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DISLOCATIONS, GRAIN BOUNDARIES AND FOCAL CONICS IN SMECTICS A

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Résumé. — Des considérations géométriques simples permettent de construire un joint de grain dans un smectique A de 3 manières différentes : soit par une simple courbure de couches, soit à l'aide d'une paroi de dislocations comme dans un cristal solide, soit, de manière spécifique, à l'aide de domaines focaux de même excentricité, les ellipses étant situées dans le plan du joint. Ces différentes situations sont illustrées par une expérience de cisaillement dans la phase smectique de CBOOA et leurs énergies sont discutées à l'aide d'un modèle.

Abstract. — Simple geometrical considerations predict 3 types of tilt grain boundaries in smectics A : curvature of the layers, arrays of dislocations and focal domains of equal eccentricity. These 3 possibilities are shown to exist in CBOOA (shear experiment). Their energies are discussed in terms of a simple model.

1. Introduction. — The solid-liquid duality of smectic liquid crystals is reflected in the main structural defects present in these mesophases, the focal conics and dislocations. There is a large elastic energy associated with any deformation which changes the interlayer spacing (compressibility coefficient $B \sim 10^7$ dyne-cm⁻¹) but the viscous relaxation within the layers allows them to glide on one another leaving only the weak energy associated with curvature (Frank constant, $K_1 \sim 10^{-6}$ dyne) (1).

Hence the most common deformations will keep constant the interlayer spacing and transform the smectic planes into parallel surfaces which have common normals and same centers of curvature along the same normal ; these centers of curvature will generally describe focal surfaces. However, in smectics these surfaces degenerate into focal lines because of the liquid character within the layers. The smectic planes are then deformed into Dupin cyclides [1] and the 2 singularities left in the structure are an ellipse and its conjugate hyperbola, the focal conics (Fig. 1). The topology of these focal domains has been studied intensively by Friedel [1] and Bouligand [2]. The dislocations have necessarily a Burgers vector b a multiple of the layer spacing d . Edge dislocations, which will be of interest here, correspond to the existence of one or (more) limited layers in the bulk (Fig. 1a). Their line tension [3]

$$\tau = \frac{\sqrt{K_1 B}}{2} \frac{b^2}{r_c} + \tau_c \tag{1}$$

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(1) The deformation free energy can be expressed in terms of the displacement u of the layers as

$$F = \frac{1}{2} B \left(\frac{\partial u}{\partial z} \right)^2 + \frac{1}{2} K_1 \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right]^2$$

The first term represents an elastic energy for compression of the layer, the second term is a curvature energy.

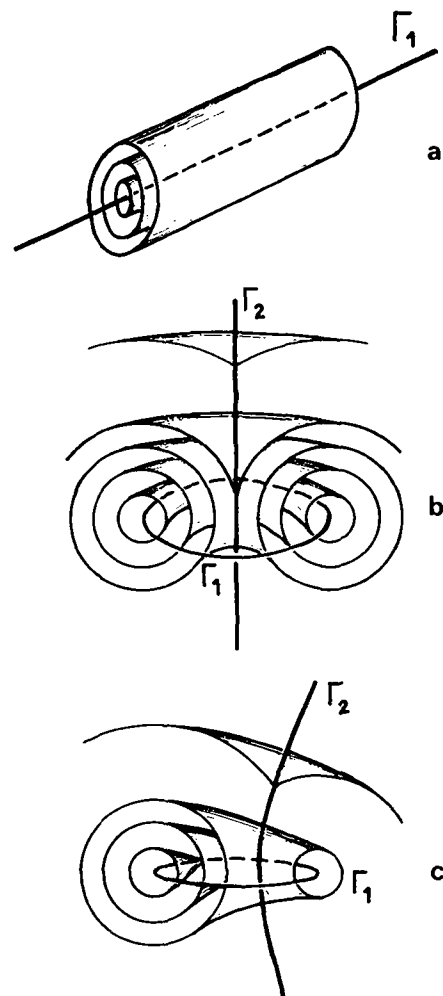


FIG. 1. — Schematic representation of the layers distribution in a confocal domain : a) Confocal domain degenerated into a cylinder. b) Ellipse degenerated into a circle and hyperbola into a straight line. The layers are tori. c) General case.

(b = Burgers vector, r_c = core radius) includes a core energy τ_c and a term due to the competition between elastic energy (dilation of the layers on one side of the line and compression on the other side) and curvature energy. The existence of these dislocations can be inferred from topological considerations and indirect effects in some experiments [4] but they have not been identified until now.

