Curvature Elasticity of Smectic-A Textures with Virtual Surface Singularities

J. B. Fournier
Laboratoire de Physique des Solides, Université Paris-Sud, Bâtiment 510, 91405 Orsay, France
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Smectic-A textures limited by special boundaries which do not fix the layer positions but only the direction of the layer normals should obey a simplified elasticity. This elasticity involves no layer dilation but only curvature energy. We present it for smectics limited to planar cells, when all the singularities due to the absence of layer dilation are virtual. We show the possibility of anchoring transitions at low threshold and the existence of a universal cycloid shape in the absence of external constraints. The link with the nucleation of smectic focal conics is discussed.

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Smectic-A liquid crystals [1] are made by the piling of liquid monolayers of rodlike molecules oriented normally to the layers. In practice, external forces induce distorted textures where the lamellae can be both curved and dilated. To face the general situation, one has to use a complete elastic theory specifying the position of every lamella [2,3]. Arbitrary constraints on the *positions* of the lamellae can produce textures where the dilation energy compares with the curvature energy, e.g., relaxation texture of an imposed lamellae undulation [4], distortion induced by a dislocation [5], etc. Besides such positional constraints, most boundaries favor specific lamellae *orientations*. Thus, antagonistic boundaries induce principally lamellae *curvature*. Indeed, the most familiar smectic textures consist in curved lamellae remaining *equidistant*. This constraint causes in counterpart the creation of characteristic *singular lines* as pairs of ellipses and hyperbolae. To describe these so-called "focal-conic" textures [6–8], *geometry* is used instead of elasticity, since giving the positions and geometrical parameters of the ellipses and hyperbolae completely determines the whole lamellar texture. Another situation is the one of free-standing films [9] (few curved equidistant lamellae between two air interfaces). Like mechanical thin plates they involve only curvature energy, the minimization of which is trivial. Recently, a new class of boundaries has appeared, which favors only the orientation of the lamellae and leaves their positions completely free (e.g., isotropic phase [10], simple liquids [11], rough interfaces [12], etc.). Such boundaries will induce only curvature (as in free-standing films), but the corresponding elasticity is no longer trivial since the lamellae can now freely intersect the boundaries. In this Letter, we study the elasticity of macroscopic smectic-A plates limited by such free boundaries. We show that the general elasticity can be reduced to a pure-curvature elasticity involving directly the boundaries' interactions. This specific elasticity acts in a continuum of new "confocal textures" with *virtual* surface singularities that generalize the discrete, geometrical, focal conics.

Some preliminary geometrical considerations on lamellar textures will be useful. One can associate to any given lamella its *focal surface* [13], defined as the surface generated by the family of the lamella normals, or equivalently as the locus of its two centers of principal curvature. It generally consists in two separated sheets (one for each principal curvature). Usually, the lamellae continuum generates a continuum of focal surfaces. Let us now consider the most general texture with curved cut strictly equidistant lamellae. The whole texture can be derived from any of its lamellae chosen arbitrarily as a reference, by simply shifting constant distances along the normals to this reference lamella. The common normals to the texture are called "*generators*." Such textures have the fundamental property that the lamellae focal surfaces degenerate into a unique surface (enveloped by the generators). For this reason, they are called *confocal textures* [3,7,8]. Their common focal surface is generally the locus of a singularity for the smectic piling. Being too energetical inside the bulk, it must degenerate into lines or points [14,15] in an infinite smectic. Geometry shows that the only confocal textures with line or point singularities are the focal conics: The singularities are a pair made up of a confocal ellipse and a hyperbola (in perpendicular planes, the focus of one coinciding with the summit of the other). The lamellae assume then the shape of the so-called "Dupin's cyclides." When the ellipse is degenerated to a point, the hyperbola vanishes and one obtains a spherical lamellae piling [8] with its point singularity. Now, for a smectic of finite size, our starting point is that the singularities can remain surfaces since they can be *virtual,* i.e., outside the physical volume of the smectic. The smectic texture will then differ from the usual focal-conic texture, without implying any dilation energy. This provides a continuum of confocal textures that will allow us to go from strict geometry to a true elasticity.

