Visualization, coarsening and flow dynamics of focal conic domains in simulated Smectic-A liquid crystals

Danilo B. Liarte,¹,² Matthew Bierbaum,² Muxin Zhang,² Brian D. Leahy,² Itai Cohen,² and James P. Sethna²

¹Institute of Physics, University of São Paulo, São Paulo, SP, Brazil
²Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY, USA

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Smectic liquid crystals vividly illustrate the subtle interplay of broken translational and orienta-
tional symmetries, by exhibiting defect structures forming geometrically perfect confocal ellipses and
hyperbolas. Here, we develop and numerically implement an effective theory to study the dynamics
of focal conic domains in smectic-A liquid crystals. We use the information about the smectic’s
structure and energy density provided by our simulations to develop several novel visualization tools
for the focal conics. Our simulations accurately describe both simple and extensional shear, which
we compare to experiments, and provide additional insight into the coarsening dynamics of focal
conic domains.

Translational broken symmetries are odd. Most broken
symmetry states respond elastically until deformations
are large. Translational order is frail. Crystals fracture
or plastically yield at strains of a few parts per thousand.
In equilibrium, they form grain boundaries – expelling
rotation gradients into walls – when subject to atomic-
scale boundary displacements. An analogous expulsion
occurs in smectics, which expel deviations from equal-
layer spacing in a manner that can be mapped onto the
Meissner/Higgs effect ¹. Instead of grain boundaries,
this expulsion of strain in smectics results in a remark-
able patterns of singular ellipses, hyperbolas, and parabo-
las known as focal conic domains (FCDs, Fig. 1), which
are the signature of the smectic one-dimensional layered
structure. Smectics provide a window into deep prop-
ties of translational order, lending insight into crystalline
behavior. FCDs have appealed to theorists and experi-
mentalists since the early days ², partially because of
their unique geometric origin. In its minimum energy
state, a smectic has lamellar layers spaced at equal dis-
tances. Equal layer spacing implies a singularity at the
centers of curvature of the surfaces. This constraint of
equal layer spacing, surprisingly, determines the allowed
shapes of the smectic’s lamella. The lamella choose sur-
faces whose centers of curvature trace out curves rather
than costly two-dimensional internal boundaries. These
surfaces are called cyclides of Dupin ³; their centers
of curvature trace out one-dimensional conic sections,
generically confocal ellipses and hyperbolas. The result-
ing structures in smectics are known as FCDs.

On a practical level, an understanding of focal conic
dynamics is necessary for the description of a variety of
liquid-crystalline states, such as smectic-A ⁴,⁵, smectic-
C and C* ⁶,⁷, lyotropic lamellar ⁸,⁹, twist-bend ¹⁰,
and even metallotropic liquid crystals ¹¹. We focus our
attention on smectic-A’s, which are the simplest case.

Our current understanding of focal conic structures in
smectics at rest includes the study of geometrical and
energetic properties ¹²,¹³, the effects of anchoring for
several substrates ¹⁴,¹⁵, the role played by dislocations
¹⁶,¹⁷, and beautiful insights extracted from a hidden
symmetry of the Poincaré group ²⁰. When a smectic
is driven by external dilatative stresses, experiments on
initially planar-aligned samples show a sequence of elas-
tic and plastic strain patterns that ultimately lead to a
polygonal array of parabolic focal conic lines ²¹. More
recently, experiments on smectic samples with antagonis-
tic anchoring conditions subjected to shear flow report on
the emergence of satellite defects ²². However, progress
in simulating smectic dynamics has been slow, perhaps
because of the challenge of incorporating defect dynamics
into Erickson-Leslie-Parodi theory.

In this letter we present results of our simulations of an
effective theory of smectic-A liquid crystals. Our dynam-
ics are an extension of Ericksen-Leslie-Parodi dynamics
and the Oseen-Frank free energy ²³,²⁴, in that we allow
focal conic singularities by allowing the order parameter
to change length, but we continue to forbid dislocations.

FIG. 1. Experimental (a and c) and simulation (b and d)
results for polarizer microscopy images of a section of smectic-
A slab for planar (a and b) and homeotropic anchoring (c and
d).
The use of modern GPU computing makes these simulations now feasible. Our simulations naturally form FCDs upon relaxation of random initial conditions and allow us to study these fascinating defects both during formation and under mechanical loading. In particular, we look at their energetics, topology, and geometry during coarsening, shear, and dilatational loading. We find good comparisons with experiments performed under similar situations. Our approach allows us to investigate focal conic structures in great detail through simulations, and provides us with an invaluable tool to understand their several aspects, ranging from energetics, topology and geometry to anchoring and mechanical strain effects that nicely complements current experimental approaches.