It should be noted also that disclinations (i. e. rotation dislocations) $\Omega = n\pi$, with the rotation axis perpendicular to the molecules, are also allowed by the symmetry of the medium and that the association of 2 disclinations $+\pi$ and $-\pi$ is equivalent to a dislocation (Fig. 2b). The structure of the core is then very different in the two cases and the importance of the transformation will be discussed later.

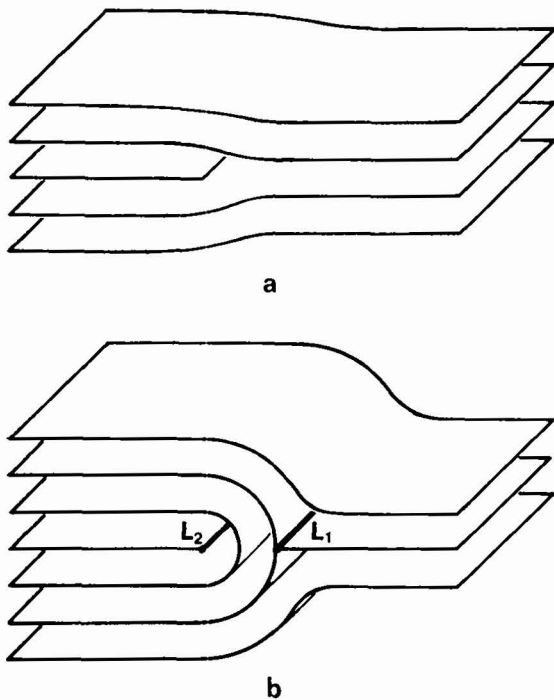


FIG. 2. — a) Edge dislocation. The end of a broken layer is treated as the core region. b) Edge dislocation. The core is split into two disclinations of opposite signs.

As an example of the competition between these different defects we shall analyse how 2 disoriented parts of a smectic can be fitted together. We shall first discuss geometrically the different possibilities and then show experimental evidence of their existence. In a final section we shall discuss briefly their energy.

2. Grain boundaries in smectics. — The 2 different types of boundaries we will be dealing with are :

2.1 A NETWORK OF FOCAL CONICS (Grandjean boundary). — In a focal domain the molecular directions coincide with the asymptotes of the hyperbola far from the ellipse ; the smectic planes are therefore perpendicular to the asymptotes and the singularity on the hyperbola disappears. Thus 2 disoriented regions of

a smectic can be matched by a network of focal conics of equal eccentricity : the ellipses are in the bisecting plane of the layers and the focal domains are cylinders with a probable iterative filling of space [5] (Fig. 3).

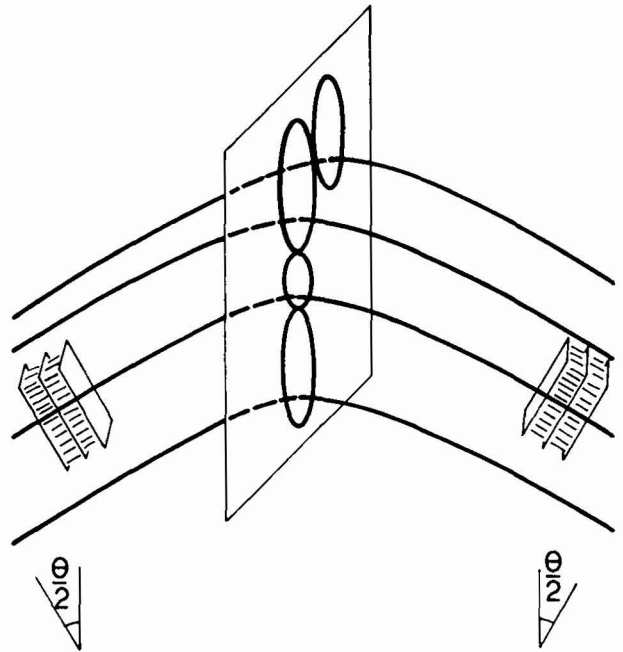


FIG. 3. — Tilt wall between two grains achieved by a system of confocal domains (Grandjean boundary, see text).

Such boundaries were observed by Grandjean [6] in a smectic lying on the cleavage plane of a solid single crystal which imposed different preferred orientations. There, the ellipses were seen edge on and the hyperbolae appeared as parallel striations (Fig. 4a and plate 1).