Let us first study whether the above-described geometrical confocal textures are physically stable. In the usual elastic description of smectic-A textures [2], the molecules are assumed strictly normal to the lamellae. A distorted state is described by the field of the normal displacements $u(x,y,z)$ of the lamellae. For small deformations, the usual elastic free-energy density reads [16]

$$f=\frac{1}{2}K\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)^2+\frac{1}{2}B\left(\frac{\partial u}{\partial z}\right)^2\equiv\frac{1}{2}K\sigma^2+\frac{1}{2}B\varepsilon^2\,, \quad (1)$$

where σ is twice the mean curvature of the lamellae and ε their relative dilation. $(K/B)^{1/2}\equiv\lambda$ is usually a molecular length [1] ~ 30 Å (far from second-order phase transitions). Minimization of the volumic integral of the free energy (1) gives the smectic bulk equilibrium equation

$$\frac{\partial^4 u}{\partial x^4}+2\frac{\partial^4 u}{\partial x^2\partial y^2}+\frac{\partial^4 u}{\partial y^4}=\frac{1}{\lambda^2}\frac{\partial^2 u}{\partial z^2}\Longleftrightarrow\Delta_\perp\sigma=\frac{1}{\lambda^2}\partial_\parallel\varepsilon\,, \quad (2)$$

where $(\partial_\parallel)_i\equiv n_i n_j\partial_j$ and $(\partial_\perp)_i\equiv(\delta_{ij}-n_i n_j)\partial_j$ refer to the direction of the local lamellae normal $n_i\equiv\delta_{iz}+O(\partial_i u)$. Rapid curvature variations are intrinsically equilibrated by layer dilation. Thus, ideal confocal textures ($\varepsilon\equiv 0$) are strictly speaking unstable versus lamellae dilation. Their intrinsic equilibrium dilation can be easily evaluated by integrating Eq. (2) along the straight generators. If the ε found is small enough, the real texture can be considered as "confocal." In practice, it is reasonable to accept as confocal any texture with both a negligible dilation, i.e., $\varepsilon\ll 1$, and a "*passive*" dilation energy, i.e.,

$$B\varepsilon^2\ll K\sigma^2\,. \quad (3)$$

Let us now consider a smectic-A limited by boundaries that the lamellae can freely intersect without feeling any positional constraint. In the absence of any imposed lamellae dilation, it is natural to look for an elasticity involving only curvature energy in the continuum of confocal textures. To simplify, we consider a smectic limited to a planar cell $\parallel(x,y)$ of thickness d (Fig. 1). The external forces are an external field $\mathbf{E}\parallel\mathbf{z}$ coupling to the smectic dielectric anisotropy $\Delta\varepsilon$, and two plate "anchorings" $\gamma_1(\theta)$ and $\gamma_2(\theta)$ assumed to favor only preferred orientations but to give no positional anchoring [17]. We look for an equilibrium confocal texture assumed invariant along y, with focal surfaces *all virtual* and well outside the cell. Integrating Eq. (2) along a generator of length L gives $\bar\varepsilon\sim l\sigma(\lambda/a)^2$, a being the curvature variations length scale. Then condition (3) reads $l^2\ll(a^2/\lambda)^2$.

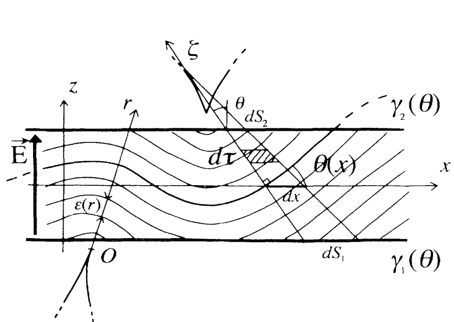

FIG. 1. Geometry of an arbitrary confocal texture with virtual focal surfaces (drawn as cusps outside the cell). The whole texture can be entirely deduced from one of its lamellae.