Our description of the smectic starts from its elastic free energy

\[ \Psi = \int \, d\mathbf{r} \left[ F(N, \partial_\mu N) + \lambda \cdot \nabla \times N \right], \tag{1} \]

which is a functional of the layer-normal field and its derivatives. The layer normal field \( N \) can be written in terms of the scalar displacement field \( u \) as \( N = N_0 - \nabla u \), where \( N_0 \) is the undeformed layer normal. The free-energy density \( F \) is given by:

\[ F = \frac{B}{4}(1 - N^4)^2 + K (\nabla \cdot N)^2 \]

\[ + \frac{1}{2}K_{24} \nabla \cdot [(N \cdot \nabla N - N (\nabla \cdot N))]. \tag{2} \]

Here, the first term penalizes compression or extension of the layers away from \( N = 1 \). The second and third terms are related to splay and saddle-splay distortions, which are inherited from the Oseen-Frank elastic free energy. We include an amplitude-dependence of \( K = N^4 \) and \( K_{24} = N^4 K_{24} \), where \( K \) and \( K_{24} \) are constants. The untraditional exponent four in the first term of the amplitude dependence of \( K \) and \( K_{24} \) result from the more general Landau-de Gennes theory using the quadrupolar parameter \( Q_{\alpha \beta} \), which imparts the quartic dependence since \( tr Q^2 \sim N^4 \) for uniaxial ordering. The Lagrange multiplier \( \lambda \) forbids dislocations by ensuring that the layer-normal field is curl-free, since the vector \( \nabla \times N \) is the density of dislocations (the Burger’s vector in units of the average layer spacing is given by the contour and area integrals \( \frac{1}{4} N \cdot d\mathbf{l} = \int_N \nabla \times N \cdot ds \)). We will treat the effects and dynamics of dislocations in a separate paper.

To arrive at the smectic’s dynamical equations of motion, we evolve the layer normal field in the simplest possible form, assuming \( N \) relaxes directly towards equilibrium. These dynamics give a partial differential equation for the gradient-descent evolution of \( N \):

\[ \gamma \dot{N} = - \left( \frac{\delta \Psi}{\delta N} - \left\langle \frac{\delta \Psi}{\delta N} \right\rangle \right), \tag{3} \]

where the angle brackets denote a spatial average and \( \gamma \) is a viscosity constant; \( \gamma \) can be written in terms of Leslie coefficients as \( \gamma = \alpha_3 - \alpha_2 \). The second term of (3) ensures that the net number of layers in the cell given by \( N_0 \) does not change during the gradient descent step. Equations (1)-(3) differ from Ericksen-Leslie-Parodi (ELP) dynamics in a few aspects. We relax the constraint of equal layer spacing \( |N| = 1 \), which is ensured in ELP theory by means of a Lagrange multiplier, and we consider amplitude-dependent elastic constants. Apart from the dependence on \( N \), our dynamics are a particular case of ELP theory in the limit of infinite fluid viscosity. As a result, our centers of mass move affinely with the external shear and only the orientation of the molecules change.

FIG. 2. Simulated energy density (white-blue density plot) and some sections of the layer surfaces (black lines) at the top section \( z = l_z \) of the system with planar anchoring (Fig 1).

To impose the external shear and extensional flows, we assume the layers are dragged with a displacement field determined by the flow. For simple shear, the layers are dragged in the \( x \) direction according to the displacement field

\[ u_x(x, y, z; t) = \frac{A}{l_z} (z - l_z) \sin(\omega t), \tag{4} \]

where \( l_z \) is the system size in the \( z \) direction, \( A \) is the amplitude, and \( \omega \) is the frequency of oscillation; our simulations are done at a fixed Ericksen number \( \gamma \omega l_z^2/K \approx 129 \). Extensional dynamics are implemented by stretching the smectic in the \( z \) direction while it contracts in the orthogonal \( x \) and \( y \) directions, as described by the set of equations

\[ l_z(t) = l_z(0) f(t), \quad l_{x,y}(t) = \frac{l_{x,y}(0)}{\sqrt{f(t)}} \]

\[ f(0) = 1, \quad f(t) > 0, \forall t \in [0, \infty) \], \tag{5} \]

where \( l_x, l_y, \) and \( l_z \) are the grid sizes in along the \( x, y, \) and \( z \) directions. To incorporate shear and dilatational dynamics simultaneously with the director relaxation, we employ an operator splitting method, alterna-
tively applying gradient-descent motion from Eq. 3 and one of the loading dynamics from Eqs. 4 & 5.

