deduced from surface anchoring energies.

### 2. Energy considerations in $B_2$ model structures

In this section, different energy contributions to the total energy of the  $B_2$  structures are outlined. First, a general description of molecular orientation is given in Section 2.1. Different terms comprising the surface anchoring energy are discussed in Section 2.2. An approximate elastic free energy density is introduced in the Section 2.3.

#### 2.1 Molecular Orientation in Layers

The orientation of bent-shaped molecules in layers can be described by three Eulerian angles  $\theta$ ,  $\phi$  and  $\psi$  (7). These angles are defined in the coordinate system with  $x$  and  $y$  axes parallel to the smectic layers and the  $z$ -axis normal to the plane of the smectic layers (Figures 1 and 2). Angle  $\theta$  describes the tilt of a long molecular axis, which coincides with molecular unit director  $\vec{n}$ . The azimuthal angle  $\phi$  characterises the director rotation around the  $z$ -axis. The unit vector of the molecular dipole moment of a bent-shaped

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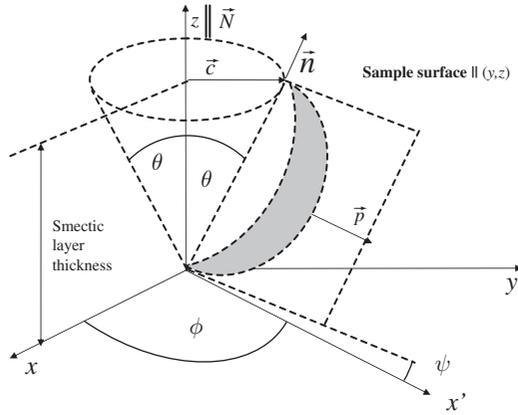


Figure 1. The coordinate system with the bent-shaped molecule. The plane of the bent-shaped molecule (which is represented by a gray banana-like object) is defined by director  $\vec{n}$  and vector  $\vec{p}$  parallel to spontaneous polarisation. The  $\vec{c}$ -director is the projection of  $\vec{n}$  onto the layer plane, the normal of which,  $\vec{N}$ , is parallel to the  $z$ -axis. Eulerian angles are defined using the coordinate system  $(x, y, z)$ : first, the plane of the molecule is tilted from the  $z$ -axis by an angle  $\theta$  (the angle  $\theta$  is the apex angle of a cone on the surface of which the director  $\vec{n}$  of a bent-shaped molecule is situated). Then the tilted molecular plane is rotated around the  $z$ -axis by an azimuthal angle  $\phi$  from the  $x$ -axis. This rotation transforms the  $x$ -axis to the  $x'$ -axis. Finally, the plane of the molecule is rotated around the director  $\vec{n}$  by an angle  $\psi$  from the  $x'$ -axis. The plane of the sample surface is the plane  $(y, z)$ . Smectic layers are perpendicular to the sample surface and thus parallel to the plane  $(x, z)$ .

molecule is denoted as  $\vec{p}$  perpendicular to  $\vec{n}$ . The plane containing the  $z$ -axis and director  $\vec{n}$  is called the tilt plane. The angle  $\psi$ , which describes the rotation of  $\vec{p}$ , is measured from this tilt plane. A detailed geometrical representation of the molecule is also given in Figure 1,

as shown in (8, 9). Sample surfaces are assumed to be perpendicular to the  $x$ -axis.

When we suppose no layer deformations, the molecular tilt angle is constant and molecular orientation depends on only two variable angles:  $\phi$  and  $\psi$ . Here the molecular orientation is determined by vectors  $\vec{n}$  and  $\vec{p}$  expressed in (7) in the form:

$$\vec{p} = (\cos \theta \cos \phi \cos \psi - \sin \phi \sin \psi, \cos \theta \sin \phi \cos \psi + \cos \phi \sin \psi, -\sin \theta \cos \psi), \quad (1)$$

$$\vec{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta).$$

With the molecular tilt angle  $\theta$  fixed, the director  $\vec{c} = (\cos \phi, \sin \phi, 0)$ , which is the projection of the director  $\vec{n}$  onto the  $(x, y)$ -plane of smectic layers, can be used to describe the molecular orientation in layers.

In order to describe geometrically an anticlinic antiferroelectric state of the  $B_2$  phase we use the bilayer continuous model proposed in (10, 11) for antiferroelectric liquid crystals with elongated molecules. Let us suppose that the molecular orientation is characterised by angles  $\phi_1$  and  $\psi_1$  in odd-numbered layers and  $\phi_2$  and  $\psi_2$  in even-numbered layers. We can then define vectors  $\vec{c}_1 = (\cos \phi_1, \sin \phi_1, 0)$ ,  $\vec{c}_2 = (\cos \phi_2, \sin \phi_2, 0)$  and  $\vec{p}_1$  and  $\vec{p}_2$  using expression (1) with angles  $\phi_1, \psi_1$  and  $\phi_2, \psi_2$ , respectively. According to Orihara and Ishibashi (10), let us introduce vectors:

$$\vec{c}_+ = (\vec{c}_1 + \vec{c}_2)/2 \text{ and } \vec{c}_- = (\vec{c}_1 - \vec{c}_2)/2, \quad (2a)$$

and

$$\vec{p}_+ = (\vec{p}_1 + \vec{p}_2)/2 \text{ and } \vec{p}_- = (\vec{p}_1 - \vec{p}_2)/2. \quad (2b)$$

