This article was downloaded by: [Tomsk State University of Control Systems and Radio]

On: 19 February 2013, At: 10:56

Publisher: Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered

office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics

Publication details, including instructions for authors and subscription information:

http://www.tandfonline.com/loi/gmcl17

Disclinations and Point-like Impurities in S_C^* Liquid Crystals

Lubor Lejček ^a

^a Institute of Physics, Czechoslovak Acad. Sci., Na Slovance 2, 18040, Prague, 8, Czechoslovakia

Version of record first published: 22 Sep 2006.

To cite this article: Lubor Lejček (1990): Disclinations and Point-like Impurities in S_C^* Liquid Crystals, Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 192:1, 245-249

To link to this article: http://dx.doi.org/10.1080/00268949008035636

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.tandfonline.com/page/terms-and-conditions

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Mol. Cryst. Liq. Cryst. 1990, Vol. 192, pp. 245-249 Reprints available directly from the publisher Photocopying permitted by license only © 1990 Gordon and Breach Science Publishers S.A. Printed in the United States of America

DISCLINATIONS AND POINT-LIKE IMPURITIES IN $S_{\mathbb{C}}*$ LIQUID CRYSTALS

LUBOR LEJČEK Institute of Physics, Czechoslovak Acad. Sci., Na Slovance 2, 18040 Prague 8, Czechoslovakia

Abstract The elastic Green function is used to determine the molecular orientation caused by disclinations of an arbitrary shape in chiral smectic C liquid crystals and their interaction energy. A special case - infinitesimal disclination loop is used to model point-like impurities.

INTRODUCTION

The investigation of properties of disclinations of an arbitrary shape in chiral smectic ($S_{\mathbb{C}}*$) liquid crystals can be based, analogously to dislocations in solids, on infinitesimal disclination loops¹.

Infinitesimal disclination loops have been used to model point-like impurities in $S_{\mathbb{C}}*$ (Refs. 2,3). In this note we use the concept of the $S_{\mathbb{C}}*$ elastic Green function to describe the orientation of $S_{\mathbb{C}}*$ molecules around a disclination loop with either infinitesimal or finite area. Also the interaction energy between disclinations will be represented by line integrals of Green function. Our study is limited to the elastic part of free energy density 4 fel describing $S_{\mathbb{C}}*$ sample with smectic layers perpendicular to x_3 -axis. Layers are supposed to be strictly parallel with fixed molecular tilt angle. Then the free energy density f_{el} can be approximated as

$$f_{el} = (B_{1}/2)((\partial \phi/\partial x_{1})^{2} + (\partial \phi/\partial x_{2})^{2}) + (B_{3}/2)(-\partial \phi/\partial x_{3} + q)^{2}.$$
(1)

Elastic constants of S_C* are B_1 and B_3 , q is connected with the S_C* helicoidal pitch p as $q=2\pi/p$. Angle $\Phi(x_1,x_2,x_3)$ is the angle between t-vector and x_1 -axis (Fig. 1). As in Ref. 3, t-vector is the projection of S_C* molecules onto a smectic layer which coincides with the plane (x_1,x_2) .

GREEN FUNCTION

The angle Φ which minimazes f_{el} can be written as $\Phi = qx_3 + \varphi(x_1,x_2,x_3)$. The function φ is an inhomogeneous correction to the perfect helicoidal order. The Green function G_{33} ($\vec{r} - \vec{r}$) satisfies the equilibrium equation \vec{r}

$$B_{1} (G_{33,11} + G_{33,22}) + B_{3}G_{33,33} + \delta(\vec{r} - \vec{r}') = 0 .$$
 (2)

Derivatives $\eth^2 G_{33}/\partial x_i \partial x_j$ or $\eth G_{33}/\partial x_k$ are shortened as $G_{33,ij}$ or $G_{33,k}$. Green function component G_{33} ($\vec{r}-\vec{r}$) gives the rotation φ of \vec{t} -vector at $\vec{r}=(x_1,x_2,x_3)$ caused by the x_3 -component of a unit moment of a point force at $\vec{r}_3=(x_1^\prime,x_2^\prime,x_3^\prime)$. The solution of (2) for an infinite medium can be written as

