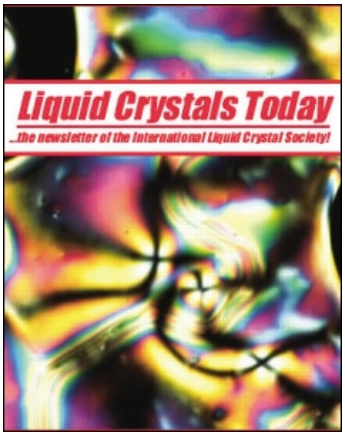

Liquid Crystals Today
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713681230

Geometry and the nonlinear elasticity of defects in smectic liquid crystals

Christian D. Santangelo[a]
[a] Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, USA

To cite this Article Santangelo, Christian D.(2006) 'Geometry and the nonlinear elasticity of defects in smectic liquid crystals', Liquid Crystals Today, 15: 3, 11 — 18
To link to this Article: DOI: 10.1080/14645180601168117
URL: http://dx.doi.org/10.1080/14645180601168117

Liquid Crystals Today, Vol. 15, No. 3, September 2006, 11–18

Taylor & Francis
Taylor & Francis Group

Geometry and the nonlinear elasticity of defects in smectic liquid crystals

CHRISTIAN D. SANTANGELO*
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, USA

(*Received 27 November 2006; in final form 13 December 2006*)

Rotation invariance imposes nonlinearities in the elastic strain of smectic liquid crystals. Though often neglected, in smectic liquid crystals these nonlinearities can generate new qualitative behavior, especially in the presence of defects such as dislocations. By exploiting geometry, I describe exact results on edge dislocations, and demonstrate a nonlinear superposition principle for certain multiple defect configurations. Though there are few exact results analogous to those of edge dislocations, results on twist-grain boundaries hint at an approximate superposition principle for multiple screw dislocations also. These superpositions, which appear to be related to the theory of minimal surfaces, exhibit unexpected symmetries that are still poorly understood.

1. Introduction

In a crystal or liquid crystal, rotation invariance requires nonlinearities in the elastic strain [1]. Typically, these nonlinearities are tractable only numerically; analytical progress is made, instead, using the equivalent linear problem, which is optimistically presumed to be valid in the limit of small strain. In studying the strain fields and energetics of dislocations in smectics-A, linear elasticity is now the stuff of textbooks [2, 3]. It has long been clear, however, that the nonlinearities induced by rotation invariance lead to qualitative phenomena in liquid crystals even in the limit of small strain, as revealed by their anomalous elasticity [4–6] and the Helfrich-Hurault instability under dilative strain [7]. Even far from the core of an edge dislocation, the induced layer deformation can differ dramatically from what is predicted by the linear theory [8–11]. Furthermore, these essential nonlinearities induce a long-range interaction between parallel screw dislocations and strongly modify their energetics [12].

In this article, I will review recent progress on understanding the nonlinear elasticity of dislocations in smectic-A liquid crystals. This progress has been made by utilizing the geometry of the smectic layers as an organizing principle. While it has long been understood that geometry is essential to understanding the bending of the individual layers, geometry in layered systems is a fully three-dimensional affair - because of the compression energy between layers, it is equally important to understand how the layers fill space. In fact, the curvature of the layers is intrinsically coupled to the spacing between them [13], and this subtle interplay leads to numerous theoretical complications. Nevertheless, this realization can also be leveraged into an *exact* solution of the layer profile around isolated dislocations, and a nonlinear superposition principle between edge dislocations. No nonlinear superposition principle is known for screw dislocations, on the other hand. However, I will describe recent work using *linear* superposition to understand the nonlinear behavior of screw dislocations in large-angle, twist-grain boundary phases. Surprisingly, there are hints of a more general, but approximate, superposition principle for screw dislocations.

Smectics-A are conveniently described using a phase field, $\phi(\mathbf{x})$, where the density of material is given by $\rho(\mathbf{x}) \approx \rho_0 + \rho_1 \cos[2\pi\phi(\mathbf{x})/a] + \ldots$ for layers with spacing a. The average density is ρ_0 and ρ_1 is the smectic order parameter. The midplane of the layers lie on surfaces of constant $\phi(\mathbf{x}) = 0, \pm a, \pm 2a, \ldots$ and, because we are concerned with smectics-A only in this article, the molecular director $\hat{n}$ always lies along the unit normal $\hat{N} = \nabla\phi/|\nabla\phi|$.

The bending energy, F_b, of the layers is inherited from the splay term of the Frank free energy for the nematic,

$$F_b = \frac{K_1}{2} \int d^3x (\nabla \cdot \hat{n})^2 \tag{1}$$

Two other terms appear in the Frank energy: the twist, $\hat{n} \cdot (\nabla \times \hat{n})$ and the bend, $\hat{n} \times (\nabla \times \hat{n})$. In smectics, the twist must vanish except at a defect core. The bend,

*Corresponding author. Email: santancd@physics.upenn.edu

Liquid Crystals Today
ISSN 1358-314X print/ISSN 1464-5181 online © 2006 Taylor & Francis
http://www.tandf.co.uk/journals
DOI: 10.1080/14645180601168117

on the other hand, is tightly coupled to the layer spacing - if it is nonzero, the compression strain is also nonzero and dominates the energy. In light of this, it is typical to neglect the bend. In many applications, it also becomes necessary to add the saddle-splay term,

$$F_{SS} = \frac{K_{24}}{2}\int d^3x \nabla\cdot[\hat{n}(\nabla\cdot\hat{n}) - (\hat{n}\cdot\nabla)\hat{n}]. \quad (2)$$

This term is a total derivative and can be evaluated on the boundaries. Though it contributes to the total energy of a dislocation, it does not affect the strain fields induced by the dislocation core in the surrounding layers.

