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Influence of surface tension on the stability of edge dislocations in smectic A liquid crystals

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Résumé. — La solution générale au problème d'une dislocation coin dans un film smectique A est présentée. Nous calculons son énergie d'interaction avec les surfaces en tenant compte rigoureusement de la tension de surface. Cette formule est utilisée pour discuter la stabilité de la dislocation vis-à-vis d'un mouvement de glissement vers la surface. Si la tension de surface domine l'élasticité smectique (caractérisée par les constantes K et B), c'est-à-dire si $\gamma > (KB)^{1/2}$, alors la dislocation se stabilise à l'intérieur du film. Si, par contre, la tension de surface est petite ($\gamma < (KB)^{1/2}$), la dislocation est attirée vers la surface.

Abstract. — The general solution describing an edge dislocation inside a smectic A film is presented. Its elastic interaction energy with the limiting surfaces is calculated by taking into account rigorously the surface tension γ . This formula is used to discuss the dislocation stability with respect to a slip motion towards the surface. If surface tension prevails over smectic A elasticity, characterized by elastic constants K and B , i.e. if $\gamma > (KB)^{1/2}$, then the dislocation is stabilized within the film. If, by contrast, the surface tension is small ($\gamma < (KB)^{1/2}$), the dislocation is attracted to the surface of the film.

1. Introduction.

The surface tension is usually neglected in problems connected with dislocations near a free surface. In solids, this constitutes a good approximation because the surface tension γ is small compared to μb , where μ is a shear modulus and b the Burgers vector of the dislocation. In smectic A liquid crystals, this criterion is different and can be expressed as $\gamma \ll \sqrt{KB}$ [1-4]. K is the curvature constant and B the elastic modulus of the layers. This condition is not always fulfilled experimentally, so that surface tension must be taken into account explicitly in the calculations. To our knowledge, this has never been done rigorously.

In this article, we give the solution to the problem of an edge dislocation lying in a smectic A film limited by two surfaces of different surface energies. The total energy of the edge dislocation and its position of stable equilibrium (when it exists!) will be also determined.

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Let us assume that the sample surfaces are situated at $z = D$ and $z = 0$ and let γ_1 and γ_2 be their surface energies, respectively. The layers, parallel to the sample surfaces, are perpendicular to the z -axis and parallel to the (x, y) -plane. The edge dislocation is situated at $z = z'$ and lies along the y -axis (Fig. 1).

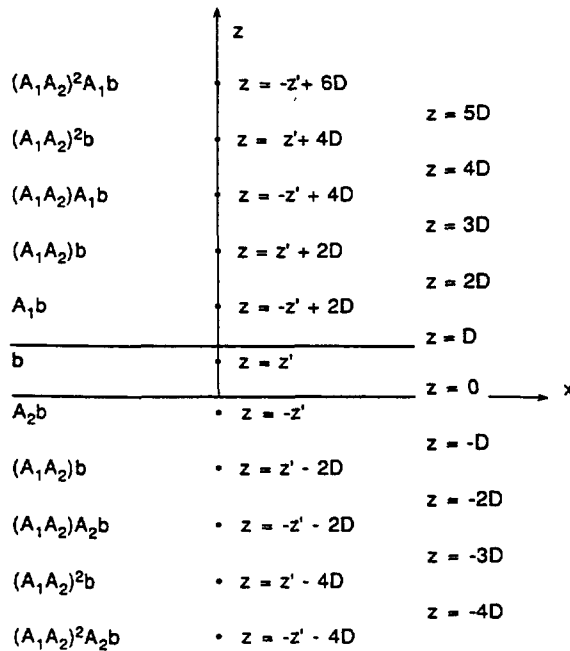


Fig. 1. — Burgers vectors and positions of the first five image dislocations. The sample of thickness D is between $z = 0$ and $z = D$ and contains an edge dislocation of Burgers vector b at $z = z'$. Coordinates x, z are also displayed

