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Behaviour of a Sm C disclination line $s = + 1/2$ with a partial twist under a magnetic field

H. P. Hinov

Institute of Solid State Physics, Boul. Lenin 72, Sofia 1184, Bulgaria

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Résumé. — Les résultats théoriques de Allet, Kléman et Vidal [15] sur le comportement d'une disinclinaison $s = + 1/2$ avec torsion partielle dans un smectique C ont été étendus au cas où un champ magnétique est appliqué le long de l'axe cylindrique. On montre qu'il existe un champ magnétique critique au-dessus duquel la disinclinaison avec saut se transforme en une disinclinaison ordinaire sans torsion. On peut déterminer expérimentalement les combinaisons de constantes élastiques $2 A_{21} - A_{11}$ et $2 A_{12} - A_{11}$ lorsque A_{11} est négatif ou $A_{11} - 2 A_{21}$ et $A_{11} - 2 A_{12}$ lorsque A_{11} est positif.

Abstract. — The theoretical results of Allet, Kléman and Vidal [15] for the behaviour of the Sm C disclination $s = + 1/2$ with a partial twist are extended to the case of a magnetic field applied along the cylinder axis. The solution has shown that a critical magnetic field exists above which the disclination with a jump is transformed into a usual edge-disclination without twist. This makes possible the experimental determination of the $2 A_{21} - A_{11}$ and $2 A_{12} - A_{11}$ Sm C coefficient combination when $A_{11} < 0$ and $A_{11} - 2 A_{21}$ and $A_{11} - 2 A_{12}$ when $A_{11} > 0$.

The elastic energy of the smectic C (Sm C) liquid crystal (LC) consists of three parts. The first part was obtained for the first time by Saupe [1] and includes all the possible reorientations of the Sm C director around the normal to the Sm C plane :

$$F_{c_1} = (1/2) B_1 \left(\frac{\partial \varphi}{\partial x} \right)^2 + (1/2) B_2 \left(\frac{\partial \varphi}{\partial y} \right)^2 + (1/2) B_3 \left(\frac{\partial \varphi}{\partial z} \right)^2 + B_{13} \frac{\partial \varphi}{\partial x} \cdot \frac{\partial \varphi}{\partial z} \quad (1)$$

where φ is the angle between the projection of the molecular director on the Sm C plane and the axis Y, B_1 , B_2 , B_3 and B_{13} are the elastic coefficients describing the resistance of the Sm C LC to all the possible reorientations of the Sm C director.

The second part of the Sm C elastic energy, obtained for the first time by the Orsay Liquid Crystal Group [2], includes the curvature elasticity and the dilation (or compression) of the Sm C layers :

$$F_{c_2} = (1/2) A_{11} \left(\frac{\partial^2 u}{\partial x \partial y} \right)^2 + (1/2) A_{12} \left(\frac{\partial^2 u}{\partial x^2} \right)^2 + (1/2) A_{21} \left(\frac{\partial^2 u}{\partial y^2} \right)^2 + (1/2) \bar{B} \left\{ \frac{\partial u}{\partial z} - (1/2) \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right] \right\} \quad (2)$$

where u is the displacement of the Sm C layers in the direction of the Z axis (i.e. normal to the Sm C plane), A_{11} , A_{12} and A_{21} are the elastic coefficients describing the resistance of the Sm C to the curvature of the Sm C layers and $\bar{B}$ is the dilation elastic coefficient.

The third part of the Sm C elastic energy, also obtained by the Orsay Liquid Crystal Group [2], describes the coupling between the layer curvature and the director field :

$$F_{c_3} = C_1 \frac{\partial^2 u}{\partial x \partial y} \frac{\partial \varphi}{\partial x} + C_2 \frac{\partial^2 u}{\partial y^2} \frac{\partial \varphi}{\partial y}. \quad (3)$$

In addition, a number of inequalities about various combinations of the Sm C elastic coefficients are obtained from the considerations of stability :

$$\begin{aligned} A_{11}^2 - 4 A_{21} A_{12} &< 0 & A_{12}, A_{21} &> 0 \\ B_1 B_3 - B_{13}^2 &> 0 & B_1, B_2, B_3 &> 0, \quad \bar{B} > 0 \\ A_{12} B_1 - C_1^2 &> 0 & A_{12} B_2 - C_2^2 &> 0 \end{aligned} \quad (4)$$

