Screw dislocation interaction in smectic A liquid crystals in an anharmonic approximation

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ABSTRACT

The interaction of two screw dislocations in smectic-A liquid crystals is treated using an anharmonic correction to the elastic energy density. In the present contribution the elastic energy and the force between two screw dislocations is evaluated and discussed. It is shown that the interaction force has the similar behavior as in the case of screw dislocations in solids.

Keywords: screw dislocations, anharmonic term, smectic A

1. Introduction

The classical solution describing a screw dislocation in the system of smectic layers of the smectic A liquid crystal is known for long time [1 - 4]. This classical solution determined within the smectic elasticity described by the elastic constant of layer curvature $K$ and the layer compression $B$ in infinite medium has the zero self-energy. Similarly, the interaction energy of two screw dislocations calculated in infinite medium is also zero [3,4].

On the other hand, when an anharmonic correction of layer compression to the smectic elasticity is taken in account, the contribution to the elastic self-energy of screw dislocation is non-zero [3, 4, 6]. This anharmonic contribution was also used to determine the critical undulations of smectic layers subjected to the dilatational deformations [4].

Screw dislocations were treated not only in linear approach as in [1,2] but also in non-linear approach, see e.g. [5, 7, 8]. Then the screw dislocation interaction in non-linear approach can

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be approximately determined [5] giving approximately logarithmic dependence for dislocation separations much greater then dislocation core radius.

In [7] the energy of a wall formed of parallel screw dislocations in the smectic-A was evaluated using anharmonic term and discussed in the connection with twist-grain-boundaries.

A classical solution of screw dislocation was reexamined in [9]. There screw dislocation deformation is modelled as a hollow cylinder of inner radius $r_c$ and outer radius $R$ with proper boundary conditions. In [9] a solution describing the screw dislocation in the cylinder of finite radius $R$ contains other terms with respect to the classical solution [1 - 4]. It should be noted, however, that in the limit of infinite outer radius $R$, i.e. $R \to \infty$, the solution given in [9] is transformed to the classical solution for the screw dislocation. When calculating the screw dislocation self-energy, Ref. [9] considers not only the classical elastic energy density but also adds the term proportional to the anharmonic correction to the energy (see expression $U_2$ in (17) of [9]). Then the energy $U_2$ leads to the Kléman´s contribution [6] of the screw dislocation energy in the limit $R \to \infty$.

In the present contribution we will examine the classical problem of the interaction of two isolated screw dislocations in infinite smectic A liquid crystal. The anharmonic approximation [4] used in this contribution gives the expression for the interaction energy and for the force between dislocations in the analytical form. Anyway, the anharmonic term is just a corrective term. It gives interaction forces between screw dislocations about of two orders smaller as compared with edge dislocation interaction forces.

In this contribution the screw dislocation core is not treated as it was well discussed e.g. in [10, 11].

2. The free energy density of smectic A liquid crystal

Let the system of smectic layers is parallel to the plane $(x,y)$ and the layer normal oriented along the $z$-axis is perpendicular to layers (Fig. 1). The free energy density $f$ of smectic A liquid crystal can be written in the well-known form [3, 4, 12]:

$$f = \frac{B}{2} \left( \frac{\partial u}{\partial z} \right)^2 + \frac{K}{2} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)^2,$$

where $u$ is the layer displacement in $z$-direction. Parameter $B$ is the layer compression elastic constant and $K$ is the elastic constant characterizing the smectic layer curvature in one-constant approximation.
Fig. 1: Smectic A layers and coordinate system. \( b \) is the smectic layer thickness and the Burgers vector.

Supposing the screw dislocation be parallel to the \( z \)-direction we expect that the dislocation displacement does not depend on the \( z \) coordinate. Therefore the calculus of variation applied to the dislocation energy

\[
\int \nu f \, dV, \tag{2}
\]

leads to the equilibrium equation:

\[
\Delta \Delta u = 0, \tag{3}
\]

where \( \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \) and \( u = u(x, y) \).

The classical solution describing the screw dislocation in an infinite smectic A liquid crystal was found in form [1 - 4]:

\[
u = \frac{b}{2\pi} \arctan \frac{y}{x}, \tag{4}
\]

with \( b \) as the value of Burgers vector oriented along the \( z \)-direction. The solution (4) satisfies the condition:

\[
\oint_{\Gamma} du = b, \tag{5}
\]

where the integral taken along the closed loop \( \Gamma \) around the dislocation core gives the value of Burgers vector \( b \).

