Spheric domains in smectic liquid crystals

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We study smectic-A defect structures which preserve layer thickness. We deduce that the interstitial regions between the well-known focal conic domains are filled with concentric spheres.

The study of defects in condensed matter systems has flourished in the past few years. It has grown from the classical investigation of line defects in solids to include everything from boojums in superfluids to defect mediated phase transitions in films.

Topology has been a basic tool in this study; the far field topological structure of the order parameter determines the simple configurational properties of most defects. Smectics form a striking exception to this pattern. The singular lines of the focal domains found in smectic liquid crystals form remarkably precise ellipses and hyperbolas (see Fig. 1). These simple forms cannot be understood using topology (topology treats ellipses as rubber bands). Geometry is a better tool here; it was used by Friedel and Grandjean[1] in 1910 to explain the focal conic defect as a consequence of their proposed layered smectic structure.

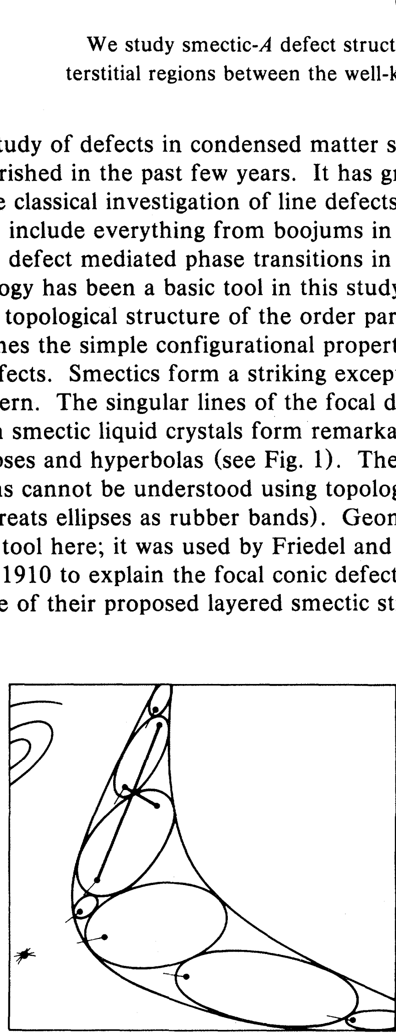

FIG. 1. The singular lines in smectic-A samples often form remarkably precise ellipses and hyperbolas. The ellipses here are attached to one of the glass slides. The dark lines extending from one focus of each ellipse are the conjugate hyperbolas; they lie perpendicular to the plane of the glass and go out of focus. Note that the major axes of the ellipses all pass through the pont marked with an asterisk. Note also that the point of tangency between two neighboring ellipses is the point of intersection of the lines connecting opposing foci. The original photograph is by C. Williams; it is reproduced in Ref. 2.

In this Communication, we will use geometry to study the simple smectic defects, and the ways in which they may be matched together to form compound defects. We will mostly study distortions which preserve the layer thickness (i.e., we ignore dislocations). We emphasize the importance of concentric spheres in the construction of compound defects. To be specific, we show that the ubiquitous polygonal field structures are spheric domains, with embedded focal conics which act to relax stresses imposed by the boundary conditions.

The smectic ground state is characterized by the segregation of molecules into a series of flat, parallel layers with liquid motion within each layer. Stresses which bend or compress these layers will cause elastic deformations; other stresses will cause viscous flow. Often the elastic constant $\bar{B}$ associated with compressing the interlayer spacing is large compared to the bending elastic constant K_1. More precisely, there is a characteristic length $\lambda=(K_1/\bar{B})^{1/2}$ which is normally comparable to the layer thickness.[2] Compression will be unimportant if the amplitude of the deformation is large compared to λ. (For example, compression is important in dislocations, where the amplitude is a layer thickness.) We shall temporarily ignore compression and treat our layers as strictly parallel, although bendable.