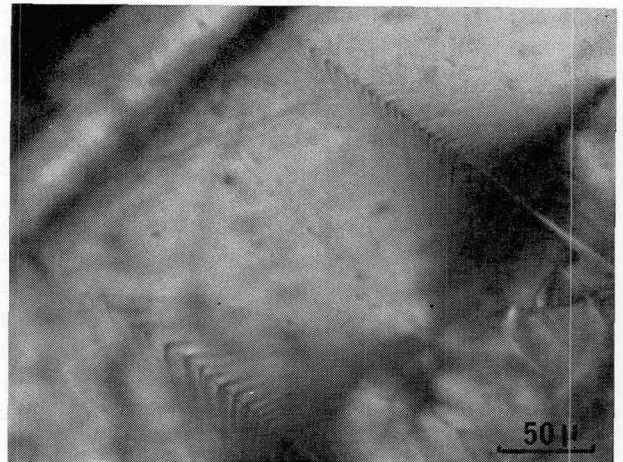


PLATE 1. — Grandjean tilt wall made of focal conics.

2.2 BENDING OF THE LAYERS AND DISLOCATIONS. — Let us start with a perfect planar sample and suppose we bend it. The curvature of the layers will be concentrated in a boundary between 2 disoriented parts with an associated dilation of the layers if no dislocations

are present. This type of boundary has been studied by Bidaux *et al.* for small disorientation $\theta \ll 1$ (Fig. 4a). However if one increases the disorientation, the stresses become large and can be relaxed by the addition of new layers in the boundary and the appearance of edge dislocations (Fig. 4b).

At the other limit, when $\theta \sim \pi$, the boundary is made up only of an array of dislocations similar to tilt boundaries in solids (Fig. 4c).

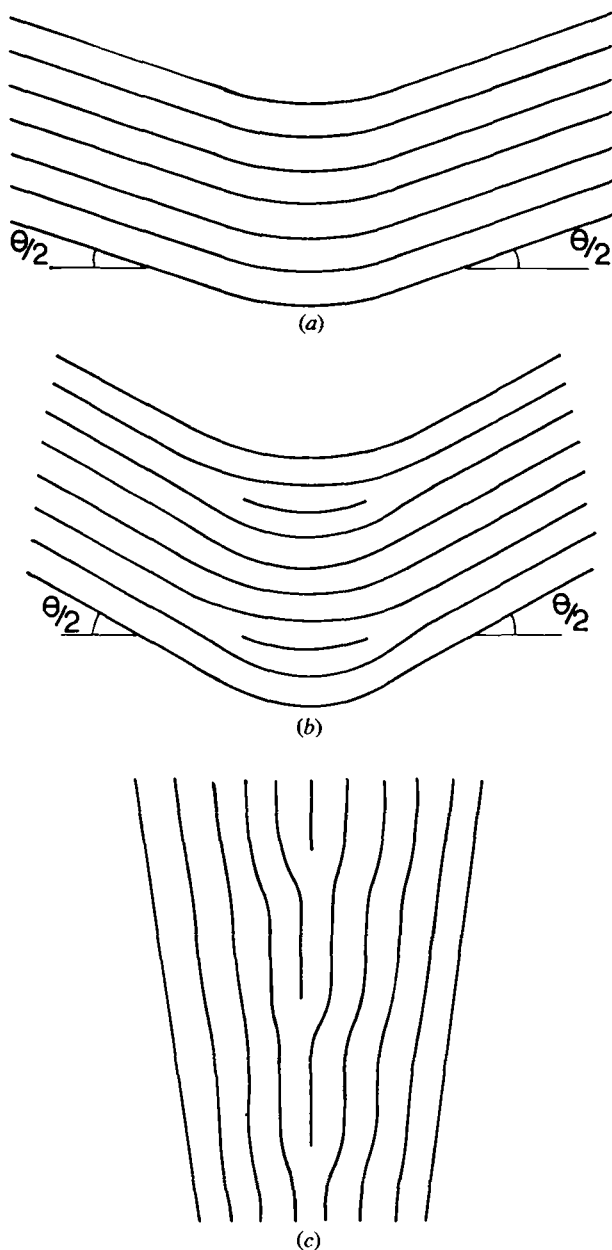


FIG. 4. — a) Tilt wall without dislocations; small disorientation. b) Tilt wall; stresses partly relaxed by dislocations. c) Tilt wall; the disorientation can be accommodated by dislocations acting alone.