Using G_{33} the rotation of \vec{t} -vector around a disclination loop of an arbitrary shape characterized by a Frank vector $\vec{\Omega}_{-} = (0,0,\Omega_{-3})$ is in the form³

$$\varphi = -\Omega_3 \int_{\Lambda} G_{\hat{\mathbf{r}}}(\hat{\mathbf{r}} - \hat{\mathbf{r}}') dA_{\hat{\mathbf{i}}}$$
 (4)

with $\vec{G}(\vec{r}-\vec{r}')=(B_1G_{33,1}',B_1G_{33,2}',B_3G_{33,3}')$ Formula (4) is analogous to the expression for displacement caused by a dislocation loop in solids⁵. The summa-

tion rule over repeating indexes from 1 to 3 is assumed. In eq. (4) the integration is carried out over the area A bounded by the disclination line. If $G_{33,i}(\vec{r}-\vec{r}')=G_{33,i}(\vec{r}-\vec{r}')$ which is also valid for G_{33} given by (3) the interaction energy E_I between two disclinations with Frank vectors $\vec{\Omega}_-$ and $\vec{\Omega}_-'$ both parallel to x_3 -axis can be expressed by line integrals

$$E_{I} = \Omega_{3} \Omega_{3}' B_{1} B_{3} \int_{C} \int_{C} G_{33}(\vec{r} - \vec{r}') d\vec{x}_{k} d\vec{x}_{k}', \qquad (5)$$

where C and C´ are the disclination lines, $d\vec{x} = (dx_1, dx_2, dx_3/\cancel{\infty})$ and $d\vec{x}' = (dx_1', dx_2', dx_3'/\cancel{\infty})$. The expression (5) is analogous to Blin´s formula of dislocation interaction in solids⁵.

The disclination self-energy $\rm E_S$ is $\rm E_I/2$ given by (5) with Ω_3 = Ω_3' and integrated along the same contours C and C´ separated only by distance $\rm r_0$ eliminating singularities. The parameter $\rm r_0$ then plays the role of a disclination core radius.

DISCLINATION LOOPS

The self-energy of the rectangular twist disclination loop of the shape shown in Fig. 2 can be evaluated in the form following from (5)

$$E_{S} = \frac{\Omega_{3}^{2}}{2\pi} (B_{1}B_{3})^{1/2} \left[2a \ln \frac{4b \exp(1+(b/a)^{2})^{1/2}}{r_{0}e^{2}(1+(1+(b/a)^{2})^{1/2})} + 2b \ln \frac{4a \exp(1+(a/b)^{2})^{1/2}}{r_{0}e^{2}(1+(1+(a/b)^{2})^{1/2})} \right].$$
(6)

The energy $\rm E_S$ coincides with the expression calculated the other way in Ref. 3. In eq. (6) it is e \approx 2.71828... The solution describing an infinitesimal disclination

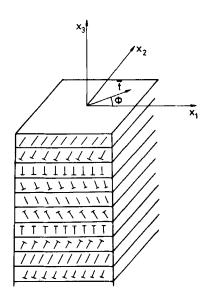


FIGURE 1 Coordinate axes and schematic representation of molecular arrangement in a perfect $S_{\mathbb{C}}*$ liquid crystal. The molecules are represented by nails the points of which are turned toward the observer.

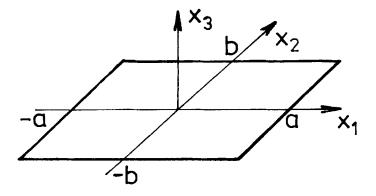


FIGURE 2 Rectangular disclination loop with the dimensions 2a and 2b in \mathbf{x}_1 - and \mathbf{x}_2 -directions, respectively.

loop of a very small area $\delta A_i'$ follows immediately from (4) by replacing the integration over dA; directly by

The interaction between straight 2%-twist disclination and infinitesimal twist disclination loop of rectangular shape shown in Fig. 2 is given by (5) in the form

$$E_{I} = (\delta A \Omega_{3})(B_{1}B_{3})^{1/2} x_{1}/(x_{1}^{2} + (x_{3}/\alpha)^{2}), \qquad (7)$$

where $oldsymbol{\delta}$ A is the loop area. Both 2 $\widetilde{oldsymbol{\pi}}$ -disclination and infinitesimal loop have Frank vectors parallel to x_3 -axis with values 2π and Ω_{-3} , respectively. Point-like impurities in S_{Γ} * like dust particles or foreign chiral or nonchiral molecules which disturb locally S_r* liquid crystal orientation were modeled by infinitesimal disclination loops in Refs. 2,3. Through E_T given by (7) the mobility of 2x-twist disclinations can be reduced by impurities what influences e.g. the temperature change of a helicoidal pitch in finite $S_{f} * samples^{6}$.

REFERENCES

- F. Kroupa, in <u>Theory of Crystal Defects</u>, edited by B. Gruber (Academia, Prague, 1966), p. 275.
- L. Lejček, Mol. Cryst. Liq. Cryst., 151, 411 (1987).
 L. Lejček and F. Kroupa, Czech. J. Phys., B38, 302 (1988).
- 4. L. Bourdon, J. Sommeria and M. Kléman, J. Physique, <u>43</u>, 77 (1982).
- 5. R. de Wit, in Solid State Physics, Vol. 10 (Academic Press, New York, 1962), p. 249. 6. L. Lejček, <u>Czech. J. Phys.</u>, <u>B40</u>, in print.