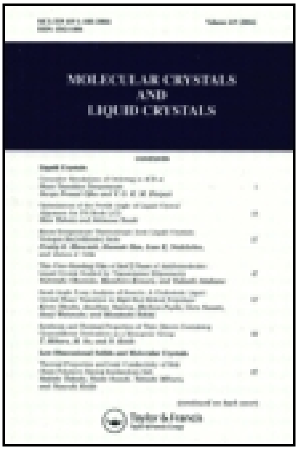

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Discontinuity Walls and Twist Disclinations in Smectic A Liquid Crystals

Lubor Lejček [a]

[a] Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 180 40, Prague 8, Czech Republic

Version of record first published: 24 Sep 2006

Mol. Cryst. Liq. Cryst., 1999, Vol. 330, pp. 259-266
Reprints available directly from the publisher
Photocopying permitted by license only

Discontinuity Walls and Twist Disclinations in Smectic A Liquid Crystals

LUBOR LEJČEK

Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 180 40 Prague 8, Czech Republic

A discontinuity wall in smectic A liquid crystals was discussed in M. Kléman, *Points, Lines and Walls in Liquid Crystals, Magnetic Systems and Various Ordered Media* (J. Wiley. Chichester 1983). Possible solutions describing a twist disclination which terminates the discontinuity wall in an infinite smectic A liquid crystal are proposed. One of solutions could be used for a description of the so called zigzag defect line which separates oppositelly oriented chevrons in a chiral smectic C liquid crystal.

Keywords: smectic liquid crystals; defects; chevrons; discontinuity walls; twist disclinations

INTRODUCTION

In Ref. [1] Kléman discussed different types of walls in the layered smectic A (S_A) phase. Among those walls there is the so called discontinuity wall which is characterized by an abrupt change of layer orientation. This discontinuity in layer orientation is also typical for both vertical[2] and horizontal[3, 4] chevrons. Chevron-type layer structures are intensively experimentally studied at the recent time (see e.g. Refs. [5, 6]) and these studies confirm previous basic theoretical representations of chevrons. Therefore one can speculate that the notion of a discontinuity wall can be also useful as a complementary description of chevron-like layer deformation.

Sheets of paper can be bent to the shape analogous to the discontinuity walls in a S_A. Intuitively the analogy between discontinuity walls in a S_A and bent sheets of paper or elastic sheets can be developed. Recently, increased attention is paid to problems of crumpled elastic sheets[7 - 9].

In this contribution a discontinuity wall terminated by a twist disclination in the S_A liquid crystal, will be treated. First, the solution describing a twist disclination terminating a discontinuity wall will be proposed within a classical S_A elasticity. Then the solution for the case of two twist disclinations of the same sign terminating two different discontinuity walls (the case of the zigzag defect) will be constructed.

DISCONTINUITY WALL TERMINATED BY A TWIST DISCLINATION

Let the coordinate system be chosen in such a way that the axes x and y are parallel to the non-deformed smectic A layers while the z-axis is along the layer normal. When layers are displaced in the direction of the z-axis this displacement is described by the function $u(x,y,z)$.

The elastic free energy density ρf can be expressed as

$$\rho f = \frac{K}{2}\left[\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)^2 + 2\left(\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \left(\frac{\partial^2 u}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2}\right)\right)\right] + \frac{\overline{B}}{2}\left(\frac{\partial u}{\partial z}\right)^2, \quad (1)$$

where K and $\overline{B}$ are S_A elastic constants of layer bend and compression. The free energy density (1) is the isotropic limit of the expression of the free energy density of smectic C (see Ref. [10]). In this contribution we limit our interest to the discontinuity wall lying along the y-axis and terminated by a singularity at $y = 0$. Therefore a singularity is parallel to the z-axis and $u = u(x,y)$. Moreover we will suppose that layers are bent to form a discontinuity wall without a volume deformation, i.e. without dilatation or compression of the smectic layers. Then the last term in (1) describing volume changes can be neglected and the equation of equilibrium which follows from the variation of the total elastic energy

