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Point-like impurity–dislocation interactions in smectic A liquid crystals

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The displacement field created in the neighbourhood of a point-like impurity, its self-energy and point-like impurity–dislocation interaction are calculated for a smectic A liquid crystal in the approximation of small deformations. The binding energy of a point defect to an edge dislocation is also estimated. The use of the Peach–Kochler formula as a basis for the calculation of the dislocation interaction with other defects is discussed.

1. Introduction

Linear defects, such as dislocations and disclinations, in layered liquid crystals have been thoroughly studied because of their clear evidence in optical microscope observations. A review of these studies can be found, for example, in the book by Kléman [1]. On the other hand, point defects are usually more localized and thus hardly noticeable in these observations. However, it can be assumed that liquid crystals can contain impurities like dust particles or complexes of foreign molecules. Those impurities can be either embedded into the smectic layer thus disturbing the molecular orientation or they can be situated between the layers to create a local layer curvature.

The properties of impurities and their interaction with externally applied stresses in smectic A (S_A) liquid crystals have been investigated in a general way [2]. In this contribution the special case, namely the interaction between a point-like impurity and dislocations in a S_A is presented. We assume such a point impurity which, situated between the layers, does not disturb the structure of a single layer in a S_A liquid crystal. This study is based on the use of the elastic free energy density, f_{el}, of a S_A liquid crystal. The energy density is taken to have the form

$$f_{el} = \frac{K}{2}\left[\left(\frac{\partial^2 u}{\partial x^2}\right)^2 + \left(\frac{\partial^2 u}{\partial y^2}\right)^2 + 2\left(\frac{\partial^2 u}{\partial x \partial y}\right)\right] + \frac{\bar{B}}{2}\left(\frac{\partial u}{\partial z}\right)^2. \tag{1}$$

Here the function $u = u(x, y, z)$ describes a small displacement of S_A layers in the direction of their normal, chosen along the z direction. The elastic properties of a smectic A liquid crystal are described by the constants K and $\bar{B}$.

Expression (1) is the isotropic limit of the part of the free energy density of a smectic C liquid crystal which describes the deformation energy connected with layer curvature [3]. The free energy density (cf. equation (1)) differs from the expression usually used for the elastic part of the S_A free energy density

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

which will be called the classical result by the term

$$\Delta_{el} = K\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \left(\frac{\partial^2 u}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2}\right). \tag{3}$$

In calculations of total elastic energy E,

$$E = \int f_{el}\, dV, \tag{4}$$

the term Δ_{el} can sometimes be important thus giving a difference between the total energies calculated using equation (1) or (2) in expression (4) as shown by Kléman and Lejček [4] and discussed recently by Dahl and Lagerwall [5]. However, expression Δ_{el} is a divergence term and thus does not influence the equilibrium equation for bulk liquid crystals

$$K\Delta\Delta u - \bar{B}\frac{\partial^2 u}{\partial z^2} = 0, \quad \left(\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right), \tag{5}$$

which follows from the variation of expression (4) with (1) or (2). The importance of the term Δ_{el} on the elastic interaction energy between defects in S_A liquid crystals and its connection with the use of the Peach–Koehler formula for configurational forces acting on defects is discussed in the Appendix.

By analogy with solids, stress components σ_{i3} ($i = 1, 2, 3$) acting on a smectic A layer can be introduced [1] in the form

$$\sigma_{13} = -K\frac{\partial}{\partial x}\Delta u, \quad \sigma_{23} = -K\frac{\partial}{\partial y}\Delta u, \quad \sigma_{33} = \bar{B}\frac{\partial u}{\partial z}. \tag{6}$$

The stresses σ_{i3} are the same for both S_A free energy densities in equations (1) and (2) and equation (5) is equivalent to the expression

$$\frac{\partial \sigma_{13}}{\partial x} + \frac{\partial \sigma_{23}}{\partial y} + \frac{\partial \sigma_{33}}{\partial z} = 0.$$

