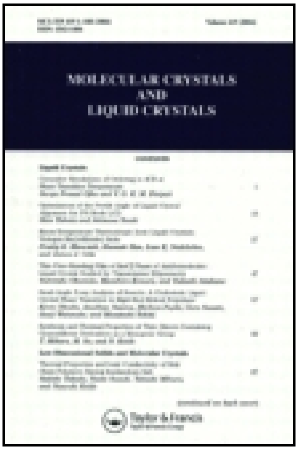

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Lubor Lejček [a]
[a] Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, 18040, Prague 8, Czechoslovakia
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A POINT-LIKE IMPURITY IN CHIRAL SMECTIC C LIQUID CRYSTALS

LUBOR LEJČEK

Institute of Physics, Czechoslovak Academy of Sciences
Na Slovance 2, 18040 Prague 8, Czechoslovakia

Abstract A small impurity which disturbs only the molecular arrangement in one chiral smectic C layer is modelled by a Somigliana twist disclination loop or by a system of infinitesimal twist disclination loops. A binding energy of a 2π-twist disclination pinned to a small impurity is estimated using the interaction energy between a straight 2π-twist disclination and an infinitesimal twist disclination loop.

INTRODUCTION

Smectic liquid crystals can be assumed to contain impurities like dust particles or complexes of foreign molecules. These impurities can be either situated between the layers to create local layer curvature or they can be embedded into the smectic layer thus disturbing the molecular orientation.

In smectic A (S_A) liquid crystals the properties of impurities and their interaction with externally applied stresses were investigated in a general way in Ref. 1. The special case, namely the interaction between a point-like impurity and dislocation in S_A was investigated in Ref. 2. In Ref. 2 the point-like impurity was supposed to be situated between layers and did not disturb the structure of a single layer.

In this note a point-like impurity in an infinite chiral smectic C (S_C*) liquid crystal will be investigated. However, we will deal only with the special case when such an impurity disturbs the molecular order in one smectic layer. This assumption permits us to use the approximation of parallel layers of S_C* when the elastic free energy density can be taken in the form

$$f_{el} = \frac{B_1}{2}\left[\left(\frac{\partial \emptyset}{\partial x_1}\right)^2 + \left(\frac{\partial \emptyset}{\partial x_2}\right)^2\right] + \frac{B_3}{2}\left(-\frac{\partial \emptyset}{\partial x_3} + q\right)^2 . \tag{1}$$

In expression (1) coefficients B_1 and B_3 are elastic constants of S_C*, q is connected with the helicoidal pitch p by the relation $q = 2\pi/p$. Angle $\emptyset$ is the angle between the projection of molecules onto the smectic layer (x_1, x_2) and the x_1-axis[3]. It should be noted that x_3-axis is perpendicular to the plane of smectic layers. The molecular projection in a smectic layer is represented by a $\vec{t}$-vector $\vec{t}$ = $(\cos \emptyset, \sin \emptyset, 0)$. The equilibrium equation $\delta f_{el}/\delta \emptyset = 0$ is the Laplace-type equation from which the Green function component U_{33} (see Ref. 4) can be determined in the form

$$U_{33}(\vec{r} - \vec{r}\,') = \frac{1}{4\pi}\frac{1}{B_1\alpha}\left[(x_1 - x_1')^2 + (x_2 - x_2')^2 + \left(\frac{x_3 - x_3'}{\alpha}\right)^2\right]^{-1/2} , \tag{2}$$

where $\alpha = (B_3/B_1)^{1/2}$ and $\vec{r} = (x_1, x_2, x_3)$. The Green function component U_{33} can be used to evaluate the director distribution near a Somigliana twist disclination loop [4]. If a Somigliana twist disclination loop is characterised by the continuous distribution of rotational vector $\vec{\omega}$ = $(0, 0, \omega_3(x_1', x_2'))$ where x_1' and x_2' are coordinates of a region A in a plane (x_1, x_2), it is [4]

$$\emptyset = qx_3 - B_3 \iint_A dx_1' dx_2' \, \omega_3(x_1', x_2') (\partial U_{33} / \partial x_3') \Big|_{x_3'=0} =$$

$$= qx_3 - \frac{x_3}{4\pi\alpha} \iint_A \frac{\omega_3(x_1', x_2') dx_1' dx_2'}{\left[(x_1 - x_1')^2 + (x_2 - x_2')^2 + (\frac{x_3}{\alpha})^2\right]^{3/2}} \tag{3}$$

If ω_3 is constant, the defect is ordinary (Volterra) twist disclination loop. For an infinitesimal area δA centered to $x_1' = x_2' = 0$ the solution $\emptyset$ corresponding to so called infinitesimal twist disclination loop can be obtained in the form [4]

$$\emptyset = qx_3 - \frac{\omega_3 \delta A}{4\pi\alpha} \frac{x_3}{\left[x_1^2 + x_2^2 + (x_3/\alpha)^2\right]^{3/2}} \tag{4}$$