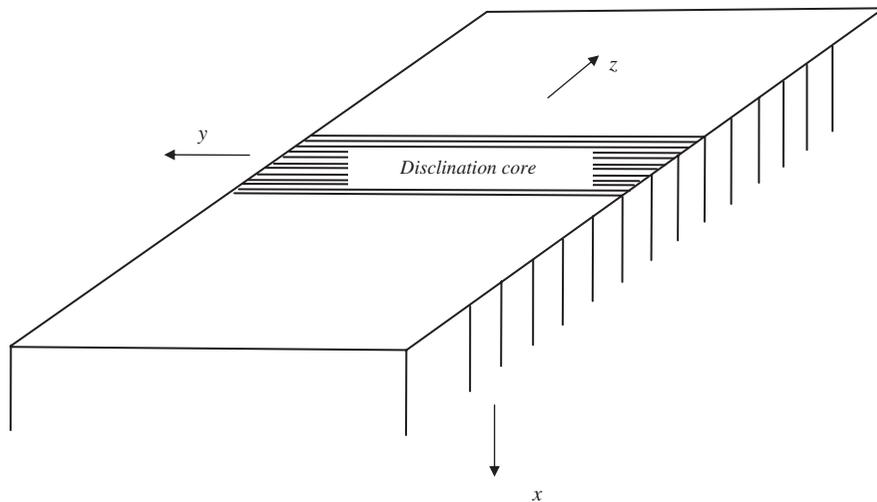


Figure 2. Surface disclination and the orientation of smectic layers. Disclination parallel to the  $y$ -axis is situated under the sample surface. The disclination core is spread on the surface along the  $z$ -axis. Smectic layers perpendicular to the sample surface  $(y, z)$  have the  $z$ -axis as the layer normal.

The combination of the above-defined vectors given by expressions (2) defines each of the synclinic or anticlinic, ferroelectric or antiferroelectric molecular structures (see also (8)). In the following, we assume the smectic layers to be perpendicular to the sample surfaces.

## 2.2 Surface anchoring energy

The anchoring of bent-shaped molecules to sample surfaces has already been discussed in (12). The possible molecular orientation on the surface was either flat or edge. As smectic layers are perpendicular to sample surfaces we expect the molecules to be attached to the surfaces by their edges.

The anchoring energy  $W_A$  can be expressed using (13):

$$W_A = -\gamma_1 (\vec{N}_S \cdot \vec{p}_+)^2 + \gamma_2 (\vec{N}_S \cdot \vec{p}_+)^2 - \gamma_3 (\vec{N}_S \cdot \vec{p}_-)^2 + \gamma_5 (\vec{N}_S \cdot \vec{c}_+)^2 + \gamma_6 (\vec{N}_S \cdot \vec{c}_-)^2. \quad (3)$$

In this expression, the external normal to the sample surface is denoted as  $\vec{N}_S$  (parallel or antiparallel to the  $x$ -axis) and parameters  $\gamma_1, \gamma_2$  and  $\gamma_3$  are the anchoring constants, which represent anchoring energies per unit surface.

The first term in (3) characterises the non-polar anchoring and it attains a minimal value for  $\vec{p}_+$  parallel or antiparallel to  $\vec{N}_S$ . The second term expresses the polar anchoring of molecules. Note that the bulk term  $\text{div } \vec{p}_+$  which can exist in the polar  $B_2$  phase (14, 15) can be transformed to a surface term which contributes to this second term in the surface anchoring energy (3). Let us suppose that the preferable orientation of  $\vec{p}_+$  points to the inside of the sample. This term then has the sign (+) in (3). The third term describes the antiferroelectric interaction of molecules with surfaces.

When polar ferroelectric anchoring dominates, parameters  $\gamma_1, \gamma_2$  and  $\gamma_3$  are expected to be positive and  $\gamma_1 + \gamma_2 > \gamma_3$  (9). Thus the antiferroelectric anchoring is unfavourable compared with the ferroelectric anchoring. On the other hand, when  $\gamma_1 + \gamma_2 \approx \gamma_3$  the ferroelectric anchoring does not stabilise the ferroelectric structure at the surfaces and antiferroelectric order from the bulk extends to the surface.

As shown in (12), other anchoring terms are possible which may prefer the plane of bent-shaped molecules to be either parallel or perpendicular to the surface. Such terms can be e.g.  $\gamma_4 (\vec{N}_S \cdot \vec{c}_+)$ ,  $\gamma_5 (\vec{N}_S \cdot \vec{c}_+)^2$  and  $\gamma_6 (\vec{N}_S \cdot \vec{c}_-)^2$ .

In the following we suppose that the polar surface anchoring is dominant, i.e.  $\gamma_2 \gg \gamma_1, \gamma_3$ , and is able to create a surface domain with a ferroelectric structure.

The term  $\gamma_4 (\vec{N}_S \cdot \vec{c}_+)$  has the tendency to orient director  $\vec{c}_+$  to be either parallel or antiparallel to the surface normal. However, for dominant polar anchoring the vector  $\vec{p}_+$  is oriented along  $\vec{N}_S$ , not the director  $\vec{c}_+$ . Thus we take  $\gamma_4 = 0$  and the anchoring energy  $W_A$  is then given in the form (3). When supposing  $\gamma_5 > 0$ ,  $\gamma_6 > 0$  the preferred anchoring of the  $\vec{c}$ -directors will be either synclinic or anticlinic with  $\vec{c}$ -directors parallel to surfaces.

## 2.3 Elastic energy of $B_2$ phase

Let layers of the  $B_2$  phase not be deformed so the tilt angle  $\theta$  is constant. In this case, bent-shaped molecules are described by the directors  $\vec{c}_1, \vec{c}_2$  and the polarisations  $\vec{p}_1, \vec{p}_2$ , respectively (9, 10). The molecular orientation in bilayers is described by the directors  $\vec{c}_1$  and  $\vec{c}_2$  as in the case of an antiferroelectric phase composed of elongated molecules. The orientation of directors in the smectic layer is determined by the azimuthal angles  $\phi_1$  and  $\phi_2$ . The polarisations  $\vec{p}_1$  and  $\vec{p}_2$  depend also on the angles  $\psi_1$  and  $\psi_2$ . All angles are functions of the variables  $x$  and  $z$ . The corresponding classic gradient energy can be constructed as in (8, 9) and considering (10, 11). In the synclinic ferroelectric structure we have  $\phi_1 = \phi_2 = \phi$  and  $\psi_1 = \psi_2 = \pi/2$ . The elastic free energy density can be written in the same form as that for chiral smectic C liquid crystals with elongated molecules:

$$f_d = \frac{K}{2} \left[ \left( \frac{\partial \phi}{\partial x} \right)^2 + \left( \frac{\partial \phi}{\partial z} - q_f \right)^2 \right], \quad (4)$$

with one elastic constant  $K$  for simplicity. The parameter  $q_f = 2\pi/p_f$  is connected with the pitch  $p_f$  of helical structures in ferroelectric phases. However, in the following we expect the structure to be unwound near the surface due to the anchoring. The form of (4) expects the wall or surface disclination to be parallel to the  $y$ -axis.