The bending energy and saddle-splay have a completely geometrical interpretation. They can be rewritten in terms of the two invariant curvatures of a surface: the mean curvature, $H=(1/r_1+1/r_2)/2$ and the Gaussian curvature, $K=1/(r_1r_2)$, where r_1 and r_2 are the two principle radii of curvature for the surface. Rewriting the curvatures in terms of the unit normal vector, the mean curvature is $H=-\nabla\cdot\hat{N}/2$ and the Gaussian curvature is $K=\nabla\cdot\left[\hat{N}\left(\nabla\cdot\hat{N}\right)-\left(\hat{N}\cdot\nabla\right)\hat{N}\right]/2$ when evaluated on the layers [14].

The compression strain is also written in terms of gradients of ϕ. The equilibrium layer spacing is given by the condition $|\nabla\phi|=1$, with a larger layer spacing when $|\nabla\phi|$ is small and smaller layer spacings when $|\nabla\phi|$ is large. There are two versions of the compression strain we will use,

$$u_{zz} = \frac{1-(\nabla\phi)^2}{2} \quad (3)$$

and

$$u'_{zz} = 1-|\nabla\phi| \quad (4)$$

Both choices are consistent with rotation invariance. Though equation (3) is more natural from the point of view of Landau theory [1, 2], equation (4) is more natural from the point of view of the layer geometry. It is typical to write the strain in terms of the Eulerian displacement field, u defined by choosing a reference direction, usually z, and writing $\phi=z-u$. Expanding equations (3) and (4) in powers of u yields,

$$\begin{aligned} u_{zz} &= \partial_z u - \frac{1}{2}(\nabla u)^2 \\ u'_{zz} &= \partial_z u - \frac{1}{2}(\nabla_\perp u)^2 + \cdots \end{aligned} \quad (5)$$

where $\nabla_\perp = \hat{x}\partial_x + \hat{y}\partial_y$. The nonlinear terms in u appearing in equations (5) enforce the rotation invariance of the strain. Unlike nonlinearities arising from, say, cubic or higher order terms in the Eulerian strain, neglecting the nonlinearities in equations (5) results in the loss of rotation symmetry in the free energy. That this can be dangerous is already apparent in the dilatative Helfrich-Hurault effect, in which the nonlinearities of the strain lead to a periodic wrinkling of the layers [7]. Nevertheless, it is typical to neglect these nonlinearities to simplify the problem of finding layer configurations around dislocations.

In what follows, I will consider the energetics and layer structure of screw and edge dislocations in the nonlinear theory in detail. Though these dislocations can be continuously rotated into one another (that is, they are topologically equivalent), they show a number of striking geometrical differences that necessitate different approaches. For example, edge dislocations, because they bend in only one direction, have no Gaussian curvature. Due to this, I will show that there is a *nonlinear* superposition principle for some configurations of edge dislocations. Screw dislocations, on the other hand, have negative Gaussian curvature so are not amenable to the same methods. Despite this, there are tantalizing hints of an analogous superposition principle for screw dislocations related to the classical theory of minimal surfaces. Defect superposition can then be used to construct topologically complex smectic phases, exemplified by the celebrated twist-grain boundary phase.

2. Linearized dislocations in smectics

The linearized smectic free energy is

$$F = \frac{B}{2}\int d^3x\left[(\partial_z u)^2 + \lambda^2\left(\nabla_\perp^2 u\right)^2\right], \quad (6)$$

where B is the bulk modulus, $\lambda=\sqrt{K_1/B}$ and $\nabla_\perp = \hat{x}\partial_x + \hat{y}\partial_y$ is the in-plane gradient. A uniform rotation of all the layers by an angle θ, given by $u(x, z)=z[\cos(\theta)-1]+x\sin(\theta)$, does not preserve this free energy. Nonetheless, equation (6) has a significant advantage over the full free energy: the Euler-Lagrange equation for the extrema is linear and, therefore, easily solved. Moreover, combinations of defects, as occurs in the TGBA phase for example, can be built up by direct linear superposition of the single defect solutions.

Screw dislocations in the linear theory have burgers vector and defect core axis along the $\hat{z}$ direction. Equation (6) is exactly minimized by [2, 3, 15]

$$u_{\text{screw}} = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right) \quad (7)$$

This has a nonzero topological charge since $\oint dl\cdot\nabla u = b$. The length $b=na$, where a is the layer

spacing and n is an integer, is the burgers scalar for the screw dislocation. Since u_{screw} is independent of z and is a harmonic function in the xy-plane, u_{screw} has vanishing linear energy. Furthermore, this implies the vanishing of the interaction energy between screw dislocations because linear superpositions of harmonic functions are still harmonic. As it happens, u_{screw} is also a solution of the nonlinear smectic free energy (with either u'_{zz} or u_{zz} as the compression strain). In computing the energy, however, it becomes evident that the linear theory has generated a significant error: the nonlinear energy diverges near the dislocation core. Introducing a microscopic cutoff, the screw dislocation line tension scales as Bb^4/ξ^2 for a characteristic core size ξ, not zero!