Eq. (1) immediately shows that the self-energy of the screw dislocation (4) is zero. Therefore, to find a contribution to the non-zero self-energy and thus the contribution to the elastic interaction energy of two screw dislocation, we add the anharmonic term in the form [4]:

\[
\frac{b^8}{8} \iint \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)^2 dxdy. \tag{6}
\]

In (6) we integrate over the surface of smectic layer (note that energy (6) is the energy per unit length of dislocation in \( z \)-direction).

The insertion of solution (4) into (6) and the use of polar coordinates \( x = r \cos \varphi, y = r \sin \varphi \) permits the evaluation of integral (6) as:

\[
\frac{Bb^4}{128\pi^4} \int_0^{2\pi} d\varphi \int_R^{\infty} \frac{r \, dr}{R^4} = \frac{Bb^4}{128\pi^3} \left( \frac{1}{r_c^2} - \frac{1}{R^2} \right) \to \frac{Bb^4}{128\pi^3 r_c^2}, \tag{7}
\]
in the limit $R \to \infty$. Parameter $r_c$ is the core radius introduced to avoid the singularity at $r = 0$. The energy given by (7) is the contribution of the screw dislocation self-energy in anharmonic approximation first introduced by Kléman [6] (see also [4]).

3. Force between two screw dislocations in anharmonic approximation

Now, the integral (6) will be evaluated for two screw dislocations, one situated at the coordinate origin and described by the solution $u_1 = \frac{b_1}{2\pi} \arctan \frac{y}{x}$ with Burgers vector $b_1$ and the other by the solution $u_2 = \frac{b_2}{2\pi} \arctan \frac{y-y_0}{x-x_0}$ with Burgers vector $b_2$ situated at coordinates $x_0$ and $y_0$. The coordinates $x_0$ and $y_0$ can be written in polar coordinates as: $x_0 = r_o \cos \phi_o$ and $y_0 = r_o \sin \phi_o$. The radial distance between two dislocations in polar coordinates is $r_o$.

Then the solution describing two screw dislocations can be written as:

$$u = u_1 + u_2. \quad \text{(8)}$$

The anharmonic contribution is expressed as:

$$\frac{B}{128\pi^4} \left( \frac{b_1 b_2 r^2 + b_1^2 r^2 + b_2^2 r^2 - 2b_1(b_1 + b_2)rr_o \cos(\phi - \phi_o)}{r^4(r^2 - r_o^2 - 2rr_o \cos(\phi - \phi_o))} \right)^2. \quad \text{(9)}$$

First, we integrate expression (9) by the coordinate $\phi$ in the interval $\phi \in (0,2\pi)$ and we obtain using Mathematica [13] the expression:

$$I_{r_o} = \frac{B}{128\pi^4} \left\{ \frac{2\pi b_1^2 (b_1 + b_2)^2}{r_o^4} + \frac{\pi b_2}{(r^2 - r_o^2)^2} \left( \frac{1}{(r + r_o)(r - r_o)} + \frac{1}{(r^2 - r_o^2)} \right) \left( \frac{4b_1 b_2 r^4 (r^2 - r_o^2)}{r^2 - r_o^2} + \frac{b_1^2 r^2 (r^2 - r_o^2)^2}{2} + \frac{b_2^2 r (r^2 - r_o^2)^2}{2} + \frac{b_1 b_2 r (5r^2 - r_o^2)^2}{2} \right) \right\}. \quad \text{(10)}$$

Expression (10) has the singularities at $r = 0$ and at $r = r_o$ where dislocations are situated. The total elastic energy of two screw dislocations, $E_T$, can be evaluated as the integral:

$$E_T = \int_{r_o}^{r_o + r_c} I_{r_o} r dr + \int_{r_o + r_c}^{R} I_{r_o} r dr. \quad \text{(11)}$$

Expression (11) is the dislocation elastic self-energy per unit length of dislocation in $z$-direction. Parameter $r_c$ in expression (11) is used to avoid the singularities. Integral (11) is divided into two parts as $|r - r_o| = r_o - r$ for the first integral and $|r - r_o| = r - r_o$ for the second one.