The equilibrium equation is then:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial z^2} = 0. \quad (5)$$

## 3. Surface disclination cores

In this section, structures of  $2\pi$ - and  $\pi$ - surface disclinations will be determined using a modified PN model. The PN model describes the disclination core spread on the sample surface where it is governed by the non-linear anchoring energy (3), while the bulk elasticity of the liquid crystal is approximated by the energy (4) (16, 17). We suppose that surface disclinations are parallel to the  $y$ -axis (Figure 2).

### 3.1 (2π)-surface disclination core

The surface disclination can be created, for example, from bulk 2π-twist disclination somehow pushed to the surface during a phase transition or by an electric field. The 2π-surface disclination may also originate from a wall stabilised by an external electric field and transformed to a surface line after the field is switched out.

As the core of the 2π-surface disclination is situated on the sample surface, we will deal with only one surface and we will assume that our sample is in fact a half-plane, for example a lower half-space ( $x < 0$ ).

Let the surface prefer a ferroelectric synclinic (SmC<sub>S</sub>P<sub>F</sub>) structure with  $\phi_1 = \phi_2 = \phi$ . Then the anchoring energy (4) on the surface at  $x = 0$  (with  $\vec{N}_S = (1, 0, 0)$ ) for the synclinic ferroelectric structure can be written as:

$$W_A = -\gamma_1 \sin^2 \phi - \gamma_2 \sin \phi + \gamma_5 \cos^2 \phi + (\gamma_1 + \gamma_2). \quad (6)$$

A constant term  $\gamma_1 + \gamma_2$  was added in (6) to identify the total minima of (6) at  $\phi = \frac{\pi}{2}, \frac{3\pi}{2}$  (synclinic order on the surface) with zero energy, i.e.  $W_{AMin} = 0$ . Energy (6) has a local minimum between two maxima.

The local minimum of (6) is situated at  $\phi = \frac{3\pi}{2}$  with the energy of  $W_{ALm} = 2\gamma_2$ . The maxima of  $W_A$  are at  $\phi = \frac{3\pi}{2} \pm \alpha$  with  $\cos \alpha = \frac{\gamma_2}{2(\gamma_1 + \gamma_5)}$ , i.e. the values of  $W_A$  at  $\phi = \frac{3\pi}{2} \pm \alpha$  are  $W_{AMax} = \frac{(2(\gamma_1 + \gamma_5) + \gamma_2)^2}{4(\gamma_1 + \gamma_5)}$ . Then the relation between energy of the maxima and local minimum

$$\frac{W_{AMax}}{W_{ALm}} = \frac{(2(\gamma_1 + \gamma_5) + \gamma_2)^2}{8\gamma_2(\gamma_1 + \gamma_5)} \geq 1,$$

is always satisfied.

The influence of the surface anchoring energy extends a thickness  $d$  towards the sample bulk, which is also the thickness of the ferroelectric domain under the surface. This thickness  $d$  can be estimated by comparing the anchoring energy (3) with the bulk energy of the antiferroelectric structure which is supposed to be preferable in the bulk:

$$w_{CMin}d + (W_{AMax} - W_{AMin}) \approx 0.$$

The parameter  $w_{CMin}$  is the minimum value of the energy density  $w_C$ . The energy  $w_C$  is the non-gradient part of the free energy density of liquid crystal which is usually used to describe structural transitions. In (9, 10) a special one-constant energy  $w_C$  was proposed, giving a minimal value  $w_{CMin} = -\beta_-/4$  for anticlinic antiferroelectric structures, while the ferroelectric synclinic structure was characterised by a maximal value  $w_{CMax} = 0$ .

Using the above relation the thickness  $d$  can be estimated as:

$$d \approx \frac{(2(\gamma_1 + \gamma_5) + \gamma_2)^2}{(\gamma_1 + \gamma_5)\beta_-}. \quad (7)$$

The core of the surface disclination in nematic liquid crystals was described by the PN model for the first time in (16, 17) and then applied to chiral smectic C liquid crystals in (5). The PN model can be used when the orientation of the director in the bulk of the liquid crystal satisfies Equation (5). Therefore we can also use the PN approach in our simplified model of the core structure of disclination in the SmC<sub>S</sub>P<sub>F</sub> phase.

Let the director on the surface situated at  $x = 0$  be described by the angle  $\varphi(z) = \phi(x = 0, z)$ . The derivative  $d\varphi(z)/dz$  is the so-called density of continuous distribution of infinitesimal disclinations spread along the  $z$ -axis (16). As the infinitesimal disclination has the strength  $d\varphi$ , then we have  $\int_{-\infty}^{+\infty} \frac{d\varphi(z)}{dz} dz = \Omega$  and  $\Omega = 2\pi$  or  $\pi$  is the total surface disclination strength (17).

As demonstrated in (16), the core structure of surface disclination is described by the PN equation in the form:

$$-\frac{dW_A}{d\varphi} = \frac{K}{\pi} \int_{-\infty}^{+\infty} \frac{d\varphi(z')}{dz'} \frac{dz'}{z - z'}. \quad (8)$$

The integral should be understood as the Cauchy principal value. The PN equation (8) is the balance between torques from all infinitesimal disclinations on the sample surface and the surface torque  $-\frac{dW_A}{d\varphi}$  due to the surface anchoring energy (3).

Equation (8) is the so-called Hilbert transformation of the density  $\frac{d\varphi(z)}{dz}$  giving the force law  $-\frac{dW_A}{d\varphi}$ . A more general method of construction of Hilbert pairs  $\frac{d\varphi(z)}{dz}$  and  $-\frac{dW_A}{d\varphi}$  is given in (18).