3. Experimental. — We shall now describe experiments showing the existence of both types of boundaries and their equivalence in reorienting the smectic planes.

We use in these experiments CBOOA (p-cyano benzylidene-p'-octyloxyaniline) which has the characteristic, apart from a nearly second order Sm \rightarrow N transition, of having a smectic interlayer distance (35 Å) larger than the extended length of the molecule (25 Å).

All observations were made with a Leitz-Orthoplan polarizing microscope. The samples were contained between parallel glass plates, 50 to 200 μ apart. A thin film of SiO evaporated from an angle of 70° on the glass [7] ensured strong anchoring of the molecules parallel to it.

Good single crystals with vertical smectic layers could be grown if cooled from a well oriented nematic phase.

A shear was then applied to the sample (by slow translation of one glass plate with respect to the other), perpendicular to the smectic planes. For a sufficiently large displacement, dislocation lines appear in the sample, parallel to the smectic planes. They are located in 2 horizontal planes close to the glass boundaries and when they are visible, they are 3 to 4 μ apart (Plate 2). It seems that the process of formation of the lines is as follows: the smectic planes remain anchored vertically to the plates during the movement but curve in the bulk. The two glass plates appear therefore as tilt boundaries: they are located along the tilt wall of figure 4a, the smectic being on one side of it only. When the curvature increases with increasing displacement, the layers break and new layers are added to relax the strain (Fig. 5a). As soon as one stops the movement of

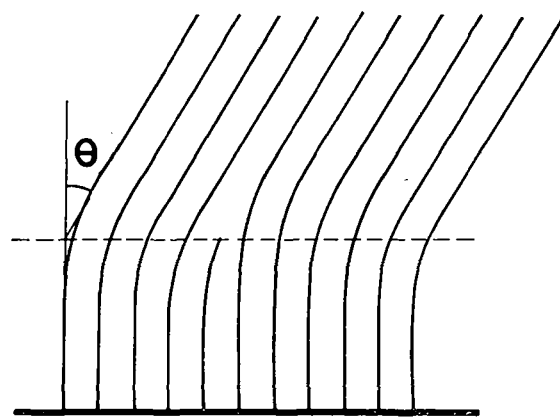


FIG. 5. — Schematic representation of the contact between the layers attached to the surface and the layers in the bulk. This epitaxial boundary is also similar to the type of dislocation boundary drawn in figure 4b.

the glass plates the lines on each boundary merge and group together and ellipses of focal domains appear in the same horizontal plane (or very close to it, within the depth of field of the microscope ~ 3 to 10 μ). Their minor axes are parallel to the dislocation lines and, whatever their size, their eccentricity is of the order of 2 (Plate 2). The lines do not cross the ellipses but are replaced by them, in a similar transformation to the one described in a previous article [8] when

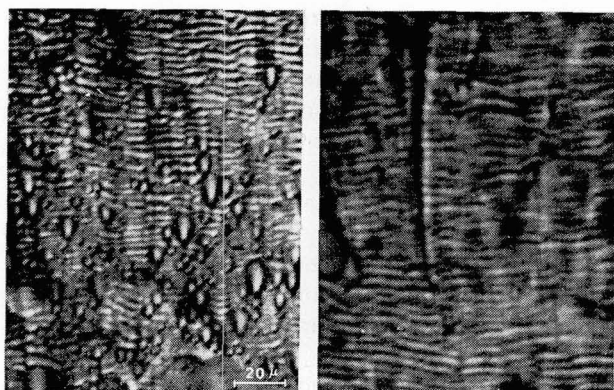


PLATE 2. — Shear experiment : dislocations near both glass surfaces. Ellipses have already appeared at one boundary. Thickness of the sample : 100 μ.

smectic samples are grown from the solid phase and dislocation lines appear near the solid-smectic phase. In both experiments, lines and focal domains are present simultaneously after relaxation. Plate 3 represents a fully relaxed sample where the grain boundary made up of dislocation lines has been partially replaced by a network of focal conics. This is a boundary identical to the one described by Grandjean but the ellipses are now in the plane of observation.

