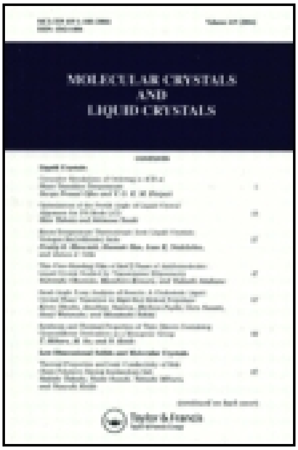

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Disclinations and Point-like Impurities in S_C* Liquid Crystals

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DISCLINATIONS AND POINT-LIKE IMPURITIES IN S_C* LIQUID CRYSTALS

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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_C*) liquid crystals can be based, analogously to dislocations in solids, on infinitesimal disclination loops[1].

Infinitesimal disclination loops have been used to model point-like impurities in S_C* (Refs. 2,3). In this note we use the concept of the S_C* elastic Green function to describe the orientation of S_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] f_{el} describing S_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

$$f_{el} = (B_1/2)((\partial\Phi/\partial x_1)^2 + (\partial\Phi/\partial x_2)^2) + + (B_3/2)(-\partial\Phi/\partial x_3 + q)^2. \quad (1)$$

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 $\vec{t}$-vector and x_1-axis (Fig. 1). As in Ref. 3, $\vec{t}$-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[3]

$$B_1 (G_{33,11} + G_{33,22}) + B_3 G_{33,33} + \delta(\vec{r} - \vec{r}') = 0 . \quad (2)$$

Derivatives $\partial^2 G_{33}/\partial x_i \partial x_j$ or $\partial G_{33}/\partial x_k'$ 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 $\vec{r}_3' = (x_1',x_2',x_3')$. The solution of (2) for an infinite medium can be written as[3]

$$G_{33} = ((x_1-x_1')^2+(x_2-x_2')^2+(x_3-x_3'/\alpha)^2)^{1/2}/4\pi B_1\alpha \quad (3)$$

with $\alpha = (B_3/B_1)^{1/2}$.

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 form[3]

$$\varphi = -\Omega_3 \int_A G_i(\vec{r} - \vec{r}')\, dA_i' \quad (4)$$

with $\vec{G}(\vec{r}-\vec{r}') = (B_1 G_{33,1'}, B_1 G_{33,2'}, B_3 G_{33,3'})$. Formula (4) is analogous to the expression for displacement caused by a dislocation loop in solids[5]. The summation 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

$$E_I = \Omega_3 \Omega_3' B_1 B_3 \int_C \int_{C'} G_{33}(\vec{r}-\vec{r}')\, d\bar{x}_k d\bar{x}_k' , \qquad (5)$$

where C and C′ are the disclination lines, $\vec{d\bar{x}} = (dx_1, dx_2, dx_3/\alpha)$ and $\vec{d\bar{x}}' = (dx_1', dx_2', dx_3'/\alpha)$. The expression (5) is analogous to Blin′s formula of dislocation interaction in solids[5].

The disclination self-energy E_S is $E_I/2$ given by (5) with $\Omega_3 = \Omega_3'$ and integrated along the same contours C and C′ separated only by distance r_0 eliminating singularities. The parameter 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)

$$E_S = \frac{\Omega_3^2}{2\pi} (B_1 B_3)^{1/2} \left[2a \ln \frac{4b \exp(1+(b/a)^2)^{1/2}}{r_0 e^2 (1+(1+(b/a)^2)^{1/2})} + 2b \ln \frac{4a \exp(1+(a/b)^2)^{1/2}}{r_0 e^2 (1+(1+(a/b)^2)^{1/2})} \right]. \qquad (6)$$

The energy 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

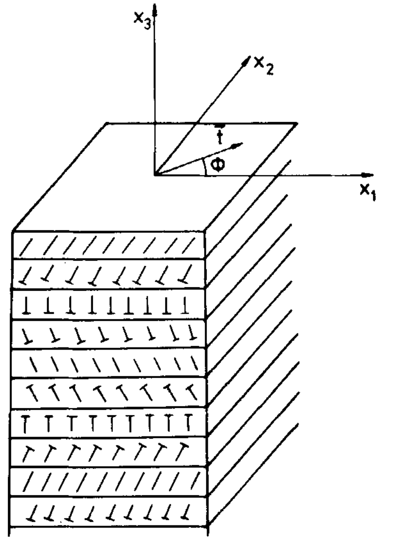

FIGURE 1 Coordinate axes and schematic representation of molecular arrangement in a perfect S_C* liquid crystal. The molecules are represented by nails the points of which are turned toward the observer.

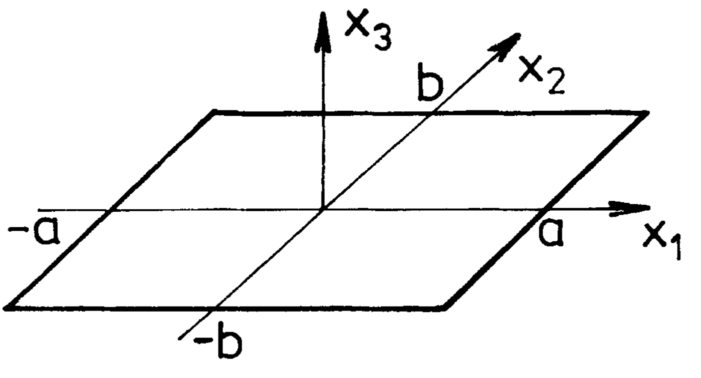

FIGURE 2 Rectangular disclination loop with the dimensions 2a and 2b in x_1- and x_2-directions, respectively.

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

The interaction between straight 2π-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 δA is the loop area. Both 2π-disclination and infinitesimal loop have Frank vectors parallel to x_3-axis with values 2π and Ω_3, respectively. Point-like impurities in S_C* like dust particles or foreign chiral or nonchiral molecules which disturb locally S_C* liquid crystal orientation were modeled by infinitesimal disclination loops in Refs. 2,3. Through E_I given by (7) the mobility of 2π-twist disclinations can be reduced by impurities what influences e.g. the temperature change of a helicoidal pitch in finite S_C* samples[6].

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