In the case of a single edge dislocation with burgers scalar b, the minimum of equation (6) is also known: [2, 3]

$$u_{\text{edge}} = \text{sgn}(z)\frac{b}{4}\left[\text{erf}\left(\frac{x}{\sqrt{4\lambda|z|}}\right)+1\right] \tag{8}$$

The topological charge of the edge dislocation is also $\oint dl\cdot\nabla u = b$. This integral is nonzero because u is singular at the origin: as $z\to 0$ from below, we have $u_-(x, 0) = -b\Theta(x)/2$, whereas $u_+(x, 0) = b\Theta(x)/2$ as $z\to 0$ from above. This singularity can be interpreted as a boundary at $z=0$ dividing the smectic into two half-spaces, one above and one below the dislocation. In this way, defect cores act as boundary conditions for the minimization of the smectic free energy. The line tension associated with the bending of the layers around the dislocation core is computed to be $\tau = B\lambda b^2/(3\sqrt{\pi}\xi)$ for a core of characteristic size ξ [2, 3].

Even in the edge dislocation case, the linear theory has developed a significant error. This is evident if we compute $\nabla_\perp u_{\text{edge}}$ and $\partial_z u_{\text{edge}}$ from equation (8): [2]

$$\begin{aligned}\partial_z u_{\text{edge}} &= -\frac{b}{8\sqrt{\pi\lambda|z|^3}}\exp\left(-\frac{x^2}{4\lambda z}\right)\\ \nabla_\perp u_{\text{edge}} &= \frac{b\hat{x}}{4\sqrt{\pi\lambda|z|^1}}\exp\left(-\frac{x^2}{4\lambda z}\right)\end{aligned} \tag{9}$$

Along the parabolas of maximum strain, $x^2 = \pm 4\lambda|z|$, we have $(\nabla_\perp u)^2 \big/ \partial_z u \sim \sqrt{|z|}$ which actually diverges as $z\to\infty$. We conclude that we were mistaken to drop $(\nabla_\perp u)^2$ relative to $\partial_z u$ in the compression strain *even in the limit of small strain* very far from the dislocation core.

Though edge and screw dislocations are topologically identical (indeed, rotating a screw dislocation into the plane of the layers converts it to an edge dislocation), the failure of the linear theory in both cases is very different. Their treatment in the nonlinear theory is, likewise, very different.

3. Nonlinear edge dislocations

Consider the compression strain u'_{zz}, yielding total free energy

$$F = \frac{B}{2}\int d^3x\left[(1-|\nabla\phi|)^2 + \lambda^2(\nabla\cdot\hat{\boldsymbol{n}})^2\right]. \tag{10}$$

Free energy (10) exhibits a class of *exact* minima that can be extracted utilizing a procedure invented by Bogomol'nyi, Prasad, and Sommerfield (BPS) for the study of magnetic monopoles and vortices in quantum field theory [16, 17]. First, complete the square in equation (10), introducing a cross-term:

$$F = \frac{B}{2}\int d^3x\left[(1-|\nabla\phi|-\lambda\nabla\cdot\hat{\boldsymbol{n}})^2 + 2\lambda(1-|\nabla\phi|)\nabla\cdot\hat{\boldsymbol{n}}\right]. \tag{11}$$

The goal of the BPS procedure is to then re-express the cross-term as a total derivative, if possible.

Notice that, for equally-spaced layers, $-\int d^3x|\nabla\phi|\nabla\cdot\hat{\boldsymbol{n}} = 2a\sum_i\int_i \mathrm{d}A_i H$, where the index i labels the layer and $\mathrm{d}A_i$ is the area element of the ith layer. For surfaces in three dimensions, there exists a geometrical relation, first discovered by Minkowski [18], relating the integral of the mean curvature over a closed surface to an integral of the Gaussian curvature. For smectics, a generalization of Minkowski's result is required [11]:

$$\int d^3x|\nabla\phi|H = \int d^3x\left[\phi K - \nabla\cdot\left(|\nabla\phi|\vec{\psi}\right)\right], \tag{12}$$

where $\vec{\psi}$ is defined by the relation $\nabla\cdot\vec{\psi}\big/2 = K$, the Gaussian curvature.

For edge dislocations, $K=0$, and equation (12) can be used to express the cross-term of equation (11) as a total derivative. The consequence of this is that the cross-term plays no role in the minimization of the surrounding layers. Because it is a total derivative, it reduces to an integral on the boundaries, *i.e.* at the dislocation core. The general form of the free energy is now

$$F = \int d^3x\,\Gamma^2 \pm 2\lambda\int \mathrm{d}A\left[1-2(\nabla\phi)\cdot\vec{\psi}\right], \tag{13}$$

where $\Gamma = 1-|\nabla\phi|\mp\lambda\nabla\cdot\hat{\boldsymbol{n}}$ and the area integral is evaluated on the boundary of the smectic. The two possible signs of equation (13) arise because we may complete-the-square with either sign.