2. Isolated point-like impurity

Let a point-like impurity be situated at the origin of the coordinate system. The introduction of this point impurity between S_A layers (cf. figure 1) leads then to the local change of volume, δV. The solution corresponding to this point impurity should follow from the equilibrium equation (5) valid in the total space with the exception of the coordinate origin. Equation (5), rewritten in the form

$$\left(\Delta + \frac{\partial}{\partial \bar{z}}\right)\left(\Delta - \frac{\partial}{\partial \bar{z}}\right) u = 0,$$

where $\bar{z} = z/\lambda$ and $\lambda = (K/\bar{B})^{1/2}$, can be solved generally using, for example, de Gennes method [6]. Here we investigate the properties of the simplest solution u^- which fulfils the equations

$$\left(\Delta - \frac{\partial}{\partial \bar{z}}\right) u^- = 0 \quad \text{for} \quad z > 0 \tag{8a}$$

and

$$\left(\Delta + \frac{\partial}{\partial \bar{z}}\right) u^- = 0 \quad \text{for} \quad z < 0. \tag{8b}$$

At the coordinate origin the solution u^- should have a singularity of the δ-function type.

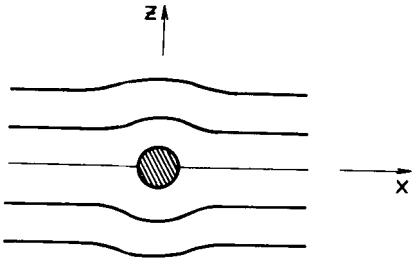

Figure 1. A small point-like impurity between smectic A layers, an example of a point-like impurity with a spherical shape.

The solution with the desired singularity can be written in the form

$$u^{-}(x,y,z) = \frac{c}{2\lambda z}\exp[-(x^2 + y^2)/4\lambda|z|], \tag{9}$$

with c an arbitrary constant, the connection of which with δV will be shown later. The displacement u^{-} given by equation (9) has the same form as the Green function of equation (8) found in [2]. The other simple solution which holds for equation (8 *a*) for $z < 0$ and for equation (8 *b*) for $z > 0$ is

$$u^{+}(x,y,z) = \frac{c}{2\lambda z}\exp[(x^2 + y^2)/4\lambda|z|].$$

The function u^{+} becomes infinite far from the origin and thus it does not represent a small inclusion or a point-like impurity at the origin.

The volume change δV in a smectic liquid crystal surrounding the point impurity described by a displacement $\mathbf{u}$ is defined as

$$\delta V = \int_S \mathbf{u}\,\mathrm{d}\mathbf{S}, \tag{10}$$

where S is a closed surface enveloping the point impurity. For the point impurity described by the solution u^{-} the cylindrical closed surface of radius R and limited at $z = \pm z_0$ can be chosen. Then in cylindrical coordinates $x = r\cos\phi$, $y = r\sin\phi$, $z = z$ the volume change δV can be expressed as

$$\begin{aligned}\delta V &= \int_0^R r\,dr \int_0^{2\pi} d\varphi[u^{-}(r, z = z_0) - u^{-}(r, z = -z_0)],\\ &= \frac{2\pi c}{\lambda z_0}\int_0^R r\,dr \exp\left(-\frac{r^2}{4\lambda|z_0|}\right),\\ &= 4\pi c\left[1 - \exp\left(-\frac{R^2}{4\lambda|z_0|}\right)\right];\end{aligned}$$

for $R^2 \gg 4\lambda|z_0|$ it is $\exp(-R^2/4\lambda|z_0|) \approx 0$. Then $\delta V = 4\pi c$ for all cylindrical surfaces with radii $R > 2(\lambda z_0)^{1/2}$ and $z_0 > 0$.