Since $l\le\sigma^{-1}$, passive dilation requires only

$$a\ge(\sigma^{-1}\lambda)^{1/2}\,. \quad (4)$$

Under this condition, the dilation energy can be neglected ($\frac{1}{2}B\varepsilon^2\ll\frac{1}{2}K\sigma^2$) and the free energy per unit length reduces to [18]

$$F=\int\!\!\int d\tau\left\{\frac{1}{2}K\sigma^2+\frac{1}{2}\frac{\Delta\varepsilon}{4\pi}E^2\sin^2\theta\right\}+\sum_{i=1,2}\int dS_i\,\gamma_i(\theta)\,. \quad (5)$$

Our confocal texture with virtual focal surfaces is entirely determined by the shape of one of its lamellae; it can be equivalently parametrized by the angle $\theta(x)$ at which the lamellae intersect the x axis (Fig. 1). From confocality, the lamella curvature radius σ^{-1} varies linearly along the generators. Calling ζ the coordinate along the generators, we have $\sigma^{-1}(x,\zeta)=\sigma^{-1}(x,0)-\zeta$, $d\tau=dx(1-\zeta\sigma)\zeta d\cos\theta$, $dS_i=dx(1-\zeta_i\sigma)$ $(i=1,2)$, and the boundary curvatures σ_i $(i=1,2)$ verify $\sigma_2-\sigma_1=l\sigma_1\sigma_2$ and $\sigma_1^{-1}+\sigma_2^{-1}=2\sigma^{-1}|_{\zeta=0}$. Without any assumption on the lamellae shape, the free energy (5) can be integrated along the generators:

$$F[\theta(x)]=\int dx\cos\theta\left\{\frac{1}{2}K\sigma\ln\frac{\sigma_2}{\sigma_1}+\sum_{i=1,2}\frac{\sigma}{\sigma_i}\frac{\tilde\gamma_i(\theta)}{\cos\theta}\right\}, \quad (6)$$

where

$$\tilde\gamma_i(\theta)=\gamma_i(\theta)+\frac{1}{4}\frac{\Delta\varepsilon}{4\pi}E^2 d\sin^2\theta\,. \quad (7)$$

Surface and bulk terms are intimately mixed and the external field simply renormalizes the surface energies. Making use of $\sigma=(d\theta/dx)\cos\theta$ and $\zeta_2=-\zeta_1=d/2\cos\theta$, the free energy (6) can be expressed in terms of $\theta(x)$ and its derivatives. Standard functional minimization, followed by a derivative transformation $[d/dx\rightarrow(\partial/\partial s)|_\zeta]$ introducing the curvilinear coordinate s through $d\sigma/dx=\cos\theta(\partial\sigma/\partial s)-\sigma^2\sin\theta$, yields the texture equilibrium equation ($'\equiv d/d\theta$):

$$Kl\left\{\left(\frac{\tilde\sigma}{\sigma}\right)^2\frac{\partial\sigma}{\partial s}-\tan\theta\,\sigma_1\sigma_2\right\}=\sum_{i=1,2}\frac{\tilde\gamma_i'}{\cos\theta}\,, \quad (8)$$

where

$$\tilde\sigma=[\sigma_1\sigma_2(\sigma_1+\sigma_2)/2]^{1/2}\,. \quad (9)$$

From confocality, Eq. (8) is invariant along the generators, since $(\partial\sigma/\partial s)/\sigma^3=(-)\partial\sigma^{-1}/\partial\theta$ is itself invariant. Thus, Eq. (8) originally written along the x axis is readily the equilibrium equation of any of the lamellae [parametrized by $\theta(s)$]. It expresses the balance of the torques acting on a generator (per lamella surface unit): $\gamma_i'/\cos\theta$ are the surface and field torques, $(-)Kl(\tilde\sigma/\sigma)^3\partial\sigma/\partial s$ is exactly the integral of the lamellae curvature torques $(-)K(\partial\sigma/\partial s)(\zeta)$, and $Kl\tan\theta\,\sigma_1\sigma_2$ is an additional torque induced at constant curvature by the variation of the generator lengths $l = d/\cos\theta$. In the weak-curvature approximation $\sigma_2 \sim \sigma_1 \equiv \sigma \ll l^{-1}$, Eq. (8) simplifies to

$$Kd\frac{\partial}{\partial\theta}(\sigma^2\cos^2\theta) = \sum_{i=1,2} \tilde{\gamma}_i' \cos^2\theta\,, \tag{10}$$