In analogy with (5) we propose the 2π-disclination core structure in the form composed of solutions corresponding to two π-disclinations:

$$\varphi(z) = \arctan \frac{z - z_o}{\xi} + \arctan \frac{z + z_o}{\xi} + \frac{3\pi}{2}. \quad (9)$$

The parameter  $\xi$  determines the disclination core width. Parameters  $\pm z_o$  are positions of both partial π-disclinations (5). The constant  $3\pi/2$  assures mapping of the interval  $z \in (-\infty, +\infty)$  onto the interval  $\varphi \in (\pi/2, 5\pi/2)$ . The density of infinitesimal disclinations  $\frac{d\varphi(z)}{dz}$  is positive. Another solution of Equation (8) can be obtained from Equation (9) by the transformation  $\varphi(z) \rightarrow (3\pi - \varphi(z))$ , which maps the interval  $z \in (-\infty, +\infty)$  onto the interval  $\varphi \in (5\pi/2, \pi/2)$ . The

solution  $(3\pi - \varphi(z))$  has the derivative  $d(3\pi - \varphi(z))/dz < 0$  and describes the  $(-2\pi)$ -disclination core structure.

The core energy of the  $2\pi$ -disclination described by the solution of Equation (9) (see for example (16)) does not depend on the form of the force law  $-dW_A/d\varphi$  and it can be written as:

$$E_{core} = 2\pi K. \quad (10)$$

Using the proposed solution (9), Equation (8) gives  $-dW_A/d\varphi$  as a function of  $z$ .

Then  $W_A$  can be found by integration:

$$W_A(z) = \int_{-\infty}^z dz' \frac{dW_A}{d\varphi(z')} \frac{d\varphi(z')}{dz'}, \quad (11)$$

with  $W_A(z) = 0$  at  $z \rightarrow -\infty$ , which corresponds to the surface energy minimum equal to zero at  $\phi = \frac{\pi}{2}$  in correspondence with Equation (9). This is the reason why also in Equation (6) the energy minima were fixed to zero for  $\phi = \frac{\pi}{2}$  and  $\frac{3\pi}{2}$ .

Using Equations (8) and (9) the energy  $W_A(\varphi(z))$  given by Equation (11) can be written as:

$$W_A(z) = \frac{K}{2} \left\{ \frac{\xi}{\xi^2 + (z - z_o)^2} + \frac{\xi}{\xi^2 + (z + z_o)^2} + \frac{1}{z_o} \left( \arctan \frac{z + z_o}{\xi} - \arctan \frac{z - z_o}{\xi} \right) \right\}. \quad (12)$$

Energy expression (12) can be numerically comparable with expression (6) with  $\varphi(z)$  inserted from (9), i.e.  $W_A(\varphi)|_{\varphi=\varphi(z)}$  in order to fix parameters  $z_o$  and  $\xi$ . The starting values of those parameters for numerical calculations can be determined tentatively from the positions of the local minimum and maxima.

The position of the anchoring energy minimum corresponds to  $\phi = \frac{3\pi}{2}$ , i.e.  $z = 0$  from Equation (9).

Equation (12) then leads to the relation:

$$\frac{2\gamma_2}{K} \xi = \frac{1}{1+t^2} + \frac{1}{t} \arctan t, \quad (13)$$

with the parameter  $t = z_o/\xi$ . As  $\gamma_2 > 0$ , we also have  $\xi > 0$ .

The  $z$ -coordinate of the position of the maximum follows from the condition  $dW_A(\varphi(z))/dz = 0$ , which gives two real roots  $z = \pm \sqrt{z_o^2 - \xi^2}$  as positions of two maxima. Then, for example for the positive root, we have the second condition in the form:

$$\begin{aligned} & \frac{(2(\gamma_1/K + \gamma_5/K) + \gamma_2/K)^2}{4(\gamma_1/K + \gamma_5/K)} \xi \\ &= \frac{1}{2t} \left( t + \arctan(t - \sqrt{t^2 - 1}) \right. \\ & \quad \left. + \arctan(t + \sqrt{t^2 - 1}) \right). \end{aligned} \quad (14)$$

The elimination of  $\xi$  gives a transcendental equation yielding a numerical solution of  $t$  depending on anchoring parameters  $\gamma_1$ ,  $\gamma_2$  and  $\gamma_6$ . The determined numerical value  $t$  gives the parameter  $\xi$  from Equation (14). Thus the estimated numerical values  $t$  and  $\xi$  can be used as starting values for their more exact numerical determination, minimising squares of the difference of surface anchoring energies (6) (with inserted (9)) and (12):

$$(W_A(\varphi(z)) - W_A(z))^2.$$

The proposed core structure (10) can be extended to the lower half-space as:

$$\phi(x, z) = -\arctan \frac{z - z_o}{x - \xi} - \arctan \frac{z + z_o}{x - \xi} + \frac{3\pi}{2}, \quad (15)$$

using the method of Cauchy integrals, which extends the function on the line boundary to the half-plane (17).

This solution, valid for the lower half-space, corresponds to two  $\pi$ -twist disclinations situated at  $z = \pm z_o$  and  $x = \xi$ . Singularity of the solution is in the upper half-plane and thus at the surface  $x = 0$ ; in the half-space  $x < 0$  there is no singularity.

A schematic drawing of the molecular distribution in the core of the  $2\pi$ -disclination spread on the sample surface along the  $z$ -axis is shown in Figure 3. In the figure, bent-shaped molecules are represented by projections onto the  $(x, z)$ -plane. They are rotating on the surface of a cone with the apex angle  $\theta$  shown in Figure 1. The vector  $\vec{p}$  characterising the molecular polarisation is tangential to the cone surface, i.e. the angle  $\psi$  is fixed as  $\psi = \pi/2$ .