The energy E_s in smectic A liquid crystals due to the introduction of a point-like impurity between the layers can be calculated using expressions (1), (4) and (9). In cylindrical coordinates the energy E_s is given by

$$E_s = \frac{\bar{B}c^2}{8\lambda^2}\int_0^{2\pi} d\varphi \int_0^{+\infty} r\,dr \int_0^{+\infty} dz\, Q(r,z), \tag{11}$$

where

$$Q(r,z) = \left(3 - \frac{3r^2}{2\lambda z} + \frac{r^4}{4\lambda^2 z^2}\right)\exp\left(-\frac{r^2}{2\lambda|z|}\right)\Big/ z^4.$$

The integrals in (11) are infinite for $r \to 0$ or $z \to 0$. By introducing cut-off parameters r_0 and ξ in integrals over r and z, respectively, we can calculate E_s given by (11) approximately as

$$E_s \approx \frac{\bar{B}c^2}{8\lambda^2}\int_0^{2\pi} d\varphi\,\frac{1}{2}\left[\int_{r_0}^{+\infty} r\,dr\int_0^{+\infty} dz\,Q(r,z) + \int_0^{+\infty} r\,dr\int_{\xi}^{+\infty} dz\,Q(r,z),\right.$$

$$\left. = \frac{\pi\bar{B}c^2\lambda}{r_0^4}\left(3 + 2\frac{r_0^4}{(4\lambda\xi)^2}\right)\right]. \tag{12}$$

The parameters r_0 and ξ characterize a cylindrical surface with volume $\delta V = 2\xi(2\pi r_0^2)$ which approximates a point-like impurity. Assuming cylindrical symmetry of the problem induced by the smectic layered structure a point-like impurity is equivalent to an infinitesimal dislocation loop [7] with Burgers vector $b = 2\xi$ and surface δA. This equivalence can be expressed by taking c equal to $(\xi\delta A/2\pi)$ in equation (9). The same displacement as given by equation (9) can be obtained by integration of the general expressions given by Kléman [1, 8] and based on the use of the Green function of equation (5).

3. Screw dislocation–point-like impurity interaction

The interaction energy E_I between a dislocation and a point-like impurity in smectic A liquid crystals can be expressed as

$$E_I = \int dV\left\{K\left[\frac{\partial^2 u^D}{\partial x^2}\frac{\partial^2 u^I}{\partial x^2} + \frac{\partial^2 u^D}{\partial y^2}\frac{\partial^2 u^I}{\partial y^2} + 2\frac{\partial^2 u^D}{\partial x\partial y}\frac{\partial^2 u^I}{\partial x\partial y}\right] + \bar{B}\frac{\partial u^D}{\partial z}\frac{\partial u^I}{\partial z}\right\} \tag{13}$$

as seen from equations (5) and (1) with an inserted displacement $u = u^D + u^I$. The components u^D and u^I are the displacements due to a dislocation and an impurity, respectively.

The screw dislocation along the z axis with Burgers vector **b** creates in its neighbourhood the displacement $u^D = (b/2\pi)\,\mathrm{arctg}\,(y/x)$. Displacement u^I of the impurity situated close to the point with coordinates $(x_0, y_0, 0)$ follows from equation (9) as

$$u^I = \frac{c}{2\lambda z}\exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{4\lambda|z|}\right).$$

Because $\partial u^D/\partial z = 0$ the integration in equation (13) over z in the interval $z \in (-\infty, +\infty)$ gives zero because $u^I(x, y, z) = -u^I(x, y, -z)$. For this reason there is no interaction energy between a straight screw dislocation and an impurity. The total force by which an impurity acts on a dislocation is also zero. However, according to Kléman [1] the local force on the element of a screw dislocation can be non-zero as seen from expressions (6) with $u = u^I$. It should be noted that the local force acting on the dislocation element has the tendency to transform locally a straight screw dislocation to a helicoidal shape. The mechanism of such a helical instability of a screw dislocation is the same as that proposed by Kléman [9] and confirmed experimentally in [10]. The change of dislocation shape investigated in [9] is caused by a volume dilatation or compression of an edge dislocation situated near that of a screw. As discussed in detail in [9] this helicoidal shape change of the dislocation also leads

to the increase of the dislocation line tension which cannot be neglected although the self-energy of a straight screw dislocation calculated from formula (2) is zero [8]. In this way the presence of impurities around a screw dislocation causes its helical instability and influences its line tension.

