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On the Theory of Smectic Textures

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Abstract—The strains in smectics are considered beyond the small-angle approximation. The energies of confocal and conical textures are determined.

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The energy of elastic strains of a smectic at small deviations of layer orientations from the horizontal xy plane is [1, Eq. (44.6)]

$$E = \frac{A}{2}\int((\partial_z u)^2 + (\lambda\Delta_\perp u)^2)dV, \quad (1)$$

where $u(\mathbf{r})$ is the layer displacement along the vertical (z axis), $\Delta_\perp = \partial_x^2 + \partial_y^2$, $A > 0$ is the elastic constant, and λ is the length parameter. However, harmonic approximation (1) is applicable only for a rather limited range of problems, namely, thermal fluctuations in smectic layers [2, §137], screw dislocations [1, §45], point defects (impurities) [3], a point source of a moments of force, and a linear inclusion (see [1, expression (44.13)]) in a smectic layer [4]. The point is that nonlinear effects are often substantial in smectics even at arbitrary small deviations of layer orientations. Then, the elastic fields correspond to an energy minimum,

$$E = \frac{A}{2}\int\left(\left(\partial_z u - \frac{(\partial_\alpha u)^2}{2}\right)^2 + (\lambda\Delta_\perp u)^2\right)dV, \quad (2)$$

where $(\partial_\alpha u)^2 = (\partial_x u)^2 + (\partial_y u)^2$. Such nonlinear problems are as follows: the Helfrich instability during tension of a smectic [1, problem to §44], an edge dislocation [5, 6], deformation in an anomalously large region around a horizontal cylindrical inclusion of radius $R > 2\lambda$ [3], homogeneous shear, a vertical linear inclusion with violated symmetry $z \longrightarrow -z$, an elementary step on the basal face of a smectic, a linear distribution of a moment of force in the basal plane [4], twin boundaries [7], and point and linear force distributions [8, 9].

Textures in which stresses are low and the orientation of smectic layers changes substantially are known in smectics [10, 11]. Then, small-angle approximation (2) is inapplicable. In such cases, stress fields should be determined in terms of the general small-strain approximation

$$E = \frac{A}{2}\int\left\{\left(\frac{\delta a}{a}\right)^2 + (\lambda\mathcal{H})^2 + \beta\mathcal{K}\right\}dV, \quad (3)$$

where a is the equilibrium interlayer spacing; δa is the deviation of the interlayer spacing from a; $\mathcal{H}$ and $\mathcal{K}$ are the average and Gaussian layer curvatures, respectively; and β is the material constant on the order of λ^2. Approximation (3) holds true if all terms in the curly brackets are small. The term with the Gaussian curvature differs from the term with the average curvature in a full derivative. Nevertheless, we should take into account both terms to calculate the texture energy.

The state of smectic is fully characterized by specifying the profile of smectic layers. This profile can be specified by various methods. For example, let us consider a smectic placed between two concentric cylinders of radii $r_2 > r_1 \gg \lambda \sim a$. In the case where the minimum of the surface energy corresponds to a layer orientation parallel to the walls, the texture shown in Fig. 1a should appear.

To a first approximation, the texture represents a set of concentric layers spaced the same distance apart. The effect of curvature leads to a weak distortion of this distance. Let a certain layer be located at a dis-

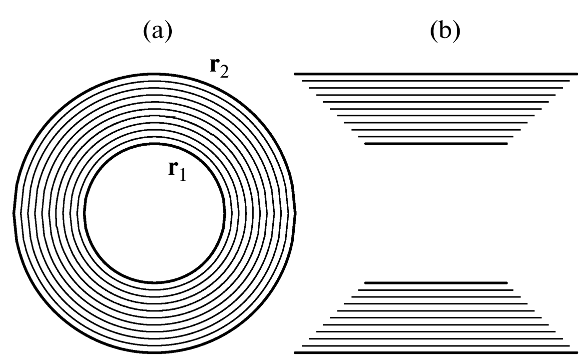

Fig. 1. (a) Cylindrical and spherical textures and (b) the corresponding undeformed states.