INFINITESIMAL TWIST DISCLINATION LOOPS AS A MODEL OF A POINT-LIKE IMPURITY IN S_C*

When a point-like impurity like a dust particle or a small cluster of foreign molecules is embedded into the molecular structure of one S_C* layer it leads to a local molecular disorientation. Such a molecular disorientation can be very general and it can depend either on the shape of an impurity or on a chemical interaction between S_C* molecules and an impurity. Thus we will assume that the disorientation of molecules around an impurity in S_C* can be modelled as a Somigliana twist disclination loop or as a distribution of infinitesimal twist disclination loops. Thus the disorientation of $\vec{t}$-vectors around an impurity in S_C* can be described by solution (3) or by a sum of solutions (4). Values of ω_3 should be found from the geometry of an impurity. In Figure 1 the examples of impurities with special shapes are shown

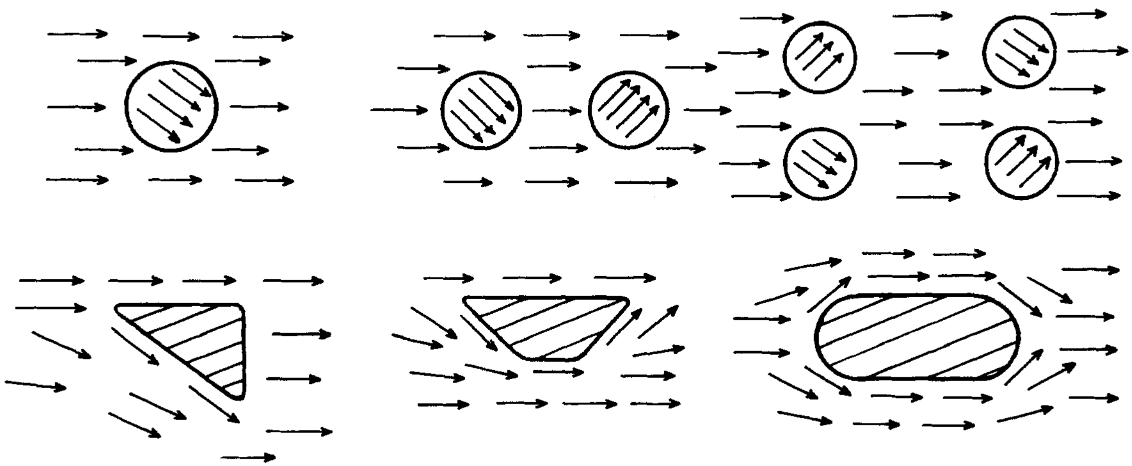

FIGURE 1. Small impurities of a special shape disorienting $\vec{t}$-vector in one S_C* layer and their modelling by infinitesimal twist disclination loops.

(a) A triangular impurity represented by a single infinitesimal twist disclination loop.

(b) A trapezoidal impurity modelled by an infinitesimal twist disclination loop dipole.

(c) An oval impurity and its representation by an infinitesimal twist disclination loop quadrupole.

as viewed from x_3-direction perpendicular to the S_C* layer (plane of Figure 1). An impurity in Figure 1c represented here by an infinitesimal twist disclination loop quadrupole is the most realistic case from those shown in Figure 1.

IMPURITY - STRAIGHT 2π-TWIST DISCLINATION INTERACTION

The interaction energy W_I between a straight 2π-twist disclination lying along x_2-axis and described by a function $\emptyset$ of the type $\mathrm{arctg}(x_3/\alpha x_1)$ and an infinitesimal twist disclination loop can be derived [4] in the form

$$W_I = \omega_3 \delta A (B_1 B_3)^{1/2} x_1/(x_1^2 + (x_3/\alpha)^2) \quad . \tag{5}$$

The binding energy w_B of a straight 2π-twist disclination to an infinitesimal twist disclination loop can be then estimated from Eq. (5) with $x_3 = 0$ and $x_1 = r_0$, where r_0 is the core radius of 2π-twist disclination. It is

$$w_B \approx |\omega_3| \, \delta A \, (B_1 B_3)^{1/2}/r_0 \quad . \tag{6}$$

The value of w_B can give an estimation of a binding energy of 2π-twist disclination to an impurity shown in Figure 1a. The value ω_3 is given by the geometry of an impurity and δA is its cross-section.

An impurity of more general shape as e.g. in Figure 1b,c is, however, represented by infinitesimal twist disclination loop dipole or quadrupole. When a straight 2π-twist disclination is far from an impurity it is $W_I \approx 0$. On the other hand, W_I is more important at small distances from an impurity where the interaction with one infinitesimal twist disclination loop representing an impurity prevails. Then again the estimation of w_B given by Eq. (6) can be used.

If an impurity is fixed in S_C* structure and is passed by a 2π-twist disclination line, there is always the possibility that the disclination can be bound to an impurity. In this way, 2π-twist disclination lines can be pinned in S_C* structure containing impurities.

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