The helical dislocation has not only a screw component but also an edge one. Through this edge component it interacts with the dilatation field of a point-like impurity as shown in the next section where a simplified case of a straight edge dislocation and a point-like impurity interaction is investigated.

4. Edge dislocation–point-like impurity interaction

Let an infinite edge dislocation lie along the y axis and a point-like impurity be situated at the point $(x_0, 0, z_0)$; the Burgers vector **b** of dislocation is oriented along the z axis. The displacements u^D and u^I describing an edge dislocation and a point defect, respectively, are

$$u^D = [\mathrm{sg}(z)]\left[\frac{b}{4} + \frac{b}{4}\int_{-\infty}^{+\infty}\frac{dq}{iq}\exp(-\lambda q^2|z| + iqx)\right] \tag{14}$$

as follows from [1, 3] and

$$u^I = u^- = c\exp\left(-\frac{(x - x_0)^2 + y^2}{4\lambda|z - z_0|}\right)\Big/2\lambda(z - z_0),$$

given by expression (9).

The interaction energy E_I can be found by the integration in equation (13). As shown in the Appendix for an edge dislocation interaction with a point-like impurity in a S_A liquid crystal the expression of the force exerted by a point defect on a unit length of dislocation can be obtained from the Peach–Koehler formula (see, for example, [1])

$$f_x = b\sigma^I_{33}, \quad f_y = 0, \quad f_z = -b\sigma^I_{13}. \tag{15}$$

Using equation (6) with u^I and equation (8) we obtain

$$\left.\begin{aligned} f_x &= b\bar{B}\left(\frac{\partial u^I}{\partial z}\right)_{\substack{x=0\\z=0}} = -\frac{\bar{B}bc}{2\lambda z_0^2}\left(1 - \frac{x_0^2 + y^2}{4\lambda|z_0|}\right)\exp\left(-\frac{x_0^2 + y^2}{4\lambda|z_0|}\right), \\ f_z &= +K\left(\frac{\partial}{\partial x}\Delta u^I\right)_{\substack{x=0\\z=0}} = +\frac{\bar{B}bcx_0}{4\lambda(z_0)^3}\left(2 - \frac{x_0^2 + y^2}{4\lambda|z_0|}\right)\exp\left(-\frac{x_0^2 + y^2}{4\lambda|z_0|}\right). \end{aligned}\right\} \tag{16}$$

The total force of the point defect–edge dislocation interaction is

$$\left.\begin{aligned} F_x &= \int_{-\infty}^{+\infty} f_x\,dy = -\frac{\bar{B}bc}{2|z_0|}\left(\frac{\pi}{\lambda|z_0|}\right)^{1/2}\left(1 - \frac{x_0^2}{2\lambda|z_0|}\right)\exp\left(-\frac{x_0^2}{4\lambda|z_0|}\right) \\ &\text{and} \\ F_z &= \int_{-\infty}^{+\infty} f_z\,dy = +\frac{\bar{B}bcx_0\,\mathrm{sg}(z_0)}{4z_0^2}\left(\frac{\pi}{\lambda|z_0|}\right)^{1/2}\left(3 - \frac{x_0^2}{2\lambda|z_0|}\right)\exp\left(-\frac{x_0^2}{4\lambda|z_0|}\right). \end{aligned}\right\} \tag{17}$$

The total force components F_x and F_z are related to the interaction energy E_I as $F_x = -\partial E_I/\partial x_0$, $F_z = -\partial E_I/\partial z_0$. Then the total energy of the interaction between a point impurity and an edge dislocation in a S_A liquid crystal is

$$E_I = \frac{\bar{B}bc}{2|z_0|}\left(\frac{\pi}{\lambda|z_0|}\right)^{1/2} x_0\exp\left(-\frac{x_0^2}{4\lambda|z_0|}\right). \tag{18}$$