The total energy W of the sample (per unit-length of dislocation) is the sum of the smectic A elastic energy W_E [1]

$$W_E = \frac{1}{2} \int dx dz \left[K \left(\frac{\partial^2 u}{\partial x^2} \right)^2 + B \left(\frac{\partial u}{\partial z} \right)^2 \right] \tag{1}$$

and the surface energies W_1 and W_2 [1, 2]

$$W_1 = \frac{\gamma_1}{2} \int_{-\infty}^{+\infty} \left(\frac{\partial u}{\partial x} \right)_{z=D}^2 dx, \quad W_2 = \frac{\gamma_2}{2} \int_{-\infty}^{+\infty} \left(\frac{\partial u}{\partial x} \right)_{z=0}^2 dx \tag{2}$$

In these equations, $u = u(x, z)$ is the layer displacement in the z -direction. Minimizing W with respect to u gives the equilibrium equation

$$K \frac{\partial^4 u}{\partial x^4} = B \frac{\partial^2 u}{\partial z^2} \tag{3}$$

in the bulk of the sample, with the two boundary conditions

$$B \frac{\partial u}{\partial z} = \gamma_1 \frac{\partial^2 u}{\partial x^2}, z = D \quad \text{and} \quad -B \frac{\partial u}{\partial z} = \gamma_2 \frac{\partial^2 u}{\partial x^2}, z = 0 \tag{4}$$

at the sample surfaces. One recognizes above the well-known Gibbs-Thomson equation, $\partial^2 u / \partial x^2$ being equal to the curvature of the surface if it is slightly distorted, while $B \partial u / \partial z$ is the elastic stress normal to the layers.

2. Displacement field around an isolated edge dislocation.

The displacement $u = u(x, y)$ around the dislocation must satisfy the equilibrium equations (3) and (4). It is given by the general method of image dislocations [4, 6]. The solution is thus obtained by adding the displacement corresponding to an isolated dislocation in an infinite medium [5, 7] to all the displacements associated with the images. The position of the image dislocations can be found using the method described in reference [6]. Their positions and their Burgers vectors are given by the recurrent relations obtained from equation (4):

$$\begin{aligned} z = z' + 2 Dm & \quad b_m = b (A_1 A_2)^m & \quad m \geq 0 \\ z = z' - 2 Dm & \quad b_m = b (A_1 A_2)^m & \quad m \geq 1 \\ z = -z' + 2 Dm & \quad b_m = b \frac{(A_1 A_2)^m}{A_2} & \quad m \geq 1 \quad m \text{ integer} \\ z = -z' - 2 Dm & \quad b_m = b (A_1 A_2)^m A_2 & \quad m \geq 0 \end{aligned}$$

Burgers vectors and positions of a few dislocations are depicted in figure 1. The resulting displacement is therefore:

$$\begin{aligned} u(x, z) = \frac{b}{4} & \left\{ \operatorname{sg}(z - z') \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z - z'|)^{1/2}} \right) + \right. \\ & + A_2 \operatorname{sg}(z + z') \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z + z'|)^{1/2}} \right) \\ & + \sum_{m=1}^{\infty} \left[(A_1 A_2)^m \operatorname{sg}(z - z' - 2 Dm) \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z - z' - 2 Dm|)^{1/2}} \right) \right. \\ & + (A_1 A_2)^m \operatorname{sg}(z - z' + 2 Dm) \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z - z' + 2 Dm|)^{1/2}} \right) \\ & + \frac{(A_1 A_2)^m}{A_2} \operatorname{sg}(z + z' - 2 Dm) \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z + z' - 2 Dm|)^{1/2}} \right) \\ & \left. \left. + (A_1 A_2)^m A_2 \operatorname{sg}(z + z' + 2 Dm) \left(1 + \operatorname{erf} \frac{x}{2(\lambda |z + z' + 2 Dm|)^{1/2}} \right) \right] \right\}. \quad (5) \end{aligned}$$