$$E_{el} = \frac{K}{2}\iint dx\,dy\left[\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)^2 + 2\left(\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \left(\frac{\partial^2 u}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2}\right)\right)\right], \quad (2)$$

can be written in the form

$$\Delta\Delta u(x,y) = 0. \quad (3)$$

The surface term

$$K\left[\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \left(\frac{\partial^2 u}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2}\right)\right]$$

does not influence the form of the equilibrium equation (3). The equilibrium equation (3) is valid everywhere with the exception of points where the singularities are situated.

Let us suppose that the discontinuity wall is parallel to the half-plane (y,z), $y \geq 0$ and it is terminated at $y = 0$. By definition, there is the jump in the derivative of $u(x,y)$ in the discontinuity wall:

$$\left(\frac{\partial u}{\partial x}\right)_{x\to 0_-} - \left(\frac{\partial u}{\partial x}\right)_{x\to 0_+} = -\frac{\Omega_y}{2}(1+\operatorname{sgn} y), \quad (4)$$

where the angle Ω_y is a (small) constant rotation angle of layer inclination with respect to x - axis. One solution of (3), more exactly the solution of the equation

$$\Delta u(x,y) = \frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2} = 0,$$

satisfying condition (4) is:

$$u(x,y) = -\frac{\Omega_t}{2\pi}\left[\frac{\pi}{2}|x| + x\arctan\frac{y}{x} + \frac{y}{2}\ln\left(x^2 + y^2\right)\right], \tag{5}$$

The solution (5) is the layer displacement around a singularity parallel to the z-axis terminating a symmetrical discontinuity wall at $x = 0$ and $y = 0$. The layer displacement $u(x,y)$ is continuous at the coordinate origin but it diverges far from the singularity. An example plot given by *Mathematica*[11] of solution (5) is shown in Fig. 1. The grid of perpendicular lines drawn on

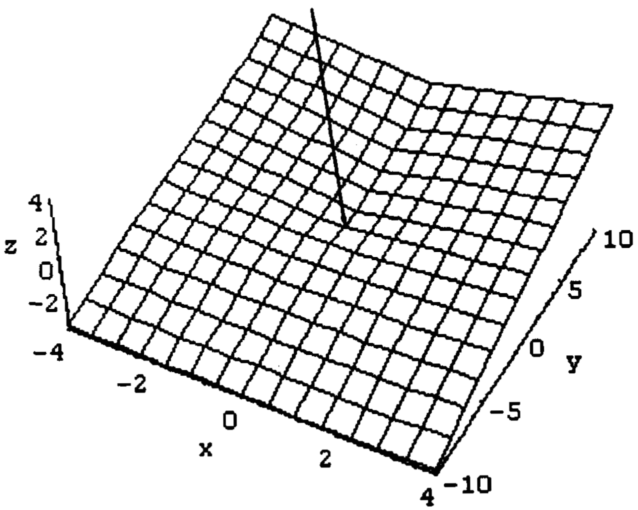

FIGURE 1 Schematic representation of the displacement of one smectic layer with a discontinuity wall (along $y > 0$) having a jump in layer orientation $\Omega_t = \pi / 3$ and terminated at a twist disclination situated at $x = 0$ and $y = 0$. The plane (x,y) is parallel to non-deformed S_A layers. The value of the angle $\Omega_t = \pi / 3$ was chosen for the purpose of graphic presentation only (the units of x and y are arbitrary in this schema). Twist disclination is represented by a solid line parallel to the z-axis.

the layer surface represents the 3D view of a deformed layer. Other smectic layers are parallel to the displayed one.