Using Mathematica [13], integral (11) can be evaluated as:
\[
E_T = \frac{B(b_1+b_2)^2}{128\pi^3} \left( \frac{1}{r_c^2} - \frac{1}{(r_c+r_0)^2} \right) + 
\frac{B}{128\pi^3} \left[ \frac{b_1^2(b_1+4b_1b_2+2b_2^2)}{(r_c+r_0)^2} + \frac{b_2^2r_0^2}{(r_c+r_0)^2} + \frac{b_2^2(4b_1+b_2)}{r_c(r_c+2r_0)} + \frac{2b_2^2}{r_0^2} \ln \left( \frac{(r_0+r_c)^2}{r_c(r_c+2r_0)} \right) \right].
\] (12)

Adding parameter \( r_c \) to the distance \( r_0 \) between both dislocations we can do limit \( r_0 \to 0 \) in (12) avoiding singularities and we obtain the expression:

\[
\frac{B(b_1+b_2)^4}{128\pi^3 r_c^2}.
\] (13)

which is the elastic self-energy of the dislocation with Burgers vector \((b_1 + b_2)\) in anharmonic correction. Expression (13) is similar to (7) in which \( b \) is changed to \((b_1 + b_2)\).

Using \( E_T \), the force between two screw dislocations can be calculated. As \( E_T \) depends on the distance between dislocations \( r_0 \) only, the force is radial an it can be evaluated as \( F_{r_0} = -\frac{\partial E_T}{\partial r_0} \).

Using Mathematica and denoting \( t = r_o/r_c \) we obtain:

\[
F_{r_0} = \frac{BB_2}{64\pi^3 r_c^3} \frac{1}{t^3} \left[ t^2 \left( b_2^3 t(1+t)^4 + 4b_1 b_2^2 t(1+t)^3(1+2t) + 2b_2^3 t(1+2t)^3 - b_2 r_0^2 (1+2t)^2 \right) (1+t)^3(1+2t)^3 \right] + 4b_2 b_2^2 t^2 \ln \left( \frac{(1+t)^2}{1+2t} \right).
\] (14)

Force (14) is the force acting on dislocations per dislocation unit length in \( z \)-direction.

4. Discussion

Expression (14) for the force between two screw dislocations can be simplified in the following important cases when we deal either with dislocations of the same sign and the same value of Burgers vector or when Burgers vectors have opposite signs.

First, let us suppose \( b_1 = b_2 = b \) where the value of Burgers vector \( b \) is equal to the thickness of the smectic layer. Then the force given by (14) takes the form:

\[
F_{r_0} = \frac{Bb^4}{64\pi^3 r_c^3} \frac{1}{t^3(1+t)^3(1+2t)^3} \left[ t^2(-4 - 16t - 10t^2 + 30t^3 + 40t^4 + 9t^5) + 4(1 + 3t + 2t^2)^3 \ln \left( \frac{(1+t)^2}{1+2t} \right) \right].
\] (15)

Fig. 2 shows the force \( F_{r_0}/(\frac{Bb^4}{64\pi^3 r_c^3}) \) as the function of \( t \):
The force between two screw dislocations of the same sign as the function of their separation $\frac{r_o}{r_c}$. The inserted scheme shows the corresponding configurations of two screw dislocation lines (oriented lines) with the same Burgers vectors $b$ (parallel arrows) separated at distance $r_o$.

The force between dislocations having the same sign is positive which means that dislocations repulse each other in the anharmonic approximation. In the limit $t \to 0$ there is the divergence in the force. This behavior is the same as the well-known interaction of dislocations of the same sign known also from solids.

Now, we will suppose $b_1 = b$, $b_2 = -b$. Then the force (14) can be expressed as:

$$F_{r_o} = -\frac{Bb^4}{64\pi^3 r_c^3} \frac{1}{t^3} \left[ \frac{t^2(4+28t^2+74t^3+90t^4+48t^4+7t^5)}{(1+3t+2t^2)^3} - 4\ln \left( \frac{(1+t)^2}{1+2t} \right) \right].$$  \hspace{1cm} (16)

The force between two screw dislocation of opposite sign is shown in Fig. 3:
Fig. 3: The force between two screw dislocations of the opposite sign as the function of their separation \( \frac{r_o}{r_c} \). The inserted scheme shows the corresponding configurations of two screw dislocation lines (oriented lines) with the opposite Burgers vectors \( b \) and \(-b\) (antiparallel arrows) separated at distance \( r_o \).