We perform analogous experiments on 8CB in the SmA phase, using a custom-built shear cell that allows precise control of the plate separation for gaps as small as 2-5 \( \mu\text{m} \) while keeping the plates parallel to \(< 1 \text{ part in } 10^3 \) \( \text{mm} \)], allowing us to explore a large range of strain amplitudes and Ericksen numbers. The shear cell is outfitted with two parallel glass plates, which we use as the sample boundaries, and imaged with cross-polarized microscopy. We treat the glass slides with cetyl-trimethylammonium bromide for homeotropic anchoring and with a polyimide treating for planar anchoring.

At the beginning of our simulations, we generate normally distributed random grids for each spatial component of the layer-normal field. We then enforce anchoring constraints, and use a Gaussian filter to smooth the field on short length scales. In order to remove the curl component of the field, we use a Helmholtz decomposition in Fourier space. The resulting components are divided by the mean length of the director field so that the field has average unit norm. We use an Euler integrator with adaptive step size \( \text{[3]} \) in order to integrate our partial differential equations. The driving code is written in Python. Each step of the integration is evaluated using parallel computing on a GPU using CUDA. Spatial derivatives are evaluated with Fourier methods (FFTs).

In this letter we present results for fixed values for the ratio \( K_{24}/K = -1.5 \) and for deGenne’s length scale \( \xi = \sqrt{K/B} = 0.2a \) (corresponding to the superconductor penetration depth), where \( a \) is the finite-difference grid spacing. (Larger \( \xi \) produces similar results with blurred features.)

From these random initial conditions, our gradient-descent dynamics forms FCDs which closely resemble those seen in experiments as shown in Fig. 1. We visualize the focal conics domains in our simulations through several techniques we have developed. We render polarizer microscopy images, as shown in Fig. 1 by ray-tracing light using the Fresnel equations for anisotropic dielectrics \( [2] \). Figure 2 shows a plot of the free energy density \( F \), overlaid with cross-sections of the layer surfaces (contours of constant \( N_0 \cdot r - u \)). The free energy is high at the focal lines, where the layer contours form cusps.

Four visualizations of the three-dimensional smectic structure are shown in figure 3. Figure 3a is a volume rendering visualization of the free energy density where each voxel is given a color and degree of transparency that is associated with its free energy density. The high energy regions (red) have organized into the characteristic focal conic structure of smectics, forming multiple ellipses, each with a hyperbola coming out of its focus. The focal conic character of the smectic structures is reinforced by the loci of the principal centers of curvature of the smectic layers, shown in Fig. 3b, which coincide with the regions of high energy density in 3a, 3c. To calculate the radii of curvature, we project each layer’s second fundamental form tensor \( \nabla_{\mu \nu} = \partial_{\mu} \partial_{\nu} u \) into the layer-surface tangent plane. The principal radii of curvature are equal to the inverse of the principal curvatures, which are the eigenvalues of the projected \( \nabla_{\mu \nu} \). The shared surface normals intersect at the centers of curvature for the layers, which form the confocal cones \( [12] \). Finally, Fig. 3c shows three-dimensional level surfaces of the mass-density field.

To study the coarsening dynamics of focal conics we simulate with no anchoring at the boundary, since the boundary constraint introduces a length scale for the distribution of the layer-surface radii of curvature. As the system evolves, our dynamics seem to energetically favor ellipses with large linear eccentricity \( c \). The layers around singular ellipses become flatter with increasing \( c \), and converge to planes when \( c \rightarrow \infty \). This is the dominant coarsening mechanism in our simulations. The coarsening of focal conics becomes slower with increasing time, but it does not stop until a uniform flat configuration is reached. (Our computational defect structures can be stabilized with simulated ‘dust’ particles on the glass slides, by introducing spatially-dependent energetic anchoring on the boundaries.) To quantify the coarsening, we investigate the probability distribution of the principal radii of curvature \( R \), which define a characteristic distance to the focal conics, and are distributed according to a function \( P(R, t) \) which also depends on time. The scaling assumption states that the morphology at late times statistically scales with a single length scale \( R^* \), so in particular \( P(R, t) \propto \Pi(R/R^*(t)) \) for some (possibly universal) function \( \Pi(X) \). In the supplemental ma-