In this expression, z' describes the dislocation position in the sample ($0 < z' < D$), b is the Burgers vector, $\lambda = (K/B)^{1/2}$ is a characteristic length of the order of the layer thickness and erf is the error function:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$$

The parameters A_1 and A_2 determine the values of the Burgers vectors of the image dislocations and have the form

$$A_1 = \frac{\alpha_1 - 1}{\alpha_1 + 1} \quad \text{with} \quad \alpha_1 = \frac{\gamma_1}{B\lambda}, \quad A_2 = \frac{\alpha_2 - 1}{\alpha_2 + 1} \quad \text{with} \quad \alpha_2 = \frac{\gamma_2}{B\lambda}.$$

The values and the signs of A_1 and A_2 depend on the ratios α_1 and α_2 which characterize the influence of surface tension on the dislocation behaviour. Many cases can be considered depending on the values of α_1 and α_2 .

For free surfaces, one usually takes $\alpha_1 = \alpha_2 = 0$. As we shall see below, this constitutes a very crude approximation which gives wrong results in general. In this limit $A_1 = A_2 = -1$ and the image dislocations have Burgers vector equal to $-b$ and b alternatively [4-6].

In order to describe a sample sandwiched between two plates, it is sufficient to take α_1 and $\alpha_2 \rightarrow +\infty$. In this limit, $A_1 = A_2 = 1$ and all the image dislocations have their Burgers vector equal to b [4, 6].

The case $\alpha_1 \neq 0$ and $\alpha_2 \rightarrow +\infty$ is also of interest. It corresponds to a free dop deposited on a solid, a situation that has been studied in detail in recent experiments [2, 8].

3. Interaction energy.

We shall first consider the general case of two parallel dislocations. Then, we shall restrict ourselves to the special case of an isolated dislocation interacting with the limiting surfaces

3.1 INTERACTION ENERGY BETWEEN TWO PARALLEL EDGE DISLOCATIONS. — Let us consider two edge dislocations with Burgers vectors b_1 and b_2 situated at points $[x_1, z_1]$ and $[x_2, z_2]$, respectively. Their interaction energy is equal to the work that is necessary to create the first dislocation in the stress field $\sigma_{zz} = B \partial u_2 / \partial z$ of the second one [6], itself characterized by the displacement field u_2 . It can be expressed in the form

$$W_I = -B b_1 \int_{x_1}^{+\infty} \left(\frac{\partial u_2}{\partial z} \right)_{z=z_1} dx. \quad (6)$$

Using equation (5) yields

$$W_I = \frac{B \lambda b_1 b_2}{4 \sqrt{\pi \lambda}} \left\{ \frac{e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 - z_2|}}{\sqrt{|z_1 - z_2|}} + A_2 \frac{e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 + z_2|}}{\sqrt{|z_1 + z_2|}} + \sum_{m=1}^{\infty} \left[(A_1 A_2)^m \frac{e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 - z_2 - 2 D m|}}{\sqrt{|z_1 - z_2 - 2 D m|}} + (A_1 A_2)^m \frac{e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 - z_2 + 2 D m|}}{\sqrt{|z_1 - z_2 + 2 D m|}} + \frac{(A_1 A_2)^m e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 + z_2 - 2 D m|}}{A_1 \sqrt{|z_1 + z_2 - 2 D m|}} + (A_1 A_2)^m A_2 \frac{e^{-(x_1 - x_2)^2 / 4 \lambda |z_1 + z_2 + 2 D m|}}{\sqrt{|z_1 + z_2 + 2 D m|}} \right] \right\} \quad (7)$$