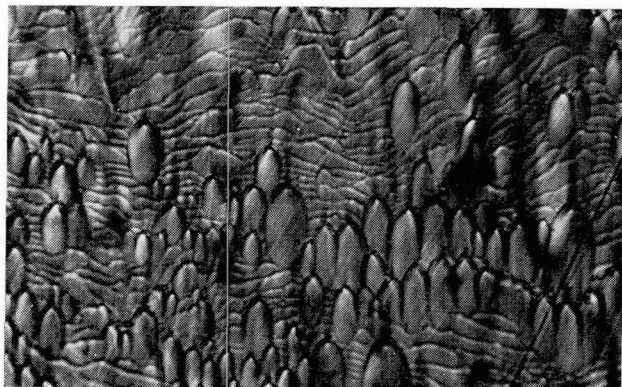


PLATE 3. — Shear experiment : after relaxation, the dislocation wall is partially replaced by a Grandjean boundary (focal domains).

What information can one deduce from such pictures ?

Firstly, the eccentricity of the ellipses, of the order of 2.2, allows us to deduce that the inclination of the smectic planes with respect to the vertical is about 25° ($\cot^2 \theta = e^2 - 1$).

Secondly, the geometry of the wall (Fig. 4b and 5) gives a relationship between disorientation, Burgers vector of the dislocation lines b and spacing between them l

$$b = l(1 - \cos \theta) \tag{2}$$

which, for a spacing l equal to 4 μ, gives a Burgers vector of 90 layers.

This contact between the region near the boundary

and the region in the bulk is reminiscent of an epitaxial boundary in a crystalline solid.

It should be noted that lines with a smaller Burgers vector could exist in the sample but they are not optically resolved for a spacing smaller than 3 to 4 μ and this has prevented us so far from determining the precise displacement of the glass plates necessary to break the layers. Further shearing does not increase the inclination of the layers in the bulk.

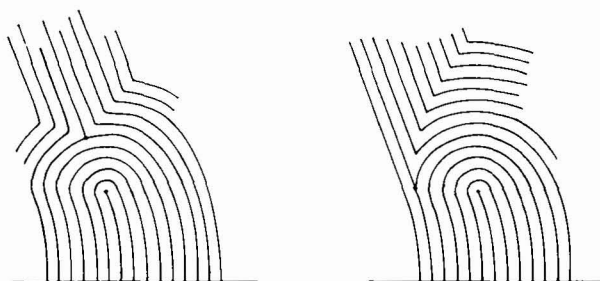


FIG. 6. — Early stage of the transformation of a dislocation line with large Burgers vector into focal conics.

4. Discussion. — We will discuss qualitatively the important features of the dislocation lines in these experiments :

- their tendency to group together to form lines with large Burgers vectors,
- and the possibility of formation of tilt walls of dislocations.

4.1 LARGE BURGERS VECTOR AND CONFIGURATION OF THE CORE. — In linear elastic theory of smectics, the line tension

$$\tau = \frac{K_1}{2} \frac{b^2}{\lambda r_c} + \tau_c \quad \left(\lambda = \left(\frac{K}{B} \right)^{1/2} \right)$$

has the same square-law dependence on b as for a dislocation line in a solid ($\tau = \frac{\mu b^2}{4\pi} \ln \frac{R}{r_c} + \tau_c$) [11] but its dependence on the other parameters is different :

- there is no divergence with the size R of the specimen,
- it is proportional to $1/r_c$ rather than to its logarithm.

If the core radius r_c is of the same order of magnitude as b , τ is proportional to b and the total energy is not decreased if the lines split as they do in solids ($b_1^2 + b_2^2 < (b_1 + b_2)^2$). This point brings up the problem of the core. For small b , there is no experimental evidence of what the core structure might be. However, for large b the observed relaxation of the lines into cofocal domains can be well described if the dislocation line is split into 2 disclination lines L_1 and L_2 (Fig. 2b). This configuration has curvature energy between L_1 and L_2 and also a large amount of elastic energy in the region outside L_1 : this can be concentrated in 2 focal regions which afterwards can relax into focal lines (Fig. 6). Such a process is also apparent in

cholesterics [9] and lyotropic lamellar phases [10]. The line tension of such a configuration with an equivalent Burgers vector $b = nd$ (n large) can be estimated. A first term takes into account the elastic energy outside the core region $L_1 L_2$. At large distance, it should be of the same order as for a dislocation line, i. e. $\sim \frac{K_1 n^2 d^2}{2 \lambda r_c} \simeq \frac{K_1 nd}{2 \lambda}$. At short distances (outside L_1) it is of the order of a Bidaux *et al.* tilt wall [5] (Fig. 4a) of angle $\theta \sim 1$, i. e. $\frac{32}{3} K_1 \frac{nd}{\lambda}$. The total contribution is $\sim 10 K \frac{nd}{\lambda}$.