We identify a special class of minima, BPS minima, found by setting the perfect square, Γ, to zero. A surprising feature of these BPS minima is that they satisfy a lower-order differential equation than the Euler-Lagrange equation for the free energy. The condition $\Gamma=0$ implies the equation

$$1-|\nabla\phi|=\pm\lambda\nabla\cdot\hat{\boldsymbol{n}}, \tag{14}$$

for which only half of the boundary conditions need to be specified.

Therefore, the procedure for finding a BPS minimum is to use half the boundary conditions and verify that the remaining desired boundary conditions are satisfied automatically; if they are not, the desired boundary conditions do not admit such a solution.

To illustrate this, consider a single edge dislocation at $z=0$. Using $\phi=(b/4)[\mathrm{erf}(x^2/\xi^2)+1]$ at $z=0$, we solve $1-|\nabla\phi|-\lambda\nabla\cdot\hat{\boldsymbol{n}}=0$ for the layers $z>0$ and $\phi=-(b/4)[\mathrm{erf}(x^2/\xi^2)+1]$ with $1-|\nabla\phi|+\lambda\nabla\cdot\hat{\boldsymbol{n}}=0$ for the layers $z<0$. The equations result in flat layers as $z\to\pm\infty$ and so satisfy the boundary conditions for an edge dislocation in a bulk smectic. The solution is shown in figure 1. The line tension is evaluated by noting that, since the perfect square is zero, the free energy of the configuration is determined entirely from the boundary terms arising from the total derivative. This yields

$$\tau=B\lambda\int d^3x\sqrt{1+\frac{b^2}{\xi^2}\exp\left(-x^2/\xi^2\right)}, \tag{15}$$

which is linear in b for $b\gg\xi$, rather than quadratic [11]. Far from the dislocation core, the first-order BPS equation becomes [10, 11]

$$\partial_z u-\frac{1}{2}(\nabla_\perp u)^2=\pm\lambda\nabla_\perp^2 u, \tag{16}$$

which has the exact displacement field

$$u=2\lambda\,\mathrm{sgn}(z)\ln\left[1+\frac{e^{b/(4\lambda)}-1}{2}\mathrm{erf}\left(x\Big/\sqrt{4\lambda|z|}\right)\right]. \tag{17}$$

This solution was originally found by Brener and Marchenko [8] by solving the Euler-Lagrange equation directly. The displacement field is vastly different from the linear theory unless $b\ll 4\lambda$. In fact, the linear solution can be distinguished from the exact solution even far from the dislocation core along the parabolas of maximum strain, $x^2=\pm 4\lambda|z|$. The deviation of the layers from the linear theory can be measured experimentally, as has been done by Ishikawa and Lavrentovich in a cholesteric finger texture [9] and again by Smalyukh and Lavrentovich [19] using confocal microscopy.

From this construction emerges a surprising nonlinear superposition principle. Consider two edge dislocations located on the plane $z=0$ (see figure 2). These two dislocations determine the shape of the first unbroken layer on either side of the dislocations, and the BPS evolution equation can be used to determine the shape of all remaining layers. In the far-field limit, we solve equation (16) to find that we can superpose the solutions *inside the logarithm*. In other words,

$$u(z>0)=2\lambda\ln\left(1+A_1u_{\mathrm{edge},1}+A_2u_{\mathrm{edge},2}\right), \tag{18}$$

where $u_{\mathrm{screw},i}$ are the *linear* solutions for each of the individual edge dislocations, and the constants A_i are determined by the boundary conditions at $z=0$. For example, a pair of dislocations with burgers scalar b has $A_1=(4/b)\exp[b/(4\lambda)-1]$ and $A_2=(4/b)\exp[b/(2\lambda)]-A_1$. Very quickly, the layer profile deviates from that found by superposing two edge dislocations in the linear

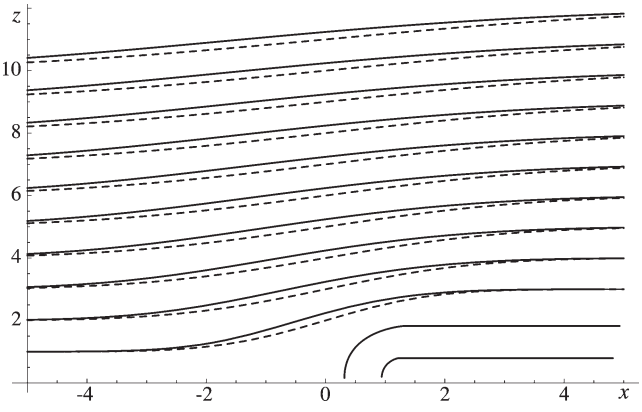

Figure 1. Edge dislocations with burgers scalar $4a$ in the far-field limit. The solid line is the BPS solution, the dashed line the solution from linear elasticity. All lengths are measured in units of λ.