### 3.2 ( $\pi$ )-surface disclination core

Another surface disclination can be realised when, at the surface, there is a line boundary between two synclinc ferroelectric domains of different chirality. This situation can be possible similarly to as in Section 3.1 when we deal with polar anchoring-preferring synclinc ferroelectric domains up to the thickness  $d$  given by expression (7) which are also able to overcome the internal barrier energy (19), at least for molecules adjacent to the sample surface. Note that this internal barrier energy keeps the molecular polarisation parallel to

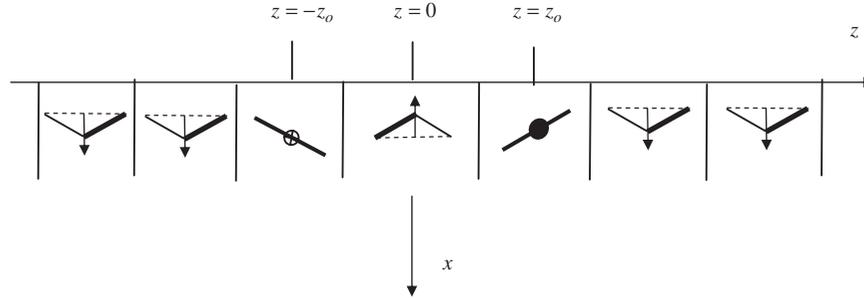


Figure 3. Schematic drawing of the director profile of  $2\pi$ -disclination core under the sample surface. Molecular orientation in neighbouring layers (having their normal parallel to the  $z$ -axis) is represented by triangles where the thicker line corresponds to the arm of the bent-shaped molecule inclined toward the observer. Dashed lines indicate the projection of the molecular director  $\vec{n}$  onto the plane of the figure. Molecular spontaneous polarisations are depicted by arrows. Symbols (•) or (×) denote polarisations pointing up or down (with respect to the  $(x, z)$ -plane), respectively. Molecules with those symbols are projected to the  $(x, z)$ -plane as lines. The disclination core is centred around  $z = 0$  where the molecular polarisation points up (i.e. towards the observer looking at the sample surface) while far from  $z = 0$  polarisation is oriented down. Both partial  $\pi$ -disclinations are centred near  $z = \pm z_0$ . In the scheme bent-shaped molecules rotate on the surface of the cone shown in Figure 1, keeping the molecular polarisation tangential to the surface of the cone. The figure presents the molecular projections onto the  $(x, z)$ -plane.

smectic layers during molecular rotation. When the surface polar anchoring is able to order dipole moments of liquid crystal molecules, the rotation of director  $\vec{c}$  is accompanied by simultaneous rotation of vector  $\vec{p}$ . For the ferroelectric order we have  $\phi_1 = \phi_2 = \phi$  and  $\psi_1 = \psi_2 = \psi$  where the angle  $\psi$  now varies. Then  $\vec{p}_+ = \vec{p}, \vec{p}_- = 0$  and  $\vec{c}_+ = \vec{c}, \vec{c}_- = 0$ .

Due to very strong polar anchoring we expect that the absolute value of projection of  $\vec{p}$  onto the surface normal, i.e.  $|\vec{N}_S \vec{p}|$ , will attain a maximal possible value during  $\vec{c}$ -director rotation given by the condition  $\partial |\vec{N}_S \vec{p}| / \partial \phi = 0$ . This last condition gives the relation between angles  $\phi$  and  $\psi$ :  $\cos \theta \sin \phi \cos \psi + \cos \phi \sin \psi = 0$ , or

$$\tan \psi = -\cos \theta \tan \phi. \tag{16}$$

Expression (16) is equivalent to the condition  $p_y = 0$  as seen from (1). The condition (16) determines the angle  $\psi$  from the angle  $\phi$ . The simultaneous rotation of the director and polarisation vector leads to the chirality change (1, 2).

Note that the elastic energy for independent angles  $\phi$  and  $\psi$  is generally non-linear, as can be seen from (7, 8). However, the use of condition (16) eliminates gradients of the angle  $\psi$  in the elastic free energy density. In one-constant elasticity we obtain (with the help of (20)) the free energy density (without the chiral term and with  $\theta = \pi/4$ ) in the form:

$$\frac{K}{2} \frac{(23 + 8 \cos 2\phi + \cos 4\phi)}{4(3 + \cos 2\phi)^2} \left[ \left( \frac{\partial \phi}{\partial x} \right)^2 + \left( \frac{\partial \phi}{\partial z} \right)^2 \right].$$

As

$$\frac{1}{2} \leq \frac{(23 + 8 \cos 2\phi + \cos 4\phi)}{4(3 + \cos 2\phi)^2} \leq 1$$

for all  $\phi \in (0, 2\pi)$ , let us approximate the above expression by its upper limit, the expression (4).

Using (1), (16) and the methods of (20), the surface energy (3) takes the form:

$$W_A = (\gamma_1 + \gamma_2) + \gamma_5 \cos^2 \phi + \frac{\left( \frac{\cos \theta}{\cos \phi} \right) \left( -\gamma_1 \left( \frac{\cos \theta}{\cos \phi} \right) + \gamma_2 \sqrt{1 + \cos^2 \theta \tan^2 \phi} \right)}{1 + \cos^2 \theta \tan^2 \phi}. \tag{17}$$

We again add the constant  $(\gamma_1 + \gamma_2)$  to  $W_A$  in order to satisfy the boundary conditions:

$$\lim_{\phi \rightarrow (\pi/2)^+} W_A = \lim_{\phi \rightarrow (3\pi/2)^-} W_A \rightarrow 0.$$

The surface energy (17) has surely one maximum when  $\gamma_1$  can be neglected with respect to  $\gamma_2$ , i.e.  $\gamma_1 \ll \gamma_2$ . We then propose the solution of (8) in a simple form (5, 16):

$$\varphi(z) = \arctan \frac{z}{\xi} + \pi, \tag{18}$$

which maps the interval  $z \in (-\infty, +\infty)$  onto the interval  $\varphi \in (\pi/2, 3\pi/2)$ .