As noted, expression (18) can be obtained by direct integration of expression (13) with u^{I} and u^{D} given by equations (9) and (14). On the other hand, expression (18) is the work necessary to create a point impurity of volume δV in the dilatation stress σ_{33}^{D} of an edge dislocation, i.e.

$$E_{\mathrm{I}} = -\delta V[\sigma_{33}^{\mathrm{D}}]_{\substack{x=x_0 \\ z=z_0}} = -\delta V \bar{B}\left[\frac{\partial u^{\mathrm{D}}}{\partial z}\right]_{\substack{x=x_0 \\ z=z_0}}.$$

5. Discussion

In this contribution we have made the assumption that the structure of the smectic A layers is not influenced by the presence of a point-like impurity. This assumption is correct in our case because we investigate only a small point-like impurity in static equilibrium.

The simplest solution describing the S_A layer displacement u^{I} caused by the presence of this impurity can be used further for the description of the interaction of this point defect with other defects in S_A liquid crystals. As an example we discuss now the interaction of a point-like impurity with an edge dislocation. In this case the interaction can be calculated simply by using the Peach–Koehler formula for the configurational force as demonstrated in the Appendix. The force between an edge dislocation and a point-like impurity is non-central, as in the case of two edge dislocations [11]. Generally the motion of a point-like impurity in the neighbourhood of an edge dislocation driven by an interaction force (cf. equation (17)) can be complicated. Let us simplify our discussion by assuming that the point-like impurity moves more easily parallel to the S_A layers than in the perpendicular direction. This assumption is in accord with our premise of undisturbed layers. The validity of this assumption was also established by de Gennes [6] in his investigation of a S_A liquid crystal flow with spherical defects and dislocations. According to de Gennes the friction coefficient of the cylindrical defect motion perpendicular to the layers is much larger than the friction coefficient of the cylinder motion in the plane of the smectic layers. Also an edge dislocation moves more easily by climb, i.e. along the layers than by slip perpendicular to the S_A layers, as seen from an investigation of its core properties [8, 12].

When a point-like impurity of strength c is situated between two layers at the position $(x_0, 0, z_0)$ (the exact position in the y direction is irrelevant due to the infinite length of an edge dislocation in this direction) the equilibrium position of this defect with respect to the edge dislocation situated at the coordinate origin follows from the relation

$$F_x = 0 \quad \text{or} \quad x_0 = \pm(2\lambda|z_0|)^{1/2}. \tag{19}$$

The stable configuration is realized at such a coordinate x_0 which satisfies the inequality

$$\partial^2 E_{\mathrm{I}}/\partial x_0^2 > 0. \tag{20}$$

Supposing $c > 0$ and $b > 0$ it can be shown that inequality (20) is fulfilled for $x_0 = -(2\lambda|z_0|)^{1/2}$. So the equilibrium position of a point-like impurity with $c > 0$ is at $x_0 = -(2\lambda|z_0|)^{1/2}$ and the unstable position at $x_0 = (2\lambda|z_0|)^{1/2}$ with respect to the edge dislocation with $b > 0$ situated in the position $x = 0, z = 0$. This result can be readily understood. A point-like impurity with $c > 0$ creates in its neighbourhood a volume dilatation. An edge dislocation with $b > 0$ is characterized by a volume

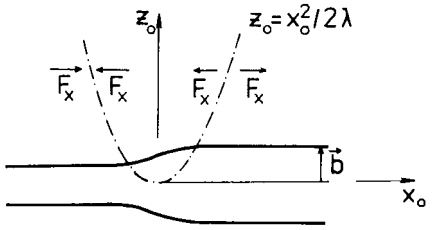

Figure 2. The equilibrium positions of point-like impurity near an edge dislocation which follow from the equation $F_x = 0$ (dashed and dotted line $z_0 = x_0^2/2\lambda$). The orientation of x-force components near the line $z_0 = x_0^2/2\lambda$ shown by the arrows corresponds to the case of both dislocation Burgers vector **b** and point-like impurity strength c positive. The situation is the same for the parabola $z_0 = -x_0^2/2\lambda$ but not depicted in the figure.

dilatation for $x > 0$ and a volume compression for $x < 0$ (cf. figure 2). So in the region $x > 0$ the point-like impurity adds more volume dilatation and thus it is expelled from this region by dislocation and directed toward the volume compression region $x < 0$ of dislocation.