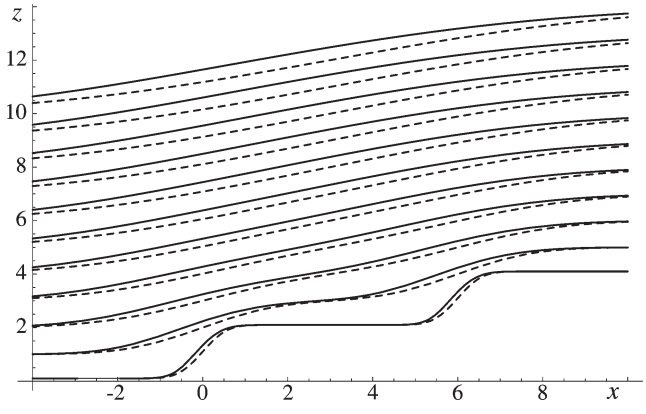

Figure 2. A pair of $b=+4a$ edge dislocations in the far-field limit. The solid line is the BPS solution, the dashed line the solution from linear elasticity, and lengths are measured in units of λ. The core region is not shown.

theory, as can be seen in figure 2. Interestingly, the interaction energy between them agrees with the linear theory, as long as their separation is much larger than their core size [11].

Exact solutions are often useful because they tease hidden structures from equations not apparent at first. However, these solutions can also be quite limited. For multiple edge dislocations with intervening layers, for example, there is no BPS solution possible. This can be traced to the failure of the solution of equation (16) to satisfy the appropriate multi-defect boundary conditions. That is, the BPS solution only allows us to set a single boundary condition in the region $z>0$ and there is no layer that can be "glued" seamlessly to another BPS edge dislocation solution unless the dislocations are infinitely far apart. How to rectify these shortcomings is a matter of current research.

4. Nonlinear screw dislocations

The BPS solution also fails when the layers have Gaussian curvature because the free energy cannot be put into the form of a perfect square plus boundary terms. Due to this, screw dislocations are not BPS minima. Nevertheless, the *linear* superposition of screw dislocations exhibits a number of surprises that suggest there is considerably more structure in the nonlinear smectic free energy than meets the eye. In this section, I will discuss the smectic structures that can be built by summing screw dislocations.

Within linear elasticity, the displacement field for a screw dislocation of burgers scalar b is given by u_{screw} in equation (7). Considering the failure of the linear theory to describe the layers in an edge dislocation, it is somewhat surprising that u_{screw} is also an exact extremum of the nonlinear energy with both u'_{zz} or u_{zz}. Another striking property of equation (7) is that $\nabla\cdot\hat{\boldsymbol{n}}=0$, implying that u_{screw} describes a *minimal surface*, that is, a surface with no mean curvature (and hence extremal area for a given topology). For $b=2$, this surface is called the helicoid (figure 3). Its existence has been known at least since 1785, when J.B. Meusnier proved it was minimal [20].

Since $\partial_z u_{\text{screw}}=0$ and $\nabla_\perp^2 u_{\text{screw}}=0$ (except at the core), the linear energy of the screw dislocation is zero! In fact, this is dramatically incorrect: substituting equation (7) into a rotationally-invariant energy yields a divergence that must be regularized by introducing a cutoff at the core. If we form a linear superposition of screw dislocations, the linear energy is still zero and the screw dislocations, therefore, do not interact. In the nonlinear theory, on the other hand, the deformations of the layer induce an interaction that, at least in some cases, is a power law [12].

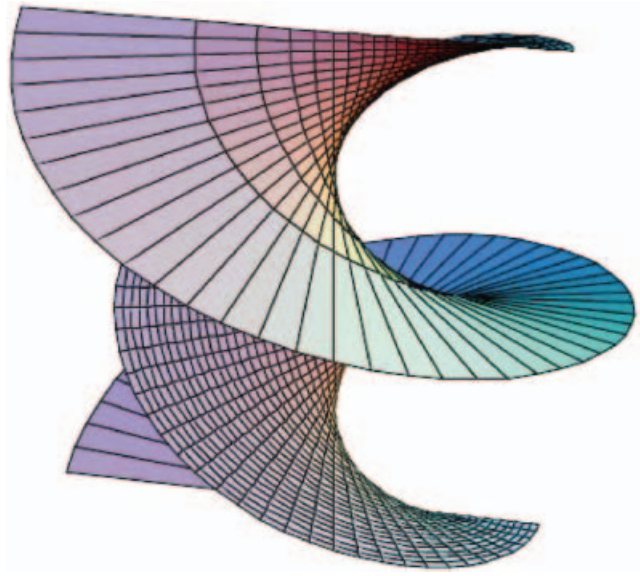

Figure 3. The helicoid corresponds to a screw dislocation with topological charge 2.

Since $H=0$, the radii of curvature are equal and opposite ($1/r_1=-1/r_2$) and the layers have negative Gaussian curvature. Subsequently, there is not a superposition principle for screw dislocations analogous to the BPS decomposition for edge dislocations. Such a principle may exist, however, at least in an approximate sense. Consider two alternate constructions for a twist-grain boundary, in which asymptotically flat layers rotate across the grain boundary by a fixed angle. Since this is incompatible with smectic order because it introduces twist, $\widehat{N}\cdot\left(\nabla\times\widehat{N}\right)$, into the layers, this frustration is alleviated by the formation of parallel screw dislocations within the grain boundary [21].

One construction was given by Kamien and Lubensky [12] by directly utilizing a linear superposition of screw dislocations of the form,

$$\phi_{\text{TGB}}=\gamma z-\frac{b}{2\pi}\sum_{n=-\infty}^{\infty}\tan^{-1}\left(\frac{y}{x+\ell_d n}\right). \qquad (19)$$

for which the twist angle is $\alpha=2\sin^{-1}[b/(2\ell_d)]$ (see figure 4). The constant γ is set by ensuring that the compression strain of the layers vanishes at infinity.