Consider now the vector field $\vec{n}$ of unit normals to a set of parallel surfaces. It is easy to see that the existence of surfaces implies $\vec{n}\cdot(\vec{\nabla}\times\vec{n})=0$, while their equal spacing implies $\vec{n}\times(\vec{\nabla}\times\vec{n})=0$. Since $n^2=1$,

$$\tfrac{1}{2}\partial_\alpha n^2=n_\beta\partial_\alpha n_\beta=0\ ,$$

$$\vec{\nabla}\times\vec{n}=\partial_\alpha n_\beta-\partial_\beta n_\alpha=0\ ,$$

$$\therefore\ n_\beta\partial_\beta n_\alpha=\lim_{\epsilon\to 0}\frac{n_\alpha(x+\epsilon n)-n_\alpha(x)}{\epsilon}=0\ .$$

One can see from this last equation that $\vec{n}$ does not change as one moves parallel to it. Thus a line perpendicular to one smectic layer will be perpendicular to any other layer it crosses. These lines are called *generators.*

These generators express very clearly the nonlocal constraints implied by the smectic structure. A single smectic layer M determines the structure in the entire region filled by the generators passing through M (Fig. 2). Any singularities in this region can be found geometrically—they are associated with the *evolute* of M.

Consider the generator G passing through point P on M. At P, M has a maximum and a minimum radius of curvature; the corresponding centers of curvature lie on G. It is easy to see that surfaces parallel to M will share these centers of curvature (Fig. 2). At these points, a radius of curvature goes to zero, and a singularity occurs in the structure. As we vary P over M, these two centers of curvature trace out the two sheets of the evolute of M. The generators for M are precisely the common tangents to the two sheets.

The sheets of the evolute (and thus the associated defects) will generically both be two dimensional. Two-dimensional defects do exist[3]; under certain circumstances their energy need not be prohibitive. On the other hand, the smectic structure introduces rigid constraints on the possible point and line defects.[4] The only surfaces with a zero-dimensional evolute are spheres; concentric spheres are the only allowed point defect. If both sheets of the evolute are one dimensional, the surface is a cyclide of Dupin, and the sheets form confocal conics. The only allowed line defects where the layers have negative curvature are the resulting focal domains of the first kind. Experimentally, light scatters off these defect lines, illuminating the striking patterns of ellipses and hyperbolas (Fig. 3).

For smectic layers of positive curvature, it is possible for one of the sheets of the evolute to be *virtual.* The radius of curvature lying on the virtual surface of centers is always larger than that of the other sheet. Thus the singularities always occur first on the other sheet; the virtual sheet hides "behind" it. The evolute for focal domains of the second kind,[5] for example, is a pair of confocal conics—but the ellipse is virtual. Focal domains of the second kind are not observed in nature. This is quite natural; there is no compelling reason for a virtual defect to remain one dimensional. Physically, these domains should be included in a wider class of defect structures, whose evolutes consist of a one-dimensional and a virtual two-dimensional sheet. The smectic layers in this class form *canal surfaces.*[6]

The elementary smectic defects do not usually occur in isolation; they normally group together into compound structures. This grouping is by no means haphazard. In assembling simple defects together, one is constrained to mesh the smectic layers smoothly at the interfaces; we explore the consequences of this constraint.

The interfaces between domains in a compound structure must, of course, be two-dimensional surfaces. [The focal conic domains in most compound structures are tangent along lines (as we shall see). The original analysis[1] concentrated upon meshing the layers along these lines, even though filing in the interstitial regions clearly involves matching along sur-

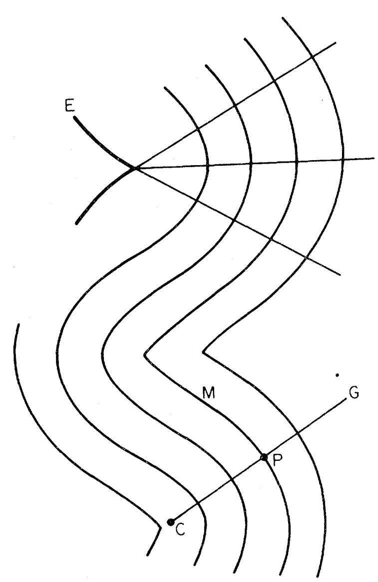

FIG. 2. A two-dimensional smectic configuration shows many of the important geometrical consequences of equally spaced layers. The generator G perpendicular to layer M at point P is perpendicular to all of the other layers. The center of curvature C is also shared by the other layers; layers to the left of C are singular. The centers of curvature form the evolute E; in three dimensions E will consist of two sheets.