FIG. 3. 3D and 2D visualizers of a simulation of smectic-A liquid crystals with planar anchoring. (a) Volume rendering visualization of the energy density; (b) loci of the centers of curvature of the layer surfaces; (c) layer surfaces; (d) polarizer microscopy image, expanded from Fig. 1b.)
terial, we propose three possible arguments yielding the cutoff radius of curvature \( R^* \approx t^{1/4}, R^* \approx [t \ln(t/\tau)]^{1/4} \), and \( R^* \approx t^{0.5} \) with \( \alpha \approx 0.28 \). Scaling collapse plots are consistent with all of these possibilities, (see Supplemental Materials for more details, and for a discussion of the decay in the energy density with time.) The approach to equilibrium by increasing eccentricity to minimize bending energy is an interesting contrast to the typical approach to equilibrium of decreasing eccentricity to minimize a surface energy.

Our simulations and experiments also provide a window to understand dynamics of focal conic domains under shear. From our simulations, simple shear oscillations parallel to the glass slides primarily act to accelerate the focal conics’ coarsening. When we shear stabilized focal conic structures, our simulations show that the focal conics are not significantly altered by the planar shear, in qualitative agreement with our experiments with strong homeotropic anchoring. In addition, our simulations allow us to tune the smectic’s anchoring at the boundary. As a result, our simulations promise to discern the effects of anchoring imperfections, such as weak or spatially-modulated anchoring, on the rich structures that can be produced in experiments (see supplemental animations [31]).

![Image](Image60x274 to 293x430)

**Fig. 4.** Simulation and experimental results for SmA under dilative stress. (a) Total free energy as a function of time. (b) Layers in the \( x-z \) plane showing undulation pattern at \( t = 120 \tau \). (c) Simulation and (d) experimental results for crossed-polarizer images showing a pattern of focal conic domains, at strain amplitudes of 0.33 and 0.13, respectively.

Under dilative strain (stretching the layer spacing), homeotropic smectic-A liquid crystals are known to release free energy by forming undulations [32–34], and focal conic domains [21, 35]. In Fig. S4a, we show simulation results for the total free energy as a function of time for a dilative dynamics with \( f(t) = 1 + A(1 - \cos \omega t) \), where \( A = 0.25 \), and \( \omega = 2\pi/1000 (\tau^{-1}) \). The first sharp peak at about \( t_1 = 100 \tau \) marks the onset of an undulation pattern, which is depicted in the layers contour plot of Fig. S4b. Linear stability analysis using the methods of [33, 34] leads to a critical strain threshold \( \epsilon_c \) that is given by the solution of the equation (see supplemental material):

\[
\epsilon_c = \frac{\pi \xi}{l_z} \sqrt{\frac{1 - 6 \epsilon_c + 6 \epsilon_c^2}{(1 - 3 \epsilon_c + 2 \epsilon_c^2)^2}} \approx \frac{\pi \xi}{l_z},
\]

since \( \epsilon_c \) is small. This analysis results in a buckling wavelength of \( \approx 9a \approx 0.04l_z \), which is consistent with our simulations (see Fig. S4c), and a time threshold that we have checked numerically. (It is smaller than our observed peak by approximately a factor of two, presumably because of the growth time of the undulation pattern.) The second peak of the free energy signals the onset of a configuration which evolves towards a complex pattern of focal conic domains. Fig. S4c and S4d show crossed-polarizer images obtained from simulations and experiments at maximum strain, respectively.

Note the fascinating fact that the critical change in length \( cl_z \approx \pi \xi \) is a microscopic length. Except near a critical point, one expects \( \xi \) to be of order a molecular size; the instability threshold [36] for a bulk material happens when one stretches it by one molecular length [37]! A simple calculation for crystals shows an analogous result for grain boundaries: a bent crystal’s ground state has dislocations once the net displacements become of order the lattice constant (up to a logarithm of the crystal size over the atomic size). Unlike crystals which are metastable, smectics are unstable under long-wavelength deformations with atomic-scale displacements – the low-energy defective state has no associated nucleation barrier. Thus the equilibrium continuum elastic theory of materials with broken translation invariance is frail [38, 39] – it is only valid in general for microscale net displacement differences over macroscale distances.