Alternatively, we might reason that, since the layers of a single screw dislocation are minimal surfaces, minimal surfaces may provide a reasonable approximation to the layers in this more complicated geometry also. In fact, a relic minimal surface known as Scherk's first surface exists for which asymptotically flat layers rotate by ninety degrees [22]. This surface has been conjectured as the structure twist-grain boundaries in diblock copolymers [23]. There are also deformed

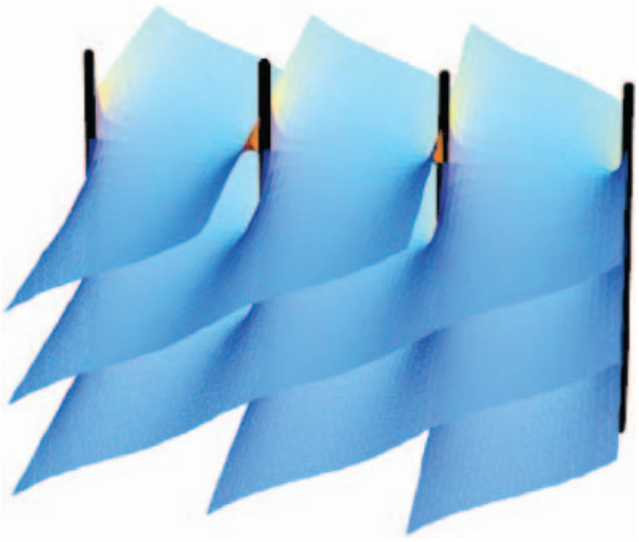

Figure 4. A twist-grain boundary can be formed by summing screw dislocations, with cores depicted here as black tubes. Shown is the twist angle $\alpha=\pi/2$.

Scherk surfaces corresponding rotation angles other than $\pi/2$. As it turns out, these two constructions of a twist-grain boundary are not so different: stretching the y coordinate of ϕ_{TGB} by $\cos(\alpha/2)$ for $b=2$ a yields Scherk's first surface or one of its deformed cousins [24]. This suggests that the mean curvature, $-(\nabla\cdot\hat{\boldsymbol{n}})/2$, though nonlinear, may exhibit a more general superposition principle.

The similarity of Scherk's first surface and the direct sum of screw dislocations suggests that these two surfaces bound the true layer configurations. Diblock copolymers in the lyotropic smectic phase are ideal for experimental characterization of layer structures because they can be directly visualized by transmission electron microscopy [23, 25]. Most recently, a transmission electron microtomography reconstruction in a polystyrene-polyisoprene diblock copolymer shows clearly that the layer structure is very well approximated by Scherk's first surface, as determined by the average mean curvature of the layers [25]. A numerical minimization for block copolymers, on the other hand, demonstrates that ϕ_{TGB} is a better approximant to the layer structure [26]. In both cases, however, the true layer structure has an average mean curvature somewhere between that of Scherk's first surface and ϕ_{TGB}. A more recent minimization of the smectic-A Landau-de Gennes free energy functional also demonstrates that ϕ_{TGB} is a reasonable approximation to the true layer structure [27]. It should be noted, however, that for large twist angle the molecular director decouples from the layer normal throughout the grain boundary.

Scherk's surface and ϕ_{TGB}, though they fail to describe the layer shapes exactly, both exhibit features that (1) inform our understanding of the true structures and (2) may be preserved experimentally in an approximate sense. For dislocations separated by a distance ℓ_d, the level sets can be written as $\phi_{\mathrm{TGB}}=\gamma z-[b/(2\pi)]\mathrm{Im}\ln\sin[(\pi/\ell_d)(x+iy)]$, where the constant γ must be set to ensure that the compression strain vanishes at infinity, $i=\sqrt{-1}$, and Im denotes the imaginary part of a complex number [11]. The layers, determined by $\phi_{\mathrm{TGB}}=na$ for integers n can be transformed into the parametric equation [12]

$$\tan\left(\frac{\pi x}{\ell_d}\right)=\tanh\left(\frac{\pi y}{\ell_d}\right). \tag{20}$$

Equation (20) exhibits a surprising symmetry under a ninety degree rotation of the defects, $(x, z)\rightarrow(-z, x)$, while taking $b\rightarrow -b$. The rotation angle $\alpha\rightarrow\pi-\alpha$ under this transformation. The sum of dislocations, ϕ_{TGB}, for example, exhibits the following startling property: there are multiple ways of superposing dislocations to construct the same set of layers! For $\alpha=\pi/2$, this gives us a dual way of constructing exactly the same structure, either with layers and defects along, say, the z axis with burgers scalar b, or defects and layers along the x axis and burgers scalar $-b$.

We continue to exploit the superposition of screw dislocations to discuss the celebrated TGBA phase [21, 28], in which smectic order coexists with a periodic array of twist-grain boundaries. This can be achieved theoretically, for example, by directly summing ϕ_{TGB}, with the substantial complication that the orientation of the screw dislocations must rotate with the layers. When the rotation angle is small, linear elasticity suffices to calculate the structure and energetics of the TGBA phase [21]. More recently, however, materials have been discovered that form TGBA phases of quite large angles, some as large as ninety degrees [29]. The layer structure of these phases are not amenable to a straightforward linear analysis [21, 30].