All the elastic coefficients, with the exception of the dilation modulus B , are very similar to those already known for the case of nematics and cholesterics and are expected to be in the range of 10^{-6} dyne [3]. The value of the Sm C elastic coefficients can be obtained, for instance, by the appropriate performance of all the possible kinds of the usual Fredericksz transition or by other, more complicated, deformations of the Sm C LC which include not only reorientations of the Sm C director but also the curvature of the Sm C layers. Although some authors have dealt with the possible Fredericksz transition of the Sm C [4-7], experimental results are very scarce [8-10] and they mainly give the value of the characteristic Sm C tilt and its temperature dependence. Recently, only Schiller and Pelzl have estimated the mean value of the elastic coefficients $B_1 \sim B_2$ for the case of 5-n-heptyl-2(4-n-nonyloxyphenyl)-pyrimidine to be in the range of 6×10^{-7} dyne [11]. In addition, the measurements of the elastic coefficients A_{11} , A_{12} and A_{21} which describe the curvature of the Sm C layers, are much more complex since the electric and magnetic fields cannot ensure one eventual optically-observable deformation of the Sm C layers by the usual Fredericksz transition [4]. Another useful way for determining these coefficients is connected with measurements of the periodicity of the Sm C layer undulations [12-14].

The aim of this communication is to present theoretical results about the behaviour of the Sm C disclination line $s = + 1/2$ with a partial twist under the action of a magnetic field applied in a suitable manner. We have chosen this Sm C disclination since, first, its energy is given in an explicit form [15] and permits a simple accounting of the magnetic field action on the orientation of the Sm C director and second, the theoretical calculations can be easily verified by the performance of eventual measurements. Indeed, we shall see that the theoretical calculations clearly show interesting phase transitions which might be useful for the determination of some combinations of the Sm C elastic coefficients.

The density of the total energy of the disclination $s = + 1/2$ with a partial twist under the action of a magnetic field consists of two parts. The elastic energy, as noted, has been already given by Allet, Kléman and Vidal (see the relation (1) in Ref. [15]). The type of magnetic field energy depends crucially on the direction of the magnetic field. It is known from the theoretical results of Allet *et al.* [15] that $\omega = \pi/2$ and $\omega = 0$ (where $(\pi/2 - \omega)$ is the angle between the projection of the molecular axis on the Sm C plane t and the cylinder axis) are minima for the disclination under study in the case of a positive sign of the elastic coefficient A_{11} . Let us for convenience denote these cases by *a*) and *b*), respectively. On the basis of these results and also from considerations of symmetry we decided to choose the simplest case when the magnetic field

is applied along the cylinder axis (see Fig. 7 in Ref. [15]). In accordance with Meirovitch *et al.* [6] we can write the following density of the magnetic energy :

$$\rho f_H = - \frac{\Delta\chi}{2} H^2 \sin^2 \psi \sin^2 \omega \quad (5)$$

where $\Delta\chi$ is the value of the magnetic anisotropy susceptibility, assumed to be positive and ψ is the characteristic tilt angle of the Sm C under study for the case *a*) when $\omega = \pi/2$ is the only minimum. It is clear that in the second case *b*), when $\omega = 0$ is the only minimum, the density of the magnetic energy has the following form :

$$f_H = - \frac{4\chi}{2} H^2 \sin^2 \psi \cos^2 \omega. \quad (6)$$

For simplicity, in the relations (5) and (6) we have neglected the usual magnetic biaxiality of the Sm C LC [4]. On the other hand, it is well known that the characteristic tilt angle ψ is nearly temperature independent for the Sm C LCs which are formed from the N phase under cooling and strongly temperature dependent for those Sm C LCs which are formed from the Sm A phase after cooling.

Before giving the detailed theoretical results let us initially stress that in all the following equations and relations the elastic terms have been already obtained by Allet, Kléman and Vidal [15]. Minimizing the total elasto-magnetic energy with respect to ω leads to the following differential equation :

$$\sin 2\omega (A_{21} \sin^2 \omega - A_{12} \cos^2 \omega + (A_{11}/2) \cos 2\omega) \pm \frac{(R^2 - r_0^2)}{\ln(R/r_0)} \frac{\Delta\chi}{2} \times \\ \times H^2 \sin^2 \psi \sin 2\omega = (B_1 \cos^2 \omega + B_2 \sin^2 \omega) \frac{d^2\omega}{d\theta^2} \quad (7)$$

where the upper sign (+) corresponds to the case *a*) and the lower sign (−) to the case *b*).