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* danilo@if.usp.br
† sethna@lassp.cornell.edu

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Supplemental Material for
Visualization, coarsening and flow dynamics of focal conic domains in simulated Smectic-A liquid crystals

In this text, we present three scaling collapses associated with the distribution of the radii of curvature during the coarsening of focal conics, and give theoretical explanations for the three possible forms. We also provide details of an application of linear stability analysis to study undulation patterns of smectic-A liquid crystals subject to dilative strain.

SCALING EXPONENT FOR THE COARSENING OF FOCAL CONICS

The principal radii of curvature $R$ define a characteristic distance to the focal conics. They are distributed in space according to a function which also depends on time $P(R|t)$. Scaling suggests that all correlation functions should scale with a single length scale $R^*(t)$ that diverges at late times, hence $P(R|t) \approx \Pi(R/R^*)/R^*$ for some perhaps universal function $\Pi(X)$. (Here the last factor preserves normalization: $\int P(R)dR = \int \Pi(X)dX = 1$.) In coarsening problems, it is often possible to use simple energetic arguments to derive the power law divergence $R^*(t) \propto t^{\alpha}$; for example, phase separation in systems without hydrodynamic flow has $\alpha = 1/3$ for conserved order parameters and $\alpha = 1/2$ for non-conserved order parameters. Here we give three possible scaling forms, of increasing sophistication and decreasing quantitative justification. The first mimics the standard energetic arguments; the second provides a refined argument including a logarithmic correction due to defect cores, and the third postulates the development of a self-similar, fractal pattern of focal conic domains of various sizes (Fig. S1).

Away from the defect cores, where $|N| \approx 1$, the free energy density scales as $R^{-2}$. So the average energy density is

$$\mathcal{E}(R^*) = \int P(R)/R^2dR. \quad (S1)$$

In traditional coarsening, one assumes that the integral for $\mathcal{E}(R^*)$ converges at zero, so $\mathcal{E}(R^*) \sim 1/(R^*)^2$. This leads to a force (tension) $T = \delta \mathcal{E}/\delta R^* \sim 1/(R^*)^3$. Since the order parameter is non-conserved,

$$\dot{R} = -\gamma T, \quad (S2)$$

where $\gamma$ is an effective inverse viscosity (see section 11.4 of [S1]). This can be solved giving $R^* \sim t^{1/4}$ (Fig. S1a), and hence $\mathcal{E}(R^*(t)) \sim 1/t^{1/2}$ (Fig. S2).

How does this change if we consider the defect cores, where $|N| < 1$? The energy in the cones, near the focal conic line singularities, scales as the length of the conics times $\ln(R/\xi)$, where $\xi$ is de Gennes’ length scale. This follows from the fact that the focal conic domains have a line singularity along which $R = 0$ and the energy density diverges. Within a single domain of size $R^*$, therefore, $P(R) \sim R$ at small $R$, so $\Pi(X) \sim X$ for small $X$. This leads to a divergence in the integrated energy near the focal conic singularities, which is cut off by $\xi$,

$$\mathcal{E}(R^*) = \int_{R^*}^{\infty} (1/R^2)\Pi(R/R^*)/R^*dR = \int_{R^*}^{\infty} \Pi(X)/(X R^*)^2dX \sim (1/R^*)^2 \int_{\xi/R^*}^{1} X/X^2dX = \log(\xi/R^*)/(R^*)^2 \quad (S3)$$

(see section 10.5 of [S2]). After some calculation, Eq. (S2) implies

$$R^* \sim [t\ln(t/\tau_c)]^{1/4}, \quad (S4)$$

in the limit of large $R$ or $t$. So if the focal domains are all of the same length scale $R^*$, and the relaxation of the core singularites dominates the coarsening, we expect a $t^{1/4}$ scaling with a logarithmic correction, as in Fig. S1b. There is a large range of values for $\tau_c$ which collapse our data. Fig. S1 shows a scaling collapse plot with the logarithmic corrections for $\tau_c = 100$.