The condition (4) can be also written in the following integral form using the definition of the vector of rotation angles[10]:

$$\vec{\Omega}(\vec{r}) = (\Omega_x(\vec{r}), \Omega_y(\vec{r}), \Omega_z(\vec{r})) = \left(\frac{\partial u}{\partial y}, -\frac{\partial u}{\partial x}, \Omega_z(\vec{r})\right).$$

Then the total vector of rotation angles integrated over the closed circuit Γ (Frank circuit) contouring the singularity line is:

$$\oint_\Gamma d\vec{\Omega}(\vec{r}) = (0, \partial u/\partial x\big|_{\substack{x\to 0_-\\ y>0}} - \partial u/\partial x\big|_{\substack{x\to 0_+\\ y>0}}, 0) = (0, \Omega_y, 0). \quad (6)$$

Expression (6) permits an identification of the singularity terminating the discontinuity wall as the twist disclination characterized by the angle Ω_y of the rotation around the y-axis.

A MODEL OF A ZIGZAG DEFECT

One possibility of a combination of discontinuity walls terminated by twist disclinations is the case of opposite walls terminated by disclinations of the same type. Such a combination can be described by a solution of the form:

$$u(x,y) = \frac{\Omega_y}{2\pi}\left[x\left(\arctan\frac{y-y_0}{x} + \arctan\frac{y+y_0}{x}\right) + \right.$$
$$\left. + \frac{y-y_0}{2}\ln\left(\frac{x^2+(y-y_0)^2}{y_0^2}\right) + \frac{y+y_0}{2}\ln\left(\frac{x^2+(y+y_0)^2}{y_0^2}\right)\right]. \quad (7)$$

The solution (7) satisfies the following discontinuity condition:

$$\left(\frac{\partial u}{\partial x}\right)_{x\to 0_+} - \left(\frac{\partial u}{\partial x}\right)_{x\to 0_-} = \frac{\Omega_y}{2}(\mathrm{sgn}(y-y_0) + \mathrm{sgn}(y+y_0)). \quad (8)$$

The condition (8) gives the jump $(+\Omega_y)$ for $y > y_0$ and $(-\Omega_y)$ for $y < -y_0$

what corresponds to discontinuity walls inclined in opposite directions which are terminated by twist disclinations of the same sign at $y = \pm y_o$. In the interval $-y_o < y < y_o$ there is not any discontinuity and the jump (8) is zero. This configuration of smectic A layers with opposite discontinuity walls is geometrically similar to the configuration of the so called thin zigzag defect line perpendicular to smectic layers, which separates domains of chiral smectic C liquid crystal with opposite chevron directions discussed in many papers e.g. in Refs. [2, 12 - 14]. The *Mathematica*[11] graphic plot of the solution (7) representing a zigzag defect is shown in Fig. 2. The layer

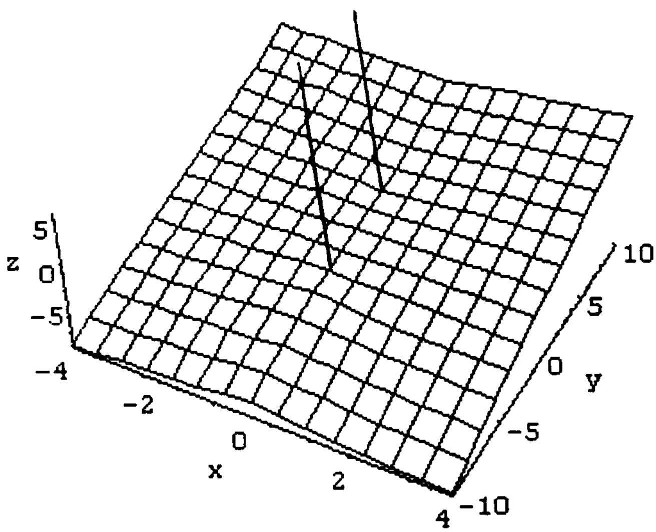

FIGURE 2 Schematic representation of the displacement of one smectic layer forming two half-plane discontinuity walls (along $y > y_o$ and $y < -y_o$ with $y_o = 2$ (in arbitrary units)) of opposite orientations with jumps in layer orientation $\Omega_x = \pm\pi/3$ and terminated at twist disclinations (solid lines parallel to the z-axis) situated at $x = 0$ and $y = \pm y_o$.

deformation in Fig. 2 is very similar to the model representation[13] of deformed smectic layers near zigzag defect using folded paper sheets.