Let us in accordance with Allet *et al.* [15] define the easy directions which minimize the elasto-magnetic energy for the case of $(d\omega/d\theta) = 0$. Then the energy has the following form :

$$f_m = (1/2) A_{11} \sin^2 \omega \cos^2 \omega + A_{12} \cos^4 \omega + A_{21} \sin^4 \omega - \\ - \frac{\Delta\chi}{2} \frac{(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi \frac{\sin^2 \omega}{\cos^2 \omega} \quad (8)$$

The extrema are obtained for

$$\frac{df_m}{d\omega} = \left((A_{11}/2) \cos 2\omega + A_{21} \sin^2 \omega - A_{12} \cos^2 \omega \mp \frac{\Delta\chi}{2} \times \right. \\ \left. \times \frac{(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi \right) \sin 2\omega \quad (9)$$

where the upper sign (−) corresponds to the case *a*) and the lower sign (+) to the case *b*), i.e. for

a) $\omega_1 = \pi/2$ (t along the cylinder axis, i.e. here the molecular axis is parallel to the anchoring direction on the glass plate)

b) $\omega_2 = 0$ (the molecular axis is in the right section of the cylinder)

$$c) \quad \cos^2 \omega_3 = \frac{1}{2(A_{12} + A_{21} - A_{11})} \left\{ -A_{11} + 2A_{21} - \frac{\Delta\chi(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi \right\} \quad (10)$$

which is a convenient form for the case *a*)

d)

$$\cos^2 \omega_3 = \frac{1}{2(A_{12} + A_{21} - A_{11})} \left\{ -A_{11} + 2A_{12} - \frac{\Delta\chi(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi \right\} \quad (11)$$

which is a convenient form for the case *b*).

The minima are obtained for $d^2 f_m / d\omega^2 > 0$:

$$\begin{aligned} \frac{d^2 f_m}{d\omega^2} = A_{11} \cos^4 \omega + (A_{12} + A_{21}) \sin^2 2\omega + 2(A_{21} \sin^2 \omega - A_{12} \cos^2 \omega) \cos 2\omega \mp \\ \mp \frac{\Delta\chi(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi \cos 2\omega \end{aligned} \quad (12)$$

where the upper sign (−) corresponds to the case *a*) and the lower sign (+) to the case *b*).

According to relations (4) the elastic coefficients A_{12} and A_{21} must be positive. On the other hand, A_{11} is the only Sm C elastic coefficient which can be either positive or negative. It is clear from equation (12) that when A_{11} , $A_{11} - 2A_{12}$, and $A_{11} - 2A_{21}$ are positive then $\omega = \pi/2$ ($A_{11} > 0$, $A_{11} - 2A_{21} > 0$) or $\omega = 0$ ($A_{11} > 0$, $A_{11} - 2A_{12} > 0$) are the only minima (as noted these cases were designated by *a*) and *b*), respectively), whereas ω_3 is necessarily a maximum of f_m , if it exists. On the other hand, for the case of a vanishing magnetic field and negative sign of the elastic coefficient A_{11} $\omega_1 = \pi/2$ (case *a*) and $\omega = 0$ (case *b*) are maxima, ω_3 exists and it is the only minimum of f_m . We shall see, however, that this is true also for small values of the magnetic field whereas for large values that are above a certain critical magnetic field the only minimum is either $\omega_1 = \pi/2$ (case *a*) or $\omega = 0$ (case *b*).

Let us consider these cases :

I. $A_{11} < 0$.

One looks for a first integral of (7) (in which we shall make $B_1 = B_2 = B$) satisfying the boundary condition $d\omega/d\theta = 0$ for $\omega = \omega_3$. This yields :

$$\begin{aligned} B \left(\frac{d\omega}{d\theta} \right)^2 = (A_{12} + A_{21} - A_{11})(\cos^2 \omega - \cos^2 \omega_3)^2 - \\ - \frac{2 \Delta\chi(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi (\cos^2 \omega - \cos^2 \omega_3) \end{aligned} \quad (13)$$

which is a convenient form for the case *a*) and

$$\begin{aligned} B \left(\frac{d\omega}{d\theta} \right)^2 = (A_{12} + A_{21} - A_{11})(\sin^2 \omega - \sin^2 \omega_3)^2 - \\ - \frac{2 \Delta\chi(R^2 - r_0^2)}{\ln(R/r_0)} H^2 \sin^2 \psi (\sin^2 \omega - \sin^2 \omega_3) \end{aligned} \quad (14)$$

for the case *b*).