Finally, we notice the increasing ‘left shoulder’ in Fig. S1 indicating a growing range of structural scales. A single focal conic domain should have $P(R) \propto R^2$ at scales small compared to the domain size, and this shoulder appears to scale with a power smaller than one. This could indicate the development of a self-similar distribution of focal conic domain sizes, perhaps a 3D variant of the ‘Apollonian packing’ of ellipses for smectics at boundaries with planar anchoring conditions [S3, S4]. This shoulder appears to be converging not to $P(R) \propto R$ at short distances, but rather to $P(R) \propto R^\kappa$ with $\kappa \sim 1/2$. If the number of conics of size $Q$ goes as $Q^{-\omega}$, the volume of conics of size $Q$ goes
as $Q^{3-\omega}$, and one can argue that $P(R) \sim R^{3-\omega} \sim R^\kappa$, so $\omega \sim 3.5$ would explain the shoulder. Given this form, so $\Pi(X) \sim X^\kappa$, we find

$$
\mathcal{E}(R^*) = \int_0^\infty (1/R^2) \Pi(R/R^*)/R^* dR = \int_0^\infty \Pi(X)/(XR^*)^2 dX \\
\sim (1/R^*)^2 \int_0^1 X^\kappa/X^2 dX \sim (1/R^*)^2 (\xi/R^*)^{\kappa-1} \sim (1/R^*)^{\kappa+1}.
$$

(S5)

Hence the tension $T = \delta \mathcal{E}/\delta R^* \sim 1/(R^*)^{\kappa+2}$, and $R^*(t) \sim t^{1/(\kappa+3)}$. For $\kappa = 1/2$, this gives $R^*(t) \sim t^{\alpha}$ with $\alpha = 2/7 \approx 0.286$ (Fig. S1c), and hence $\mathcal{E}(R^*(t)) \sim t^{-(\kappa+1)/(\kappa+3)} \sim t^{-3/7}$ (Fig. S2).

All of these scaling forms are compatible with the data, given the limited scaling regime (less than a decade in length, corresponding to less than three decades in ‘size’); $P(R,t)$ is clearly still evolving in shape. The fractal scaling form is appealing, in that it explains also the observed shape evolution – but we have not confirmed the large preponderance of small focal conic domains that would seem necessary for this scaling form ($\omega \sim 3.5$ should demand that the focal conics of 1/10 the size should occupy three times the volume).

**FIG. S1.** Scaling collapses of the layer-surface radii of curvature distribution. (a) Naive power-law scaling, $R^*(t) \sim t^{1/4}$. (b) Incorporation of logarithmic corrections to scaling, $R^*(t) \sim t \log(t/\tau_c)^{1/4}$. (c) Assuming a fractal distribution of conic domains, inspired by growing ‘left shoulder’ on the plot, $R^*(t) \sim t^\alpha$ with $\alpha = 1/(\kappa+3)$ with $\kappa \sim 1/2$. 

FIG. S2. Total free energy $\psi$ (blue circles) as a function of time. The black and blue lines correspond to the behavior predicted from the naive argument $R^* \sim t^{1/4}$ and the fractal scaling $R^* \sim t^{1/(\kappa + 3)} \approx t^{2/7}$ respectively. The dashed line is a best fit.

LINEAR STABILITY ANALYSIS FOR SMA UNDER DILATIVE STRAIN

We consider a situation where a thin slab of homeotropic smectic-A is subject to dilative stress [S2, S5–S9]. In this case, the smectic layers are parallel to the glass slides, so that the stretching of the gap promotes an increase of the interlayer spacing. Planar-layer configurations store a considerable amount of bulk energy as strain is increased, which is released with the formation of an undulation pattern after a critical strain is reached. Here we use the methods of [S5–S7] to study the formation of undulation instabilities on smectic-A liquid crystals.

The displacement field associated with an undulation pattern of a smectic-A can be written as:

$$u(x) = \epsilon z + u_0 \cos(qx) \sin(kz), \quad \text{(S6)}$$

where we take $k = \pi/l_z$ to enforce strict homeotropic anchoring. Our elastic free energy density is given by:

$$f = \frac{B}{4} (1 - N^4)^2 + K (\nabla \cdot N)^2. \quad \text{(S7)}$$

Notice that we have not included a saddle-splay term, nor have we considered amplitude dependence of the elastic constant $K$, since their effect is negligible. Also, we do not need include a Lagrange multiplier, since $N = z - \nabla u$ is curl-less if $u$ is given by Eq. (S6). The free energy density (S7) can be written in terms of the displacement field as

$$f = \frac{B}{4} \left\{ 1 - \left[ 1 + \left( \frac{\partial u}{\partial x} \right)^2 - 2 \frac{\partial u}{\partial z} \right]^2 \right\}^2 + K \left( \frac{\partial^2 u}{\partial x^2} \right)^2. \quad \text{(S8)}$$