The force \( F_{r_o} \) in Fig. 3 is negative. It corresponds to the attraction of two opposite screw dislocations in the anharmonic approximation, what was expected from the analogous behavior of dislocations in solids. However, in solids described by linear elasticity, there is a divergence of the force for \( r_o \to 0 \). For screw dislocations in anharmonic approximation of smectic A liquid crystal the force is decreasing for decreasing \( r_o \) up to about \( r_o \sim 3r_c \). In the interval \( 0 \leq r_o < 3r_c \) the influence of anharmonic approximation appears which gives \( F_{r_o} \to 0 \) when \( r_o \to 0 \).

Now, let us compare force of edge dislocations interaction with the force of screw dislocation interaction. The force component \( F_x \) of edge dislocations having Burgers vectors \( b_1 \) and \( b_2 \) can be written as [4]:

\[
F_x = \frac{BB_1b_2}{8\sqrt{\pi\lambda}} \frac{x_o}{|x_o|^{3/2}} \exp\left(-\frac{x_o^3}{4\lambda|x_o|}\right),
\]  

(16)
with one dislocation situated at the coordinate origin and the second at position \((x_o, z_o)\).

Parameter \(\lambda\) in (16) is defined as \(\lambda = \sqrt{\frac{K}{B}}\).

The comparison of \(F_x\) for \(b_1 = b_2 = b\) at \(x_o = z_o = b\), \(\lambda \sim b\) with \(F_{r_o}\) at \(t = 1\) (with \(r_c \sim b\)) gives:

\[
\frac{F_x}{F_{r_o}} = \frac{64\pi^3}{8\sqrt{\pi}} \exp\left(-\frac{1}{4}\right) \sim 100.
\]  (17)

Therefore we can conclude that the force between two screw dislocations is about two order smaller than the force between edge components. The force between screw dislocations evaluated at the anharmonic approximation can be taken as a correction in cases when we deal with individual screw dislocations only.

On the other hand, the case of TGB phases modelled by screw dislocation walls is rather complex structure. Screw dislocation walls in TGB phases were treated e.g. in [14] as the continuous distribution of screw dislocations. The evaluation of their elastic energies in anharmonic approximation in [7] gave both their self-energies and interaction energies. It is interesting that interaction energies of screw dislocations in screw dislocation wall is proportional to \(r_o^{-5}\).

The interaction force between two single screw dislocations in anharmonic approximation is proportional to \(r_o^{-2}\). This difference in the force behavior can be understood in the analogy with solids [15] where the interaction of the edge dislocations with the tilt wall decreases also more rapidly as compared with the interaction of two individual dislocations.

The nucleus of TGB phase in the form of filaments composed of finite blocks which are relatively rotated to each other by screw dislocation walls (see e.g. [16, 17]) is a more realistic case compared to TGB phases modelled just by blocks infinite in two dimensions [4, 12, 18] and separated by screw dislocation walls in the dimension parallel to the chiral axis. In filaments, the screw dislocation walls forming with edge dislocation walls finite dislocation loops. Edge dislocation walls mediate the nucleation of TGB phase in unperturbed smectic-A layers surrounding TGB filaments. When dealing with dislocation loops having both screw and edge dislocation segments, interactions between screw dislocations can be neglected with respect to the edge ones. In [16, 17] the energy of dislocation loops was taken principally as a line energy of loops, i.e. composed by the self-energies of edge and screw line dislocation segments, their interaction energies being neglected. The comparison of the elastic self-energy with the interaction energy of edge dislocations in [17] showed that the self-energy is about an order of magnitude greater than the interaction energy in the present study. The estimations also showed that interaction forces between screw dislocations are of the order smaller than interaction forces between edge dislocations. Thus we can conclude that our previous approximations in [16, 17] were valid.

5. Conclusions

Anharmonic correction to the elastic free energy of smectic A liquid crystal enables to evaluate the interaction force between two parallel screw dislocations as the function of their separation. The interaction between dislocations behaves analogously as in solids, i.e. dislocations of the same sign repulse each other while dislocations of the opposite sign are
mutually attracted. Effects of non-linearity of interaction appear when dislocations are approaching each other, say up to distances $r \sim 3r_c$. However, the interaction force between two screw dislocations is about two order smaller than this of edge dislocations. One can conclude that the corrective interaction force between two screw dislocations calculated within an anharmonic approximation is important only in cases where we deal with long and isolated segments of screw dislocations in the smectic-A.

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