Thus point-like impurities have the tendency to increase their concentration in the edge dislocation compression region. The concentration distribution C of point-like impurities near an edge dislocation in a S_A liquid crystal can be determined by classical Boltzmann statistics as (see, for example, [13])

$$C = C_0 \exp(-E_I/kT),$$

where C_0 is the impurity concentration far from an edge dislocation, T is the absolute temperature and k is the Boltzmann constant. The interaction energy E_I of the dislocation–impurity interaction is given by equation (18). Again it is seen that, for the compression region (where $E_I < 0$), $C > C_0$ and for the dilatation region ($E_I > 0$) $C < C_0$. The concentration C where $C > C_0$ of impurities near an edge dislocation thus form a cloud. In this way the situation is similar to that in metallurgy where such a cloud is called a Cottrell cloud.

The binding energy of the point-like impurity to the dislocation can be estimated by inserting into expression (18) the relation $x_0 = -(2\lambda|z_0|)^{1/2}$. Then the binding energy E_B is

$$E_B = |E_I(x_0 = -2\lambda|z_0|)| = \frac{\bar{B}bc}{|z_0|}\left(\frac{\pi}{2e}\right)^{1/2}. \tag{21}$$

If $z_0 \approx b/2$, then $E_B/\bar{B}c \approx (2\pi/e)^{1/2} \approx 1{\cdot}52$.

Through this binding energy a point-like impurity can follow the climb motion of an edge dislocation and by its own friction force it will increase the friction of the dislocation climb motion in a S_A liquid crystal. Using de Gennes results [6] the friction force, F_f, acting on the spherical point impurity of radius ξ which moves with velocity V_x in the x direction is $F_f \approx 8\pi\eta\xi V_x$; where η is the viscosity. Thus for small velocities V_x the point-like impurity increases the dislocation friction by a value F_f.

6. Conclusions

Using the elastic free energy density of S_A liquid crystals one solution of the equilibrium equation giving the displacement $u^1 = u^-$ (cf. equation (9)) in the neighbourhood of a spherical inclusion or a point-like impurity situated between smectic layers was used to investigate the dislocation-point impurity interaction.

The interaction of an edge dislocation with a point-like impurity can be described by the Peach–Koehler formula for the configurational force which is the same for both expressions (1) and (2) of the smectic A free energy density, as discussed in the Appendix. The interaction energy E_I given by formula (18) was used to estimate the binding energy (cf. equation (21)) of a point-like impurity to an edge dislocation. On the other hand, the interaction of a straight screw dislocation with a point-like impurity is zero. However, the presence of a point-like impurity near a screw dislocation leads to its helical shape instability thus influencing the dislocation line tension. The interaction between a helical dislocation and a point-like impurity can then be approximated by the interaction of a point-like impurity with a helical dislocation edge component.

Appendix

The interaction energy between a dislocation and another source of the internal stress in a smectic A liquid crystal can be expressed using equation (13) as

$$E_I = \int dV[\mathrm{div}(\mathbf{A} + \mathbf{B}) + u^D \sigma^E_{i3,i}], \tag{A 1}$$