It seems that the solution of these differential equations consists of a complex combination of elliptic integrals and we shall not deal with this problem. For our aim, it is sufficient to point out that for small values of the magnetic field ω_3 oscillates in a very complex manner in the range $(-\omega_3, +\omega_3)$ passing either through $\omega = \pi/2$ or 0. On the other hand, the equations (10) and (11) clearly show that the raising of the magnetic field up to the value H_c which is determined either from the relation :

$$H_c^2 = (2A_{21} - A_{11}) \frac{\ln(R/r_0)}{\Delta\chi \sin^2 \psi (R^2 - r_0^2)} \quad (15)$$

for the case *a*) or from the relation :

$$H_c^2 = (2 A_{12} - A_{11}) \frac{\ln(R/r_0)}{\Delta\chi \sin^2 \psi (R^2 - r_0^2)} \quad (16)$$

for the case *b*), lead to a distinct first order phase transition and the disclination $s = + 1/2$ with a partial twist is transformed with a jump into an usual wedge-disclination without twist.

It is clear that above this critical magnetic field the Sm C LC molecules prefer to stay in a position which minimizes the magnetic energy, i.e. the application of a magnetic field with a value which is above the critical one replaces the minimum ω_3 by $\omega = 0$ or $\omega = \pi/2$. In the case *a*) all the molecules go to $\pi/2$ whereas in the case *b*) they go to $\omega = 0$. Furthermore, the relations (15) and (16) can be used for the determination of the $2 A_{21} - A_{11}$ and $2 A_{12} - A_{11}$ combinations of the Sm C elastic coefficients for the case of a negative value of A_{11} . For this purpose one should estimate the value of the core radius r_0 which according to Allet *et al.* [15] is of the order of a Sm C layer thickness.

II. $A_{11} > 0$.

One finds different first integrals, according to whether the chosen minimum is $\omega = 0$:

$$f_m = (A_{12}/2) - (\Delta\chi/2) \frac{(R^2 - r_0^2)}{\ln(R/r_0)} \sin^2 \psi H^2 \quad (17)$$

or $\omega = \pi/2$

$$f_m = (A_{21}/2) - (\Delta\chi/2) \frac{(R^2 - r_0^2)}{\ln(R/r_0)} \sin^2 \psi H^2 \quad (18)$$

case *a*) $\omega = \pi/2$, $A_{12} > A_{21}$, $A_{11} > 2 A_{21}$.

The first integral is

$$B \left(\frac{d\omega}{d\theta} \right)^2 = \left(A_{12} - A_{21} - \frac{(R^2 - r_0^2) \sin^2 \psi}{\ln(R/r_0)} H^2 \right) \cos^2 \omega + (1/4)(A_{11} - A_{12} - A_{21}) \sin^2 2\omega \quad (19)$$

Equation (19) integrates to :

$$\pm \int_0^\omega \frac{d\alpha}{\cos \alpha (1 - m \sin^2 \alpha)^{1/2}} = \left(\frac{A_{12} - A_{21}}{B} \right)^{1/2} (\theta - \pi/2) \quad (20)$$

where

$$m = \frac{A_{12} + A_{21} - A_{11}}{A_{12} - A_{21} - \frac{(R^2 - r_0^2) \sin^2 \psi H^2}{\ln(R/r_0)}} \quad (21)$$

It is clear that m should be positive. The case when m goes to unity i.e. when

$$2 A_{21} - A_{11} + \frac{\Delta\chi(R^2 - r_0^2) \sin^2 \psi}{\ln(R/r_0)} H^2 = 0 \quad (22)$$

the disclination $s = + 1/2$ with a partial twist is transformed with a jump to the usual edge-disclination $s = + 1/2$ without twist.

The critical magnetic field can be determined from the relation (22) :

$$H_c^2 = \frac{(A_{11} - 2 A_{21}) \ln (R/r_0)}{\Delta\chi(R^2 - r_0^2) \sin^2 \psi} \quad (23)$$

case b) $\omega = 0$, $A_{21} > A_{12}$, $A_{11} > 2 A_{12}$.