To develop a theory for the $\pi/2$ TGB structure, we again try to form a sum a screw dislocations. Though we should, in principle, sum grain boundaries with dislocations that alternate being along the $\hat{z}$ and $\hat{x}$ directions, this sum is quite difficult, and probably impossible, to perform analytically. Since in the $\pi/2$ TGBA structure, the defect axes lie along the z and x axes alternately, the duality in ϕ_{TGB} allows us to rotate all the defects to the z axis. Since they are now parallel, it is reasonable to conjecture an approximate structure

for the $\pi/2$ TGB phase [31].

$$\phi_{\mathrm{TGBA}} = \gamma z - \frac{b}{2\pi} \sum_{n,m=-\infty}^{\infty} (-1)^m \mathrm{Im}\ln(x + iy + \ell_d n + i\ell_b m + \ell_d m/2), \tag{21}$$

for grain boundaries separated by a distance ℓ_b. Notice that this structure has adjacent grain boundaries with opposite sign and shifted by half a period (see figure 5) - this choice is arbitrary but yields some simplifications. Here, γ should be chosen to minimize the compression energy, but a suitable *ansatz* is to choose it so that the compression energy vanishes along lines midway between adjacent grain boundaries [31]. This sum can be performed exactly to give

$$\phi_{\mathrm{TGBA}} = \gamma z - \frac{b}{2\pi} \mathrm{Im}\ln \mathrm{sn}(\theta x + i\psi y, k), \tag{22}$$

where sn is a Jacobi elliptic function, θ and ψ are scale factors selected to yield the appropriate separations between defects, and $k^2<0$ is the elliptic modulus. The resulting layers, dubbed *Schnerk's first surface*, is shown in figure 5 [31].

Schnerk's first surface is necessarily achiral since it is developed from a set of defects with neutral total topological charge. While there is no known way to scale Schnerk's first surface to be a minimal surface, the surface is triply-periodic and shares the same topology as another relic minimal surface, the Schwartz D surface [31]. This generalizes the surprising superposition of a single TGB, but the superposition is merely approximate. Interestingly, though the interaction energy between dislocations within a single grain boundary is a power law [12], the interaction energy between multiple grain boundaries is exponential at long distances, as it is in the linear theory. In the nonlinear theory, however, the interaction length scale is given by ℓ_d and arises from the nonlinearities whereas in the linear theory it arises from the director modes [21].

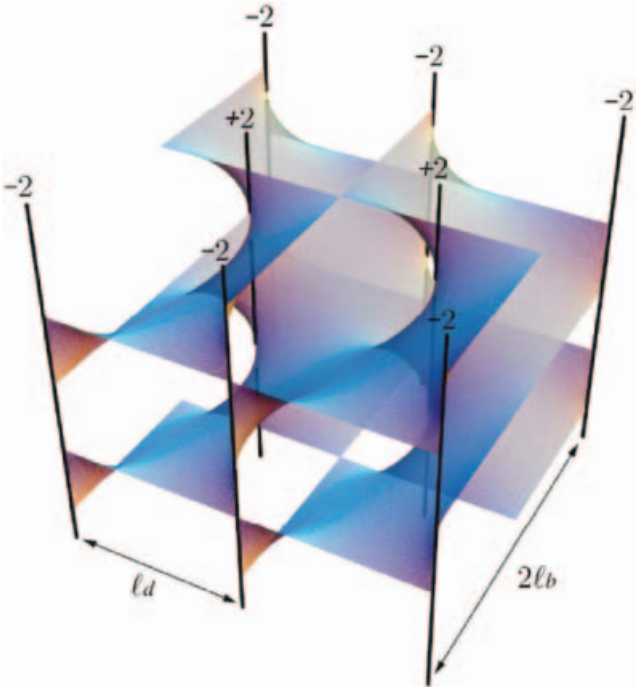

Figure 5. Schnerk's first surface is composed of parallel $\pi/2$ twist-grain boundaries formed by the linear superposition of parallel screw dislocations [31].

5. Nonlinear elasticity and general defect configurations

Understanding the nonlinear elasticity of defects in smectics is crucial if one wants to construct complex smectic textures by thinking of the defects as the primary degrees of freedom. In fact, many layered structures of complex topology can be built up by superposition of an underlying defect network, and the energetics and elasticity of these structures are bound up with our understanding of how these defects superpose in the nonlinear theory for smectics.

To illustrate the utility of this view, consider the TGBA phase once again. As we have seen, a single twist-grain boundary can be built from two equivalent sets of screw dislocations. In Schnerk's first surface, this duality becomes a triality: the structure can be constructed from any one of three orthogonal arrangements of parallel screw dislocations. This exotic set of defects can be used to understand some aspects of TGBA phases with twist angles smaller than $\pi/2$. In particular, a general angle α can be made by twisting Schnerk's surface by an angle $\delta=\pi/2-\alpha$ at each grain boundary. For sufficiently small δ, the screw dislocations along the pitch axis should twist along with the structure, endowing them with an edge component and, presumably, raising the energy [32].