DISCUSSION

A smectic A liquid crystal with elasticity described by a free energy density (1) was taken as a model material for the simple description of a special type of discontinuity wall terminated by a line disclination. This discontinuity wall terminated by disclination can be described analytically by equation (5). The twist disclination is oriented perpendicularly to smectic layers and solution (5) in an infinite media is valid far from the disclination line and from the discontinuity wall.

The present solution is thus complementary to that one in Ref. [15] where a disclination was oriented parallel to layers. Then the layer compression cannot be neglected and we deal with a wedge disclination terminating the so called curvature wall[1].

The model of a zigzag line between chevrons of opposite orientation is of particular interest. In Refs. [2, 12 - 14] the geometry of layer deformation near a zigzag line was well established and the dependence of the layer inclination angle Ω_i as a function of the temperature and anchoring conditions was measured and $\Omega_i \leq 18°$ was found[12]. The layer geometry near a zigzag line schematically modeled by folded paper sheets[13, 16] can be described, at least for small Ω_i, by solution (7). In the future publication[17] the elastic energy of a zigzag line in S_A liquid crystal will be estimated what can be a starting point to the real case of a chiral smectic C liquid crystal.

Acknowledgments
This work was supported by Grant No.: 202/99/1120 of the Grant Agency of the Czech Republic.

References

[1] M. Kléman, *Points, Lines and Walls in Liquid Crystals, Magnetic Systems and Various Ordered Media* (J. Wiley, Chichester 1983).
[2] N.A. Clark, and T.P. Rieker, *Phys. Rev.* **A37**(3), 1053 (1988).
[3] I. Dierking. F. Giesselmann, J. Schacht, and P. Zugenmaier, *Liquid Crystals* **19**(2), 179 (1995).
[4] R.F. Shao, P.C. Willis, and N.A. Clark, *Ferroelectrics* **121,** 127 (1991).
[5] A. Iida, T. Noma, and K. Hirano, *Ferroelectrics* **149,** 117 (1993).
[6] Y. Takanishi, A. Iida, K. Ishikawa. H. Takezoe, and A. Fukuda, *Jpn J. Appl. Phys.* **35,** 683 (1996).
[7] Y. Pomerau, *C.R. Acad. Sci. Paris,* **320I,** 975 (1995).
[8] S. Chaib, F. Melo, and J.-C. Geminard, *Phys. Rev. Lett.* **80**(11), 2354 (1998).
[9] E. Cerda, and L. Mahadevan, *Phys. Rev. Lett.* **80**(11), 2358 (1998).
[10] P.G. de Gennes, and J. Prost, *The Physics of Liquid Crystals* (2^{nd} edition, Oxford University Press, 1993).
[11] S. Wolfram : Mathematica (3^{rd}edition, Cambridge University Press, 1996).
[12] N.A. Clark, T.P. Rieker, and J.E. Maclennan, *Ferroelectrics* **85**, 467 (1988).
[13] Y. Ouchi, H. Takano. H. Takezoe, and A. Fukuda, *Jpn. J. Appl. Phys.* **27**(1), 1 (1988).
[14] A. Fukuda, Y. Ouchi, H. Arai, H. Takano, K. Ishikawa, and H. Takezoe, *Liquid Crystals* **5**(4), 1055 (1989).
[15] L. Lejček. *Czech. J. Phys.* **B40,** 1250 (1990).
[16] L. Limat. *Europhys. Lett.*, **44**(2), 205 (1998).
[17] L. Lejček, *Czech. J. Phys.*, to be published.