which is directly integrable for any surface anchorings and external field. In the absence of external forces, it becomes simply $\partial(\sigma^{-1}l)/\partial\theta = 0$: The lamellae are not curved at constant radius σ^{-1} (as free-standing films) but at constant product $\sigma^{-1}l$. The corresponding shape is a *cycloid*, $s(\theta) = A\sin\theta$, whose integration constant is to be chosen according to the lateral boundary conditions (here nondefined). The striking feature of the texture equation (8) is the "nonlocal" character of the external forces, due to the rigidity of the generators. Indeed, opposite anchorings $\gamma_1(\theta) = -\gamma_2(\theta)$ and indifferent anchorings $\gamma_1(\theta) = \gamma_2(\theta) = 0$ yield the same set of solutions. Another interesting feature is the effect of the external field. Expanding $\gamma_i(\theta) \sim \gamma_i^{(0)} + \gamma_i^{(2)}\sin^2\theta + \gamma_i^{(4)}\sin^4\theta$, only the coefficient $\gamma_i^{(2)}$ (usually $\gg \gamma_i^{(4)}$) is renormalized by the electrical field. Assuming $\Delta\varepsilon < 0$, $\gamma_i^{(2)}$ can be compensated, which allows for second-order and first-order texture transitions according to the sign of $\gamma_i^{(4)}$. Even with a strong anchoring $l_a \equiv K/\gamma^{(2)} \sim 1000$ Å ($K \sim 5 \times 10^{-7}$ cgs) and a low $|\Delta\varepsilon| \sim 0.1$, the threshold $\Delta\varepsilon V_c^2/d \sim \gamma_i^{(2)}$ corresponds to a low tension $V_c \sim 7$ V for a 10 μm thick cell. This value is $(l_a/\lambda)^{1/2} \sim 10$ times lower than the Helfrich-Hurault [1,19] so-called "ghost" transition. In practice, due to permeation [1], the above discussed transitions should be slow (unless the smectic order is melted near the boundaries [20]).

The equilibrium confocal textures may sometimes attract the focal surfaces and yield the nucleation of focal conics. First, we expect the most general confocal texture to have *virtual surfaces* degenerating into *real lines* as they penetrate the smectic bulk (Fig. 2). This raises some interesting problems. Consider in Fig. 1 the penetration of a focal-surface cusp. Along the cusp generator, since $\partial\sigma/\partial s = 0$, we have $\partial^2\sigma/\partial s^2 = -\sigma^4\partial^2(\sigma^{-1})/\partial\theta^2$.

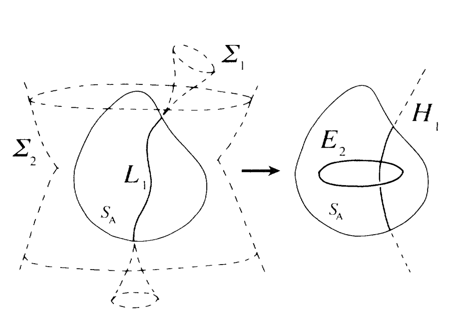

FIG. 2. Virtual focal surfaces degenerating into real lines as they penetrate the smectic. If both focal sheets enter, they degenerate into parts of conjugated conics. Once the ellipse is completely embedded, the hyperbola cannot transform to a surface outside the bulk.

From confocality, $\partial^2(\sigma^{-1})/\partial\theta^2 \equiv \Lambda$ is a (macroscopic) generator's constant; then $\partial^2\sigma/\partial s^2 = -\Lambda\sigma^4$. Integrating Eq. (2) up to a distance r ($=\sigma^{-1}$) to the cusp, ε diverges as $\sim\Lambda\lambda^2/r^3$, and the stability condition (3) requires $r \geq r_c \sim (\Lambda\lambda)^{1/2}$. Closer than r_c, which is a mesoscopic distance, the texture is no more confocal and dilation will repel the singularity (unless it is topologically required). In practice $\Lambda \sim 100$ μm gives $r_c \sim 5000$ Å, still below optical microscopy resolution. If one sheet of the focal surface is forced to penetrate the bulk, it will degenerate into a line [21]. We know from geometry [22] that the most general surface where focal sheets are one surface and one *line* (parametrized by u) is generated by the envelope of a family of spheres centered on the line, with varying radii $r(u)$. Regarding the elasticity this case is more delicate: To define the reference lamella one needs an additional variable defining the shape of the focal line; the saddle-splay term will generally contribute; the generators will be articulated along the line singularity and their lengths will be complicated functions of the smectic volume shape. Because of this articulation, the electrical field will not simply renormalize the surface energies. If the two focal sheets both enter the bulk, they must degenerate into pieces of an ellipse and its confocal hyperbola (Fig. 2). To this degeneracy will correspond an energy barrier of *geometrical* origin associated with the nucleation of focal conics. Once the ellipse is completely embedded inside the bulk, the whole texture is geometrically determined, and the conics cannot transform to surfaces outside the bulk (unless introducing some dilation corresponding to the classical curvature discontinuities between domains [7]). When the ellipse is partially virtual or simply lying on the interface, the transformation to virtual surfaces is possible. This point is important as the interfacial lamellae can be affected, and together the interfacial energy which is generally responsible for the very existence of the focal conics [10,11].