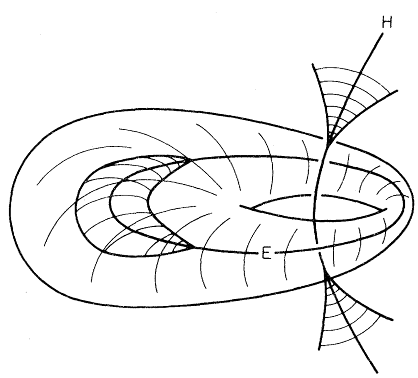

FIG. 3. The singularities within a focal domain of the first kind are an ellipse E and a hyperbola H in confocal poisiton. That is, they lie in perpendicular planes, and they pass through one another's foci. The smectic surfaces are cyclides of Dupin. Hilbert and Cohn-Vossen[4] have photographs of models of these cyclides, as well as examples of canal surfaces. Other views (including cross sections) are common in the literature (Refs. 2,5,9).

faces.] Friedel has pointed out that these surfaces must be composed of generators. (If generators cross a surface, the only smooth way of matching smectic layers at the surface is to "analytically continue" along the generators. This, of course, implies that both sides of the surface belong to the same smectic domain.)

Generically, it is unlikely that two smectic domains can be smoothly joined along any surface. Focal domains are special in that they can be joined along a cone of generators; all known two-dimensional interfaces are along these cones. The cone can be generated by linking any point on one conic with all the points on the other; because the conics are confocal, it is always a right circular cone.

Consider now a right circular cone of generators in a concentric sphere domain. The apex of the cone lies at the center of the spheres. The spheres intersect the cone in circles whose planes are normal to the axis of the cone. This is also the manner in which the Dupin cyclides would intersect it, and thus this cone forms a smooth interface between a focal domain and a structure of concentric spheres[7] (Fig. 4).

This happy construction allows us (and nature) to assemble lots of compound defects. We may start with a concentric sphere structure, and drill out right circular cones in any pattern we wish. On each cone we choose a conic section; its confocal partner will pass through the center of the spheres. We then fill in the cones with cyclides of Dupin. The structure can be thought of as an insect eye, with focal domains in each face and concentric spheres in the interstitial regions.

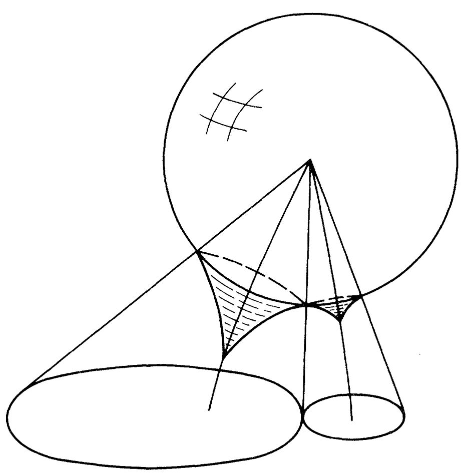

FIG. 4. The cyclides of Dupin mesh smoothly onto spheres. The interface is along a cone of generators; the apex of the cone lies on the hyperbola and is the center of the sphere. The apex of the cones of two adjacent focal domains must coincide at this point; this gives Friedel's "law of corresponding cones."

We have shown that the gaps between focal domains can be filled with concentric spheres; it remains to be resolved if they ever are so filled. Normally, focal domains form to relax stresses imposed by boundary conditions. For example, the ellipses in the photograph traced in Fig. 1 are attached to one of the microscope slides. Inside the ellipses, the layers attach normal to the slide, thus satisfying the boundary condition. The concentric spheres which (potentially) fill the clear regions between the ellipses do not satisfy this condition. Two questions must be answered. First, how far will the boundary effects propagate into the bulk? Secondly, will other structures (i.e., smaller focal domains) fill these regions instead?