We can combine Eqs. (S8) and (S6) in order to write

$$\frac{f}{B} = \xi^2 q^4 u_0^2 \sin^2(kz) \cos^2(qx) + \frac{1}{4} \left\{ \left[ q^2 u_0^2 \sin^2(kz) \sin^2(qx) \right. \right. \right.$$

$$- 2(ku_0 \cos(kz) \cos(qx) + \epsilon) + 1 \right\}^2, \quad \text{(S9)}$$

where $\xi = \sqrt{K/B}$ is de Gennes’ length scale. To find the stability threshold we integrate out the free energy density over one period in the $x$-direction, and from 0 to $l_z$ in the $z$-direction:

$$F = \int_{0}^{2\pi} dx \int_{0}^{l_z} dz f(x, z). \quad \text{(S10)}$$
The stability threshold is given by the solution of the equation:

$$\frac{\partial^2 F}{\partial u_0^2} = 0,$$

(S11)

or,

$$4k^2 \left( 6\epsilon^2 - 6\epsilon + 1 \right) + q^2 \left( \xi^2 q^2 - 8\epsilon^3 + 12\epsilon^2 - 4\epsilon \right) = 0.$$

(S12)

For given $\xi$ and $l_z$, this equation defines a curve in the $\epsilon \times q$ plane. Fig S3 shows the critical strain as a function of $q$ for $\xi = 0.2a$ and $l_z = 64a$, corresponding to our simulation parameters, where $a$ is the finite-difference grid spacing.

The strain is minimal for

$$q = \frac{\sqrt{4\epsilon^3 - 6\epsilon^2 + 2\epsilon}}{\xi}.$$

(S13)

Eq. (S13) can be plugged back into Eq. (S12), so that,

$$\epsilon_c = \frac{\pi \xi}{l_z} \sqrt{\frac{1 - 6\epsilon_c + 6\epsilon_c^2}{(1 - 3\epsilon_c + 2\epsilon_c^2)^2}} \approx \frac{\pi \xi}{l_z},$$

(S14)

where the approximate solution on the r.h.s. of (S14) is valid since $\epsilon$ is small. Notice that our approximate critical strain ($\pi \xi / l_z$) corresponds to half of the value obtained in [S5–S7]. Also, it is interesting to point out that the critical change in length $\epsilon_c l_z \approx \pi \xi$ is a microscopic length (see main text).

Fig S4 shows simulation results for smectic-A liquid crystals under dilative stress with $\xi = 0.2a$ and $l_z = 64a$. We consider $f(t) = 1 + A(1 - \cos(\omega t))$ (see Eq. (6) of main text), with $A = 0.25$, and $\omega = 2\pi / 1000 \tau^{-1}$. Eq (S14) predicts a strain threshold of $\epsilon_c \approx 0.01$, and a critical wavelength of $q \approx 9a \approx 0.04l_z$, which is consistent with our simulations (Fig S4b). However, since $\epsilon = 1 - f^{-1}$, we can rearrange $f(t)$ in order to write

$$t_c = \frac{1}{\omega} \cos^{-1} \left( 1 - \frac{\epsilon_c}{A(1 - \epsilon_c)} \right) \approx 45\tau,$$

(S15)

which is about half of the time threshold associated with the first peak of Fig S4a. We suggest that the time scale associated with the growth of the undulation pattern accounts for the discrepancy between the simulation threshold and the analytical estimate. We can also investigate the stability threshold by adding a small perturbation $\delta N$ to $N_0$. Under a gradient descent infinitesimal evolution of $N$, we expect that $\mathcal{F}[\delta N_z(t + \delta t)] = \exp(\lambda_k \delta t)\mathcal{F}[\delta N_z(t)]$, where $\mathcal{F}$ denotes a Fourier transform operator. An exponent $\lambda_k$ is less than zero for stable planar configurations, and reaches...
FIG. S4. Simulation results for SmA under dilative stress. (a) Total free energy as a function of time. (b) Layers in the $x$-$z$ plane showing undulation pattern at $t = 120\tau$.

zero at the critical strain for some wavenumber $q$. Careful numerical calculations for $\lambda_k$ lead to $t_c \approx 45\tau$, and $q \approx 9a$, in agreement with our analytical estimate.

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