where the vector fields **A** and **B** are of the form

$$\left.\begin{aligned} A_1 &= K\left[\frac{\partial u^D}{\partial x}\frac{\partial^2 u^E}{\partial x^2} + \frac{\partial u^D}{\partial y}\frac{\partial^2 u^E}{\partial x \partial y}\right], \\ A_2 &= K\left[\frac{\partial u^D}{\partial y}\frac{\partial^2 u^E}{\partial y^2} + \frac{\partial u^D}{\partial x}\frac{\partial^2 u^E}{\partial x \partial y}\right], \\ A_3 &= 0, \end{aligned}\right\} \tag{A 2}$$

and $B_i = u^D \sigma^E_{i3}$, $(i = 1, 2, 3)$. Displacements u^D and u^E are created by a dislocation and another stress source, respectively. By analogy with Eshelby [14] let surface S_D be the surface enveloping the dislocation cut half-plane as depicted schematically in figure 3. The volume integral (cf. equation (A 1)) can then be transformed to the surface integral

$$E_I = \int_{S_D} A_i n_i \, dS + \int_{S_D} u^D \sigma^E_{i3} n_i \, dS + \int u^D \sigma^E_{i3,i} \, dV. \tag{A 3}$$

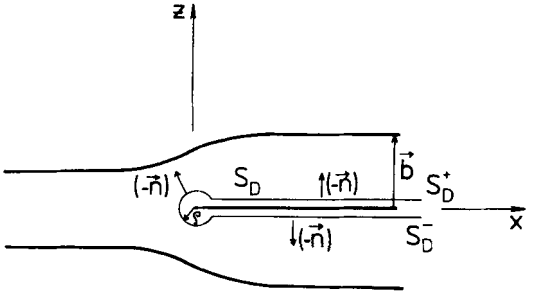

Figure 3. A schematic representation of the surface S_D enveloping the dislocation cut half-plane $x > 0$. The surface S_D is composed of the upper (S_D^+) and lower (S_D^-) lip both connected by the cylindrical surface of radius around the dislocation line (perpendicular to the figure plane). The outer normal to the surface S_D is **n** but the inner normal ($-\mathbf{n}$) is depicted for convenience.

In expressions (A 1) and (A 3) the usual summation convention over repeated indexes $i = 1, 2, 3$ is adopted. The vector $\mathbf{n}$ in equation (A 3) is the outer normal of S_D. With respect to the surface S_D it is convenient to express the vector field $\mathbf{A}$ in the unsymmetrical form (cf. equations (A 2)). The summation of stress component derivatives

$$\sigma^E_{i3,i} = \frac{\partial \sigma^E_{13}}{\partial x} + \frac{\partial \sigma^E_{23}}{\partial y} + \frac{\partial \sigma^E_{33}}{\partial z} = 0$$

is the equilibrium condition for displacement u^E with stress components given by equation (6) with $u = u^E$. Displacement u^D changes by b on S_D and finally E_I can be expressed as

$$E_I = \int_{S_D} A_i n_i \, dS + b \int_{S_D^+} \sigma^E_{i3} n_i \, dS. \tag{A 4}$$

Comparison of the interaction energy (equation (A 4)) in a S_A with the analogous expression in elasticity of solid crystals [14, 15] shows that the derivatives of the integral $b \int_{S_D} \sigma^E_{i3} n_i \, dS$ with respect to the position coordinates of stress source σ^E_{i3} give the configurational force acting on a dislocation. This configurational force can also be obtained from the well-known Peach–Koehler formula (see, for example, Eshelby [14], Kléman [1]). The difference between the interaction energy in a S_A and in the classical elasticity of solids is the term $\int_{S_D} A_i n_i \, dS$. The field $\mathbf{A}$ is composed of derivatives of displacements u^D and u^E continuous across the cut half-plane. So the integral $\int_{S_D} A_i n_i \, dS$ could contribute only on the cylindrical surface of radius enveloping the line dislocation singularity at the edge of dislocation cut half-plane (cf. figure 3). The role of the term $\int_{S_D} A_i n_i \, dS$ was demonstrated during the study of the interaction of two parallel screw dislocations in a smectic C or at the smectic A limit of the smectic C free energy density, by Kléman and Lejček [3]. For