If strains propagated a macroscopic distance in from the boundaries, they would presumably disrupt the precise geometry of the ellipses. Strong anchoring conditions will, in general, impose a structure on the boundary which is incompatible with the bulk structure; the transition will, in general, involve bending the layers through a large angle and changing the layer spacing by a large fraction. If the transition region is of width λ, the free energy per unit area $K_1\lambda/\lambda^2+\bar{B}\lambda$ is minimized with $\lambda=(K_1/\bar{B})^{1/2}$. As mentioned earlier, λ is usually roughly the interlayer spacing. Thus any strain which disrupts the equally spaced layer smectic structure will heal on a microscopic length λ, and spheres will remain spheres in the bulk. This is the macrosocopic rigidity which makes geometry a useful tool in studying smectics.

The second question is a serious one. The accepted method for filling these interstitial regions is through a hierarchy of focal domains.[8] The surface tension associated with the spheres $\sim(K_1\bar{B})^{1/2}$ by the above arguments; the free energy of a substituting focal domain goes roughly as K_1 times the perimeter. Thus focal domains of characteristic contact radius R can nucleate favorably until $(K_1\bar{B})^{1/2}R^2\sim K_1R$ or $R\sim\lambda$. Experimentally, some systems do seem to show this cascade of domains. However, the photograph sketched in Fig. 1 shows unquestionably clear regions between the ellipses. Presumably, the system is not in equilibrium—the free energy needed to nucleate a new domain must be large compared to kT. This energy will be roughly the surface tension times the square of the nucleation radius. If we assume, following Ref. 8, that the nucleation radius is about ten times the interlayer spacing, and the latter ~20 Å, then thermal activation will only be important for surface tensions $\sim10^{-4}$ ergs/cm^2. Characteristic surface tensions of organic compounds are ~50 ergs/cm^2.

This leads to one final observation. The existence of concentric spheres as metastable structures is more plausible if they nucleate first. The compound defects give strong evidence for this. Here the aforementioned insect eye pattern is a recurrent theme. This structure is naturally explained by the nucleation of concentric spheres, say, on the upper microscope slide; when they reach the bottom face the focal domains form to relax the boundary conditions.

We hope to have communicated some of the elegance with which nature has expressed itself in the smectic system.

ACKNOWLEDGMENT

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[1]G. Friedel and F. Grandjean, Bull. Soc. Fr. Min. Crist. 33, 192, 409 (1910). See also the review artical by G. Friedel, Ann. Phys. (Paris) 18, 273 (1922).

[2]P. G. de Gennes, *The Physics of Liquid Crystals* (Clarendon, Oxford, 1974), p. 291.

[3]M. Kléman and F. C. Frank (unpublished).

[4]D. Hilbert and S. Cohn-Vossen, *Geometry and the Imagination* (Chelesea, New York, 1952), p. 217ff.

[5]Y. Bouligand, J. Phys. (Paris) 33, 525 (1972).

[6]Canal surfaces, if they exist in current observations, have not yet been identified as such. Domains filled with canal surfaces would have low free energies, but would not always be static solutions. (The stability of the observed focal domains must be due to the rigid constraint of forcing both evolutes to be one dimensional.) Canal surfaces are nicely described by Hilbert and Cohn-Vossen (Ref. 4). J. A. Geurst [Phys. Lett. 34A, 283 (1971)] has shown (although he claims otherwise) that cyclides of Dupin exert no pressure; this might be useful. Professor F. J. Almgren, Jr. (private communication) has noted the possible importance of the infinitesimal nucleation of new layers in studying the static solutions.

[7]Alternatively, two focal domains could join along this cone, the outer domain forming a hat over the inner. This has been noted by Y. Bouligand (Ref. 4, Fig. 17b). Although this could be a static, low-energy solution, it plays no role in relaxing stress; it has not been observed.

[8]R. Bidaux, N. Boccara, G. Sarma, L. De Seze, P. G. de Gennes, and O. Parodi, J. Phys. (Paris) 34, 661 (1973).

[9]M. Kléman, *Points, Lines, and Walls* (Wiley, New York, 1981).