The expression (16) can be solved as  $\psi = \arctan(-\cos \theta \tan \phi) - \pi$ . This branch of the function arctan is chosen to assure that the direction

of polarisation  $\vec{p}$  is preferentially oriented along the surface polarisation, i.e. along the  $x$ -axis. The angle  $\psi$  then lies in the interval  $\psi \in (-\pi/2, -3\pi/2)$ .

In Figure 4 the core structure of the  $\pi$ -disclination described by the solution (18) on the sample surface is shown schematically. In this case molecules rotate simultaneously on the surface of the cone (change of the azimuthal angle  $\phi$ ) and around the director  $\vec{n}$  (see

Figure 1). In Figure 4(a) projections of bent-shaped molecules onto the  $(x, z)$ -plane are shown. Note that molecules are inclined with respect to the  $(x, z)$ -plane while polarisations are always situated in this plane because the condition (16) assures that the  $y$ -component of  $\vec{p}$  is zero, i.e.  $p_y = 0$ .

Flank molecules of Figure 4(a) are shown in perspective in Figure 4(b) and 4(c). The ends of molecules

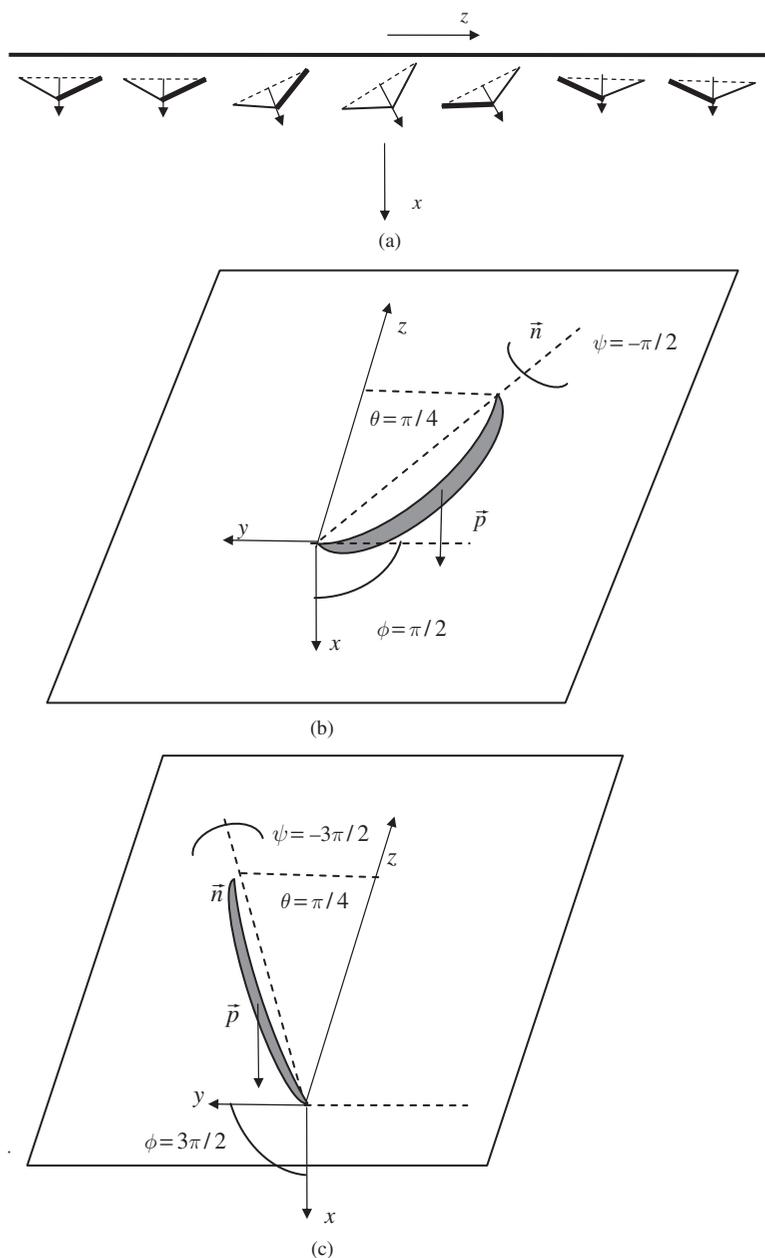


Figure 4. Schematic drawing of the director profile of  $\pi$ -disclination core just under the sample surface  $(y, z)$ . In (a) a row of molecules projected onto the plane  $(x, z)$  is displayed. With the exception of the molecule in the central column, molecules are inclined with respect to the  $(x, z)$ -plane while molecular polarisations are always in the  $(x, z)$ -plane. The molecule in the central column lies in the  $(x, z)$ -plane and it is tilted with respect to the surface by a tilt angle  $\theta$ . In (b) and (c) the molecules are shown in perspective. The molecule in (b) is the left molecule in (a) and in (c) the right molecule of (a) is shown, respectively.

in Figure 4(b) and (c) lie on the sample surface. The molecular orientations are characterised by angles  $\phi = \pi/2$ ,  $\psi = \pi/2$  and  $\phi = 3\pi/2$ ,  $\psi = \pi/2$ , respectively.

Boundary solution (18) and Equation (8) are valid when the elastic behaviour of the liquid crystals is approximated by the expression (4). The bulk solution  $\phi$  again satisfies the equation  $\Delta\phi(x, z) = 0$ . In this case the energy  $W_A(\varphi(z))$  takes a simple form:

$$W_A(z) = \frac{K}{2} \left( \frac{\xi}{\xi^2 + z^2} \right). \quad (19)$$

The position of the maximum of (19) corresponds to  $z = 0$  (i.e.  $\varphi(z = 0) = \pi$ ). Then:

$$W_A(\varphi = \pi) = \gamma_2(1 - \cos \theta) + \gamma_5, \quad (20)$$

is the maximum value of  $W_A$ . By comparing  $W_A(z = 0) = \frac{K}{2\xi}$  with (20) we obtain the parameter  $\xi$ :

$$\xi = \frac{K}{2[\gamma_2(1 - \cos \theta) + \gamma_5]}. \quad (21)$$

Using (16) the core energy of the  $\pi$ -disclination described by the solution (18) can be written as:

$$E_{core} = \pi K/2. \quad (22)$$

The proposed core structure (18) can be extended to the lower half-space as:

$$\phi(x, z) = -\arctan \frac{z}{x - \xi} + \pi. \quad (23)$$

#### 4. Discussion

Strong polar surface anchoring and preference for synclinic structure induces a ferroelectric synclinic structure near the surface. An external electric field can create in surface synclinic ferroelectric structures either  $2\pi$ -walls (with no chirality change) or  $\pi$ -walls accompanied by chirality change (4). Switching off the field leads to the collapse of walls in the sample bulk. However, strong surface anchoring can eventually keep remnants of walls at the surface as  $2\pi$ - and  $\pi$ -surface disclinations. Here we have investigated the core structures of those disclinations spread on the sample surface.