The first integral is

$$B\left(\frac{d\omega}{d\theta}\right)^2 = \left(A_{21} - A_{12} - \frac{\Delta\chi(R^2 - r_0^2) \sin^2 \psi}{\ln (R/r_0)} H^2\right) \sin^2 \omega + \\ + (1/4)(A_{11} - A_{12} - A_{21}) \sin^2 2\omega \quad (24)$$

Similarly, the corresponding critical magnetic field is expressed by the following relation :

$$H_c^2 = \frac{(A_{11} - 2 A_{12}) \ln (R/r_0)}{\Delta\chi(R^2 - r_0^2) \sin^2 \psi}. \quad (25)$$

It is clear that the relations (24) and (25) can be used for the determination of the following $A_{11} - 2 A_{21}$ and $A_{11} - 2 A_{12}$ combinations of Sm C elastic coefficients in the case when $A_{11} > 0$.

The preliminary estimations show that the critical magnetic field is around several thousand gauss.

The theory hitherto developed is for the ideal case of a single disclination $s = + 1/2$ with a partial twist. In fact, in cases when $\omega = \pi/2$ and $\omega = 0$ are minima, this disclination usually appears in a combination with the complementary disclination $s = - 1/2$ forming in this way a Néel wall. This disclination can significantly disturb the orientation of the Sm C molecules inside the Sm C layers of the disclination and can additionally lead to the dilation of the Sm C layers being around the disclination under study (see Fig. 6 in Ref. [15]). In addition, these disturbances will be large for small distances between the alternating disclinations $+ 1/2$ and $- 1/2$ when the radius of the cylinder under consideration is considerably smaller than the LC layer thickness. On the other hand, the undulation around the disclination under study can be considerable or negligible depending on the experimental circumstances such as the type of the LC cell, the surface treatment, the initial orientation of the Sm C LC etc. For instance, it seems that these undulations will be large for a Sm C disclination $s = + 1/2$ with a partial twist formed in a Sm C LC confined between two glass plates and will be small for the case of a Sm C droplet. The latter case has been confirmed by Allet *et al.* [15].

It is interesting to consider the influence of the magnetic field on the Sm C disclination line $s = + 1/2$ with a partial twist including the layer undulations for the simple case when the twisting of the molecules inside the layers and the radius of the cylinder under consideration on one hand, and the twisting of the molecules and the wave number of the layer undulation on the other hand are uncoupled. For clarity, we shall use the theoretical calculations already developed by Allet *et al.* for the case of a Sm C droplet [15]. In the same circumstances discussed by these authors, the application of a magnetic field along the cylinder axis leads to the drastic change in the algebraic equation describing the R -variations :

$$\Delta\chi H^2 R^2 + \left(\frac{16 \alpha^2 \lambda^3 \bar{B}^2}{\gamma} + 2 K + A'\right) R - \frac{32 \alpha^2 \lambda^3 \bar{B}^2}{\gamma} D = 0. \quad (26)$$

(For the meaning of the material constants which enter in this equation see Ref. [15].)

It is clear that the application of the magnetic field leads to the inclusion of a cubic term in the initially linear equation. This equation has a solution for each value of the material constants of

the Sm C LC. Unfortunately, this solution might be only numerical. An analytic solution is possible for the case of a Sm C disclination $s = + 1/2$ with a partial twist when the undulations that are outside the cylinder are hindered :

$$R \sim (1/H) \left(\frac{2K + A'}{\Delta\chi} \right)^{1/2}. \quad (27)$$

Let us mention that the parameter $2K + A'$ is a function of ω and consequently of H when the magnetic field has a value smaller than the critical one (see Eqs. (15), (16), (23) and (25)). For larger values of the magnetic field in these parameters enter only the elastic Sm C coefficients.

In conclusion, the raising of a magnetic field applied along the cylinder axis of a disclination line $s = + 1/2$ with a partial twist strongly anchored on the glass plate up to a certain critical (threshold value leads to a first-order phase transition with a sudden transformation of the disclination into the usual edge-disclination. On the basis of these theoretical results one can experimentally measure the following $2A_{21} - A_{11}$, $2A_{12} - A_{11}$ ($A_{11} < 0$), $A_{11} - 2A_{21}$, $A_{11} - 2A_{12}$ ($A_{11} > 0$) combinations of the Sm C elastic coefficients.

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