In summary, the possible existence of boundaries producing a smectic *orientational* anchoring, but not positional anchoring, yields a new class of problems. Such interfaces exist naturally (e.g., liquid mesophases) or could be produced by suitable surface treatments (e.g., liquid coatings [11], controlled roughness [12], etc.). The expected smectic textures belong to a new class of confocal textures with virtual singularities outside the smectic bulk, that generalize the usual focal conics. These textures can be described by a reduced set of variables; this allows us to work out a specific elasticity that contains only curvature energy and directly involves the external constraints. We have explicitly derived the elastic equilibrium equation for planar cells, when the singularities are all virtual. We find the possibility of field-induced texture transitions with a very low threshold and the existence of a universal shape (cycloid) in the absence of external forces. Finally, the possibility of confocal textures with both real focal lines and virtual focal surfaces provides a new framework to study the nucleation of focal conics and should yield a reinterpretation of focal conic textures in the vicinity of free interfaces.

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[1] P. G. de Gennes, *The Physics of Liquid Crystals* (Academic, New York, 1974).
[2] P. G. de Gennes, J. Phys (Paris), Colloq. **30**, C4-65 (1969).
[3] M. Kleman and O. Parodi, J. Phys (Paris) **36**, 671 (1975).
[4] G. Durand, C.R. Hebd. Seances Acad. Sci. Ser. B **275**, 629 (1972).
[5] P. G. de Gennes, C.R. Hebd. Seances Acad. Sci. Ser. B **275**, 939 (1972).
[6] G. Friedel and F. Grandjean, Bull. Soc. Fr. Mineral Cristallogr. **33**, 192 (1910). See also G. Friedel, Ann. Phys. (Paris) **18**, 273 (1922).
[7] Y. Bouligand, J. Phys (Paris) **33**, 525 (1972).
[8] J. P. Sethna and M. Kleman, Phys. Rev. A **26**, 3037 (1982).
[9] C. Rosenblatt and N. Amer, Appl. Phys. Lett. **36**, 432 (1980).
[10] J. B. Fournier and G. Durand, J. Phys. II (France) **1**, 845–870 (1991), and references therein.
[11] O. D. Lavrentovich, Zh. Eksp. Teor. Fiz. **91**, 1666 (1986) [Sov. Phys. JETP **64**, 984 (1986)].
[12] M. Monkade, M. Boix, and G. Durand, Europhys. Lett. **5**, 697–702 (1988).
[13] G. Salmon, *Analytic Geometry of Three Dimensions* (Chelsea, New York, 1952).
[14] M. Kleman, *Points, Lines and Walls* (Wiley, New York, 1981).
[15] As mentioned in Ref. [9], a pair of one real line and one nonmaterialized surface is also possible.
[16] The saddle-splay term being a *surface* term, it need not be introduced at this point.
[17] G. Durand, in "Liquid Crystals," Proceedings of the Fourteenth ILCC, Pisa, 1992 (to be published).
[18] The saddle splay is zero as the Gaussian curvature is zero from invariance along y.
[19] W. Helfrich, Appl. Phys. Lett. **17**, 531 (1970).
[20] M. Cagnon and G. Durand (to be published).
[21] Focal lines having a higher symmetry, the divergence of ε is generally weaker.
[22] D. Hilbert and S. Cohn-Vossen, *Geometry and the Imagination* (Chelsea, New York, 1952).