The first term of this expression corresponds to the interaction energy between two dislocations in an infinite medium [5]. All the other terms come from the image dislocations which model the sample surfaces. Their presence modifies quantitatively the interaction between the two dislocations. If α_1 and α_2 are both greater than 1, then A_1 and A_2 are positive and the term in brackets in equation (7) is always positive. In consequence, two dislocations of the same sign repulse each other whereas dislocations of opposite signs attract each other, as expected. In the other cases, when one at least of the A_i 's is negative, the behaviour is more difficult to analyze but it is qualitatively similar (except when dislocations are very close together in the same climb plane [10]). In the next subsection, we analyze in more detail the case of a single dislocation. In particular, we shall discuss its stability with respect to a slip motion perpendicular to the layers

3.2 INTERACTION OF A SINGLE DISLOCATION WITH SURFACES. — The interaction energy between a single dislocation and the surfaces can be easily found by putting $b_1 = b_2 = b$, $x_1 = x_2$ and $z_1 = z_2 = z_0$ in equation (7). If the δ -function corresponding to the dislocation self-energy in an infinite medium is omitted, W_1 can be rewritten as

$$W_1 = \frac{B\lambda b^2}{8\sqrt{2}\pi\lambda} \left[\frac{A_2}{\sqrt{z_0}} + \sum_{m=1}^{\infty} \left(\frac{2(A_1 A_2)^m}{\sqrt{Dm}} + \frac{(A_1 A_2)^m}{A_2} \frac{1}{\sqrt{|z_0 - Dm|}} + \frac{(A_1 A_2)^m A_2}{\sqrt{|z_0 + Dm|}} \right) \right]. \tag{8}$$

The equilibrium position z_0 of the dislocation can be found from the condition $\partial W_1 / \partial z_0 = 0$. After putting $t = z_0 / D$, this condition reads

$$\frac{A_2}{\sqrt{t^3}} = \sum_{m=1}^{\infty} \left[\frac{(A_1 A_2)^m}{A_2} \frac{1}{\sqrt{|t - m|^3}} - \frac{(A_1 A_2)^m A_2}{\sqrt{|t + m|^3}} \right]. \tag{9}$$

This equation invites several comments :

— first, it is satisfied whatever z_0 when $\alpha_1 = \alpha_2 = 1$ (i.e. $\gamma_1 = \gamma_2 = \sqrt{KB}$). In this peculiar case, the dislocation has no preferred position inside the film, because elastic effects compensate exactly for surface tension effects,

— second, when $\alpha_1 = \alpha_2 = \alpha \neq 1$ (i.e. $\gamma_1 = \gamma_2 = \gamma \neq \sqrt{KB}$), there is a unique solution $t = 1/2$. In equilibrium, the dislocation lies in the middle of the sample, which is obvious in view of the symmetry of the problem. On the other hand, this position is not always stable. If $\alpha = \gamma / \sqrt{KB} > 1$, the dislocation is repulsed by both surfaces so that the equilibrium is stable. By contrast, the dislocation is attracted to the surfaces when $\alpha < 1$. As a result, the equilibrium is unstable and the dislocation slips to the surface :

— third, equation (9) allows us to find the equilibrium position in the general case $\gamma_1 \neq \gamma_2$. An approximate calculation, taking into account the first images only, gives :

$$t = \frac{1}{1 + Q} \quad \text{with} \quad Q = \left(\frac{A_1}{A_2} \right)^{2/3} \tag{10}$$

As before, this equilibrium is unstable from the moment that one of the α_i 's is smaller than 1. One case that is particularly interesting is the one of a smectic droplet deposited on a solid surface. As $\alpha_2 \rightarrow \infty$ and $A_2 \rightarrow 1$ on the solid support, the solution (10) takes the form

$$z_0 \approx \frac{D}{1 + A^{2/3}} \quad \text{with} \quad A = \left(\frac{\gamma - \sqrt{KB}}{\gamma + \sqrt{KB}} \right) \tag{11}$$

where γ is the surface tension at the free surface.