$$u^D = \frac{b^{(1)}}{2\pi} \operatorname{arctg} \frac{y}{x}$$

and

$$u^E = \frac{b^{(2)}}{2\pi} \operatorname{arctg} \frac{y - y_0}{x - x_0}$$

describing two parallel screw dislocations with Burgers vectors $b^{(1)}$ and $b^{(2)}$ at $x = y = 0$ and $x = x_0$, $y = y_0$, respectively, the integral $\int_{S_D} A_i n_i \, dS$ is

$$\lim_{\varrho \to 0} \int_0^{2\pi} \varrho \, d\alpha [-A_1 \cos\alpha - A_2 \sin\alpha] = \frac{K b^{(1)} b^{(2)}}{2\pi r^2}$$

(per unit length in the z direction) where cylindrical coordinates $x = \varrho \cos\alpha$, $y = \varrho \sin\alpha$, $z = z$ were used, and $\mathbf{n} = (-\cos\alpha, -\sin\alpha, 0)$, $r^2 = x_0^2 + y_0^2$. The term $b \int \sigma^E_{i3} n_i \, dS$ does not contribute because $\Delta u^E = 0$. In a classical smectic A liquid crystal the interaction energy can be written analogously to equation (A 4) as

$$E_I = \int_{S_D} A'_i n_i \, dS + b \int_{S_D^+} \sigma^E_{i3} n_i \, dS, \tag{A 5}$$

with

$$A'_1 = K \frac{\partial u^D}{\partial x} \Delta u^E, \quad A'_2 = K \frac{\partial u^D}{\partial y} \Delta u^E, \quad A'_3 = 0. \tag{A 6}$$

For a screw dislocation $\Delta u^E = 0$ and then $E_I = 0$. So in a classical S_A liquid crystal there is no interaction between parallel screw dislocations [8]. The difference between the expressions (A 4) and (A 5) is connected with the term Δ_{el} (equation (3)) and thus its importance was demonstrated.

For an edge dislocation along the y axis the dislocation displacement does not depend on the y coordinate. Then

$$\int_{S_D} A_i n_i \, dS = -K\varrho \int_0^{2\pi} d\alpha \int_{-\infty}^{+\infty} dy \left[\cos\alpha \frac{\partial u^D}{\partial x} \frac{\partial^2 u^E}{\partial x^2} \right]$$

in cylindrical coordinates $x = \varrho\cos\alpha$, $y = y$, $z = \varrho\sin\alpha$ and $\mathbf{n} = (-\cos\alpha, 0, -\sin\alpha)$. Using u^D given by equation (14) it is [1]

$$\frac{\partial u^D}{\partial x} = \frac{b\,\mathrm{sg}(\sin\alpha)}{4(\pi\lambda\varrho|\sin\alpha|)^{1/2}} \exp(-\varrho\cos^2\alpha/4\lambda|\sin\alpha|),$$

which behaves as $\varrho^{-1/2}$. If $(\partial^2 u^E/\partial x^2)$ has no singularity for $\varrho \to 0$ then

$$\lim_{\varrho\to 0} \int_{S_D} A_i n_i \, dS \to 0.$$

The same procedure can also be used for a classical smectic A. Thus for both S_A and classical S_A liquid crystals the interaction of an edge dislocation with the displacement field, u^D, from the other source of stresses the interaction energy is of the form

$$E_I = b \int_{S_D^+} \sigma_{i3}^E n_i \, dS, \tag{A 7}$$

which is equivalent to the use of the Peach–Koehler formula for the configurational force (15). The displacement u^E can be either the displacement created by another parallel edge dislocation as studied in smectic A liquid crystals by Kléman and Williams [11] or u^I of a point-like impurity (see §§3 and 4).

In conclusion of this schematic analysis it should be noted that the Peach–Koehler formula for the configurational force cannot be simply used without further discussion in liquid crystals such as smectic A, smectic C or chiral smectic C whose free energy densities contain the powers of second layer displacement derivatives.

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