In the case of  $2\pi$ -surface disclination we assume that the molecular polarisation was fixed with respect to the molecular director and that it rotates in the same manner as the director. The core structure of  $2\pi$ -disclination was proposed in the form of two  $\pi$ -disclinations positioned at  $z = \pm z_o$  with a core width  $2\xi$ . When

anchoring parameters  $\gamma_1, \gamma_2$  and  $\gamma_5$  are known, parameters  $z_o$  and  $\xi$  can be determined. The estimation of the order of parameters  $z_o$  and  $\xi$  can be carried out using the approximate determination of anchoring parameters in (9). In (9)  $\gamma_1 \approx 0$ ,  $\gamma_2 \approx 10^{-3} \text{ J m}^{-2}$  and  $\gamma_5 \approx 2 \times 10^{-3} \text{ J m}^{-2}$  were determined for materials denoted 10WDVI and 11BVID11 (3, 9). Using an approximate value of the parameter  $\beta_- \approx 10^3\text{--}10^5 \text{ J m}^{-3}$  (9) the thickness  $d$  within which the surface anchoring induces ferroelectric order near surface can be estimated as  $d \approx 0.1\text{--}10 \text{ }\mu\text{m}$ .

Let the order of the elastic constant of the liquid crystal be  $K \approx 10^{-11} \text{ J m}^{-1}$  (21). Then  $\gamma_2/K \approx 10^2 \text{ }\mu\text{m}^{-1}$  and  $\gamma_5/K \approx 2 \times 10^2 \text{ }\mu\text{m}^{-1}$ . Conditions (13) and (14) give numerically  $\xi \approx 0.0024 \text{ }\mu\text{m}$  and  $z_o \approx 0.008 \text{ }\mu\text{m}$ . The values of those parameters change only slightly when minimising squares of surface anchoring energies.

Profiles of the anchoring energy  $W_A\xi/K$  (in non-dimensional units) as a function of  $\phi/\pi$  and the corresponding density of the infinitesimal surface disclinations  $d\varphi(z)/dz$  for the above-listed parameters are

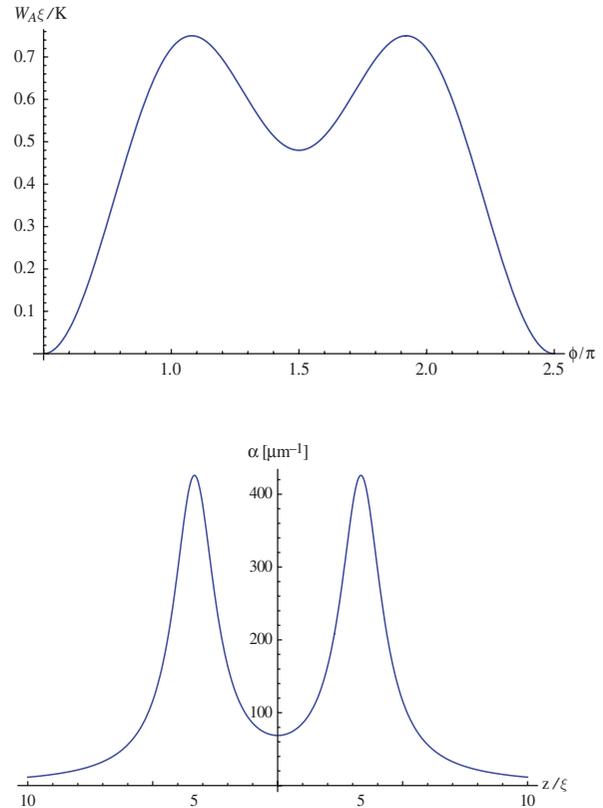


Figure 5. Plots of (a) surface anchoring energy  $W_A\xi/K$  (in non-dimensional units) as a function of  $\phi/\pi \in (1/2, 5/2)$ , and (b) the density of infinitesimal surface disclinations representing the core of  $2\pi$ -surface disclination. Both plots are calculated for parameters:  $\gamma_1 \approx 0$ ,  $\gamma_2 \approx 10^{-3} \text{ J m}^{-2}$ ,  $\gamma_5 \approx 2 \times 10^{-3} \text{ J m}^{-2}$ ,  $\xi \approx 0.0024 \text{ }\mu\text{m}$ ,  $z_o \approx 0.008 \text{ }\mu\text{m}$  and  $K \approx 10^{-11} \text{ J m}^{-1}$ .

illustrated in Figures 5(a) and 5(b), respectively. A local minimum in the anchoring energy leads to a local minimum in the disclination density, meaning that  $2\pi$ -disclination is dissociated into two partial  $\pi$ -surface disclinations. The separation of both  $\pi$ -disclinations is  $2z_o \approx 0.016 \mu\text{m}$  and the width of the  $2\pi$ -surface disclination core is then  $2(z_o + \xi) \approx 0.021 \mu\text{m}$ , which is a very thin core.