A second term due to curvature energy in the half-cylindrical region between L_1 and L_2 is estimated to be $\frac{\pi K_1}{2} \ln \frac{n}{2}$ for large n . A last term τ'_c comes from the 2 core regions L_1 and L_2 . Finally, we get

$$\tau_{L_1 L_2} \simeq 10 K_1 \frac{nd}{\lambda} + \frac{\pi K_1}{2} \ln \frac{n}{2} + \tau'_c. \quad (3)$$

In this model τ'_c does not depend on n , so that at *short distances* dislocations of the same sign can attract each other if they are on the same climb plane; this is the plane where the elastic interactions are minimal [3]. The second term also gives rise to an attraction between lines of the same sign if n is large. In conclusion, the proposed core model would favour large Burgers vectors.

4.2 ENERGY OF A DISLOCATION WALL (Fig. 5). — The energy per unit area of a tilt dislocation wall can be estimated as the sum of contributions due to individual dislocations of Burgers vector $b = nd = l(1 - \cos \theta)$ (see eq. (2)), neglecting the mutual interactions between dislocations and with the boundaries. Using eq. (3), we get

$$\sigma_d \sim 5 \frac{\theta^2 K_1}{\lambda} + \frac{4 K_1}{\pi} \frac{\theta^2}{nd} \ln \frac{n}{2} + \frac{\theta^2}{2 nd} \tau'_c. \quad (4)$$

Large values of n will lower the energy even more than in the case of an isolated dislocation.

This energy can be compared with the energy of a tilt wall without dislocations calculated by Bidaux *et al.* [5] in the limit of small θ 's :

$$\sigma_w = \frac{16}{3} B \lambda \theta^3. \quad (5)$$

For small disorientation σ_w , of order θ^3 , is smaller than σ_d , of order θ^2 , but for large disorientation the wall of dislocations has a lower energy. This is true for all

values of n and there exists an angle $\theta_c(n)$ for which $\sigma_w(\theta_c)$ and $\sigma_d(\theta_c)$ are equal. Let us remark that

$$\left(\frac{\partial \sigma_d}{\partial n} \right)_\theta = - \frac{\pi}{8 b} K_1 \theta^2 \frac{\ln n/2}{n^2} - \frac{\theta^2}{2 n^2 b} \left(\tau'_c - \frac{\pi K_1}{2} \right) \quad (6)$$

is probably negative so that θ_c decreases as n increases; but the 2 curves are not tangent at the origin so that for n infinite they cross at a finite θ .

When one shears the smectic sample, one can therefore think that the following process takes place : a tilt wall without dislocation first appears. Then the layers break and form dislocations with the smallest possible Burgers vector at the value of θ for which σ_w equals σ_d . For $n = 2$, this leads to $\theta \sim 1$, i. e. a large angle. Afterwards, σ_d is relaxed by increasing n and the dislocations group with large Burgers vector.

An important remark remains to be made concerning this model of the tilt dislocation boundary. The difference with solids, in which tilt walls are well known, is striking : in solids the dislocations form an array of lines whose Burgers vector is perpendicular to the wall; one speaks of a coherent tilt wall. In our case, we have clearly an incoherent tilt wall, since the Burgers vector is (more or less) in the plane of the wall. This corresponds physically to the fact that the dislocations we introduce cannot relax all the curvature energy σ_w , but that a *minimum* amount of curvature subsists, whose energy has not been taken into account. This curvature of the layers is *not* at constant layer thickness, and is relaxed by the formation of confocal domains. This transformation of lines with large Burgers vector into focal conics will be discussed in a forthcoming paper.

5. **Conclusion.** — Shearing of a single-domain crystal of CBOOA in its smectic A phase allowed us to create tilt walls. We have shown that :

(i) The tilt walls predicted by simple geometrical considerations do exist in smectics.

(ii) For a small disorientation angle the layers are simply curved; for a larger angle θ_c layers break and dislocation lines appear in the boundary. These group together to form lines with very large Burgers vectors. Simple energetic considerations explain these transformations.

(iii) The tilt wall of dislocations transform afterwards into a wall made up of focal domains of equal eccentricity, all the ellipses being in the plane of the boundary.

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