4. Concluding remarks.

We have shown that surface tension plays an important role in problems related to dislocations in smectic A liquid crystals and that it can be taken into account rigorously. Our main conclusion is that edge dislocations are repulsed from the free surface as soon as its surface tension γ is greater than $B\lambda = \sqrt{KB}$. This inequality is satisfied very often experimentally. For instance, at the contact with air we have $\gamma \approx 25 \text{ erg/cm}^2$ while $\sqrt{KB} \approx 10 \text{ erg/cm}^2$ if one takes $K \approx 10^{-6} \text{ dyn}$ and $B \approx 10^8 \text{ erg/cm}^3$. Thus, the common

assumption of free surface with zero surface tension turns out to be completely wrong and leads to erroneous conclusions concerning the stability of bulk dislocations. Our theoretical results are moreover in accordance with certain experimental observations of Williams [2] who found that dislocations are not attracted by the free surface; rather they are found at large distances from it. Williams note also that bulk dislocations influence the free surface of the sample, leading to fine lines that are visible through the microscope in reflected light [2]. It is possible to calculate, within the framework of this model, the surface distortion. For the sake of simplicity, we shall only consider the simplest case of an edge dislocation sandwiched between two free surfaces of surface tension $\gamma > \sqrt{KB}$. We shall assume the dislocation in equilibrium at $z' = D/2$. The surface deformation is characterized by the inclination θ of the superficial layers with respect to the (x, y) plane and by the width ξ over which θ varies significantly.

$$\theta = \frac{\partial u}{\partial x} \Big|_{z=D, z'=D/2} \quad \text{and} \quad \xi = |x_1 - x_2|$$

where x_1 and x_2 are the solutions of the equation

$$\frac{\partial^2 \theta}{\partial x^2} \Big|_{z=D, z'=D/2} = 0.$$

By taking into account the first image dislocations only, it is possible to calculate approximately ξ and the maximum tilt angle $\theta_M = \theta(x=0)$.

$$\xi \approx 2 \sqrt{\lambda D} \quad \text{and} \quad \theta_M \approx \frac{b(1-A)}{2 \sqrt{2 \pi \lambda D}} = \frac{b(1-A)}{\xi \sqrt{2 \pi}}$$

In order to evaluate these geometrical factors, let us take $\alpha \approx 5$ [2], $\lambda \approx 20 \text{ \AA}$ and $D = 10 \text{ \mu m}$. We obtain $\xi \approx 0.28 \text{ \mu m}$ and $\theta_M (\approx 27 \text{ b} (\text{\mu m}))$. For « giant » dislocations, that are very numerous in smectics [2], the angle θ_M can be fairly important and clearly visible through the microscope. It increases as the film thickness D decreases and it can even reach large values in the thinnest films. Thus, for $b = 10$ layers $\approx 3 \times 10^{-2} \text{ \mu m}$ we get $\theta_M \approx 0.8^\circ$ with $D = 10 \text{ \mu m}$ whereas θ_M reaches 2.5° for $D = 1 \text{ \mu m}$.

Experimentally, the condition $\alpha < 1$ is rarely observed at the contact with air in thermotropic liquid crystals. Conversely, it should be fulfilled at the interface between the smectic A and its isotropic liquid because the surface tension is expected to be much smaller in this case. Thus, the smectic A-isotropic interface should attract the bulk edge dislocations. This phenomenon is perhaps important in explaining certain anomalies observed in recent experiments on the shape of smectic A droplets [9]. Analogous situations may be encountered in lyotropic liquid crystals where surface tensions are very small too. Nevertheless, very little is known about dislocations in these systems.

Finally, situations with two interfaces of different surface tensions could be investigated experimentally, for example by spreading a smectic A on a suitable liquid.

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- [10] When the two dislocations are in the same climb plane and when one at least of the A_i 's is negative, the interaction energy and the force between the two dislocations can change sign as a function of their distance. Thus, two dislocations of the same sign can attract when they are very close together (typically for $|x_1 - x_2| < (\lambda D)^{1/2}$) whereas they repulse if they are of opposite sign. Nevertheless, this peculiar phenomenon is not of great interest because both dislocations are unstable with respect to a slip motion towards the surface (see Sect 3.2)