In principal, there is another possibility to realise  $2\pi$ -surface disclination by transition through a ferroelectric-like structure in the core, i.e. it can be supposed that  $\phi_1 = \phi, \phi_2 = \pi/2$  and  $\psi_1 = \psi_2 = \pi/2$ . This means that the molecular rotation for  $2\pi$  is realised in odd planes while molecules in even planes rest fixed in the minimum of the anchoring energy. In this case the core structure is determined by a balance between the surface anchoring energy, elastic energy and antiferroelectric energy  $w_C$ . However, such a model leads to a non-linear equilibrium equation in the bulk of the liquid crystal and we cannot use the PN model for description of the disclination core. We cannot therefore consider this solution in the present work.

When strong polar anchoring prefers synclinc ferroelectric domains and overcomes the internal energy barrier of the polarisation rotation (19) near surfaces then a  $\pi$ -surface disclination separating two synclinc ferroelectric domains of different chirality can exist. As discussed above in Section 3.2, the rotation of the molecular director  $\vec{n}$  around the layer normal in the disclination core is accompanied by the simultaneous rotation of the molecular polarisation unit vector  $\vec{p}$  around  $\vec{n}$  in such a way that molecular dipole moments are parallel to the surface polarisation. For this reason the  $\pi$ -surface disclination connects surface domains of opposite chirality. As an illustration we again used the estimated parameters of 10WDVI and 11BVID11 (3, 9). Then the core width  $2\xi$  is given as  $2\xi \approx 0.0044 \mu\text{m}$ . The core width is in this case very thin, and so the  $\pi$ -surface disclination is probably hardly detectable. The description of the  $\pi$ -disclination above (in Section 3.2) using the PN model is valid when the elasticity of the liquid crystal can be approximated by the energy density (4).

A  $\pi$ -disclination core distributed along the  $z$ -axis is schematically represented in Figure 4. Due to the anchoring, the main part of the molecular polarisation points inside the sample, preferably along the  $x$ -axis. Due to the condition (16) there is no  $y$ -component of polarisation.

When the  $B_2$  structure is characterised by the tilt angle  $\theta = \pi/4$  no optical contrast can be distinguished on both sides of a line as in (4). In other cases domains of different contrast separated by the  $\pi$ -disclination can be expected.

A wider core of the  $\pi$ -surface disclination can be found with compounds which have lower anchoring

energies. Taking model values, e.g.  $\gamma_2/K \approx 1 \mu\text{m}^{-1}$  and  $\gamma_5/K \approx 0.7 \mu\text{m}^{-1}$ , the expression (21) gives  $2\zeta \approx 1 \mu\text{m}$ . In contrast, the thickness  $d$  can be estimated as  $d \approx 0.1\text{--}0.001 \mu\text{m}$  in this case because the parameter  $\beta_-$  is the same.

In the case of strong anchoring keeping molecular dipole moments mostly oriented along the surface normal, a  $2\pi$ -surface disclination core will also be modified. Both partial  $\pi$ -surface disclinations will have a structure similar to that shown in Figure 4. Nevertheless, far from the core, structures have the same chirality.

Finally, let us discuss the behaviour of the core of surface disclinations in a weak external electric field. In the sample of thickness  $d$ , the near-surface energy density of the electric field  $P_s E \sin \phi$  (with spontaneous polarisation  $P_s$  and intensity of an electric field  $E$ ) competes with polar anchoring. Therefore the energy of the field can be estimated as  $dP_s E \sin \phi$  (small field).

In order to discuss qualitatively the behaviour of the  $2\pi$ -core at small fields we simply change  $\gamma_2 \rightarrow \gamma_2 - dP_s E$  in (13), which gives approximate values of  $\xi$  and  $t$ . We can distinguish two cases differing in the sign of  $P_s E$ . When  $P_s E < 0$ , an electric field increases the anchoring and the core width  $2(z_o + \xi)$  decreases. This is seen by taking e.g.  $z_o \approx \xi$  and a modified equation (13), which leads to a decrease of  $\xi$  for a small increase of  $P_s E$ . As we expect, for stronger fields disclination will transform in a wall in the sample bulk. When  $P_s E > 0$ , an electric field has a tendency to compensate for the polar anchoring acting against it. Suppose now, for simplicity, that widths of partial  $\pi$ -disclinations do not change with field but can relatively simply displace themselves in the field. This means their positions  $z_o$  change. Then Equation (13), simplified to the form  $\frac{2(\gamma_2 - dP_s E)}{K} \xi \approx \frac{\pi}{2t}$ , shows that  $t$  (respectively  $z_o$ ) has a tendency to increase with the increase of the electric field. In fact, the core region acts as a nucleus of opposite polarisation, i.e. molecules have polarisations oriented against the surface anchoring polarisation. As an external applied electric field is also oriented against surface polarisation, it increases the core region. The approximations used are valid in a small field. A similar qualitative conclusion can be obtained using a simplified Equation (14).

In the case of  $\pi$ -surface disclination, its core width  $2\xi$  has a tendency to decrease under an external electric field for which  $P_s E < 0$  (and eventually create a wall in a sample bulk). On the other hand, when  $P_s E > 0$ , the width  $2\xi$  increases with the increasing field.

There is an important difference between  $2\pi$ - and  $\pi$ -surface disclinations: the core of the  $2\pi$ -disclination is already a nucleus of ferroelectric structure with opposite polarisation which can spread in an opposite electric field. For structures separated by a  $\pi$ -disclination, the opposite field should first nucleate a nucleus

of opposite polarisation. Therefore the switching of the electric field could be simpler for  $2\pi$ -surface disclination.

In conclusion, the structures of surface  $2\pi$ - and  $\pi$ -disclination cores stabilised by surface anchoring were investigated using the Peierls–Nabarro model. Model parameters such as core width and separation of partial disclinations were estimated. Estimations of the core width of 10WDVI and 11BVID11 materials give very thin cores. The disclination core width depends inversely on the anchoring energy parameters (see e.g. expression (21)). In liquid crystals with smaller anchoring parameters the disclination core width  $2\xi$  is greater.

The present model considers only a particular case of possible surface disclinations in the  $B_2$  phase, but we hope it opens the path to more complex studies concerning walls in  $B_2$  structures under an electric field, which are frequently observed (see e.g. (4, 6)).

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