However, the energetics and structure of such a screw-edge hybrid dislocation is a completely open question in the nonlinear theory. In general, one might expect the energetics to differ dramatically from the linear theory, in analogy to pure screw dislocations. At the same time, the layer configurations will also disagree with the linear theory as they do for edge dislocations. While it is possible to make some general topological statements about the underlying defect network in a TGBA phase [32], it is difficult to make much progress about the energetics of such phases without a more generic theory for the nonlinear elasticity of defects. Another open problem has to do with edge dislocations separated by intervening layers or in smectic films. Since these are not BPS minima because they do not satisfy the appropriate BPS boundary conditions, they must be

treated with a more general theory of nonlinear elasticity.

To summarize, rotation invariance requires layered systems to have essential nonlinearities in their elastic strains. These nonlinearities are crucial for a precise understanding of defects in these phases - linear elastic theory makes incorrect predictions about the energetics and layer structure around dislocations. It is by understanding the geometry of smectics that allows progress. Surprisingly, even with these nonlinearities edge dislocations can exhibit an exact superposition principle and screw dislocations an approximate one.

Acknowledgements

I have benefited from guidance and discussions with Randy Kamien and Fyl Pincus. I acknowledge NSF grant DMR05-47230, the ACS Petroleum Research Fund, and a gift from L.J. Bernstein.

References

[1] P. Chaikin, T.C. Lubensky. *Principles of Condensed matter*. Cambridge University Press, Cambridge (1995).
[2] P.G. de Gennes, J. Prost. *The Physics of Liquid Crystals* (2nd edition), Oxford University Press, New York (1993).
[3] M. Kleman. *Points, Lines, and Walls*. John Wiley and Sons, New York (1983).
[4] G. Grinstein, R. Pelcovits. *Phys. Rev. Lett.*, **47**, 856 (1981).
[5] G. Grinstein, R. Pelcovits. *Phys. Rev. A*, **26**, 915 (1982).
[6] L. Golubović, Z.-G. Wang. *Phys. Rev. E*, **49**, 2567 (1994).
[7] W. Helfrich. *J. Chem. Phys.*, **55**, 839 (1971); J.P. Hurault, *J. Chem. Phys*. **59** 2068 (1973); M. Boucif, H.E. Wesfreid, E. Guyon, *J. Phys. Lett*. **45** 413 (1984).
[8] E.A. Brener, V.I. Marchenko. *Phys. Rev. E*, **59**, R4752 (1999).
[9] T. Ishikawa, O.D. Lavrentovich. *Phys. Rev. E*, **60**, R5037 (1999).
[10] C.D. Santangelo, R.D. Kamien. *Phys. Rev. Lett.*, **91**, 045506 (2003).
[11] C.D. Santangelo, R.D. Kamien. *Proc. R. Soc. A*, **461**, 2911 (2005).
[12] R.D. Kamien, T.C. Lubensky. *Phys. Rev. Lett.*, **82**, 2892 (1999).
[13] B.A. DiDonna, R.D. Kamien. *Phys. Rev. Lett.*, **89**, 215504 (2002).
[14] R.D. Kamien. *Rev. Mod. Phys.*, **74**, 953 (2002).
[15] M. Kleman. *Rep. Prog. Phys.*, **52**, 555 (1989).
[16] E. Bogomol'nyi. *Sov. J. Nucl. Phys.*, **24**, 449 (1976).
[17] M.K. Prasad, C.H. Sommerfield. *Phys. Rev. Lett.*, **35**, 760 (1975).
[18] H. Minkowski. *Math. Ann.*, **57**, 447 (1903).
[19] I.I. Smalyukh, O.D. Lavrentovich. *Phys. Rev. Lett.*, **90**, 085503 (2003).
[20] J.B. Meusnier. *Mém. des savans étrangers*, **10**, 477 (1785).
[21] S.R. Renn, T.C. Lubensky. *Phys. Rev. A*, **38**, 2132 (1988).
[22] H.F. Scherk. *J. Reine Angew. Math.*, **13**, 185 (1834).
[23] S.P. Gido, J. Gunther, E.L. Thomas, D. Hoffman. *Macromolecules*, **26**, 4506 (1993).
[24] In fact, the surface is minimal for any b/a, but for even b/a the layers at the dislocation core join to make a continuous surface.
[25] H. Jinnai, K. Sawa, T. Nishi. *Macromolecules*, **39**, 5815 (2006).
[26] D. Duque, M. Shick. *J. Chem. Phys.*, **113**, 5525 (2000).
[27] H. Ogawa, N. Uchida. *Phys. Rev. E*, **73**, 060701(R) (2006).
[28] J.W. Goodby, M.A. Waugh, S.M. Stein, E. Chin, R. Pindak, J.S. Patel. *Nature*, **337**, 449 (1989).
[29] J. Fernsler, et al. *Proc. Nat. Acad. Sci.*, **102**, 14191 (2005).
[30] I. Bluestein, R.D. Kamien, T.C. Lubensky. *Phys. Rev. E*, **63**, 061702 (2001).
[31] C.D. Santangelo, R.D. Kamien. *Phys. Rev. Lett.*, **96**, 137801 (2001).
[32] C.D. Santangelo, R.D. Kamien. *Phys. Rev. E*, **75**, 011702 (2007).