tance $r + \eta(r)$ from the center, where r is the layer radius in the initial equidistant state. The energy of such a texture is

$$E = \pi A \int_{r_1}^{r_2} \left(\dot{\eta}^2 + \frac{\lambda^2}{(r+\eta)^2} \right) r dr, \tag{4}$$

where $\dot{\eta} = \partial_r \eta$. In this case, the equation of mechanical equilibrium takes the form

$$\ddot{\eta} + \frac{\dot{\eta}}{r} + \frac{\lambda^2}{(r+\eta)^3} = 0. \tag{5}$$

Without regard for the deformation of the walls, we have boundary conditions $\eta(r_1) = \eta(r_2) = 0$. Radial layer displacement η turns out to be small, and Eq. (5) is reduced to the equation

$$\ddot{\eta} + \frac{\dot{\eta}}{r} + \frac{\lambda^2}{r^3} = 0. \tag{6}$$

Its general solution is

$$\eta = -\frac{\lambda^2}{r} + C \ln \frac{r}{b},$$

where C and b are the constants of integration. With allowance for the boundary conditions, we obtain

$$\eta = \lambda^2 \left\{ \frac{1}{r_1} - \frac{1}{r} + \left(\frac{1}{r_2} - \frac{1}{r_1} \right) \frac{\ln(r/r_1)}{\ln(r_2/r_1)} \right\}. \tag{7}$$

Indeed, the deviations from the equilibrium interplanar spacings are small, and we may assume that $\eta = 0$ to find energy (4); then, we have

$$E = \pi A \lambda^2 \ln \frac{r_2}{r_1}. \tag{8}$$

This texture energy is paid for the decrease in the energy of smectic–wall contact, which is proportional to the contact surface area. If the internal cylinder is absent, we have $r_1 \sim a$. Such a defect represents a disclination in a smectic.

For an analogous problem with spherical symmetry, it is convenient to introduce a radial layer displacement. With the same designations, for the texture energy we obtain

$$E = 2\pi A \int_{r_1}^{r_2} \left(\dot{\eta}^2 + \frac{s}{(r+\eta)^2} \right) r^2 dr, \tag{9}$$

where $s = 4\lambda^2 + \beta$. For a sphere of radius R, we have

$$\mathcal{H} = \frac{2}{R}, \quad \mathcal{K} = \frac{1}{R^2}.$$

When neglecting displacement η, we find

$$E = 2\pi A s (r_2 - r_1). \tag{10}$$

For the displacement field, we obtain

$$\eta = \frac{s}{r} \left(\frac{r - r_1}{r_2 - r_1} \ln \frac{r_2}{r_1} - \ln \frac{r}{r_1} \right). \tag{11}$$

In the general case as well as in small-angle limit (1), the theory of elasticity for smectics can be formulated in terms of displacement field $u(\mathbf{r})$ with respect to a certain initial equidistant plane state. Indeed, we have $\delta a = a \partial_z u$ for uniform compression (along the z axis) of a state with horizontal smectic layers and equilibrium period a. When creating uniform strain $\partial_x u$, we obtain the interplanar spacing

$$a + \delta a = a(1 + \partial_z u)\cos\varphi,$$

where $\tan\varphi = \partial_x u$. In the second operation, every layer is rotated through angle φ at the same interlayer spacing along the vertical. From stereometry, we have

$$\tan^2\varphi = (\partial_x u)^2 + (\partial_y u)^2 = (\partial_\alpha u)^2. \tag{12}$$

Thus, we obtain

$$\delta a = \{(1 + \partial_z u)\cos\varphi - 1\} a. \tag{13}$$

For this parametrization of the profile of smectic layers, the cylindrical texture considered above in the initial undeformed state represents two isolated sections (Fig. 1b, trapezoid in the section). The displacement fields are

$$u = -\sqrt{z^2 - x^2} - z$$

for the lower trapezoid ($z < 0$) and

$$u = \sqrt{z^2 - x^2} - z$$

for the upper trapezoid ($z > 0$). The edges of the upper and lower layers are joined and the texture shown in Fig. 1a is formed. Correspondingly, for the spherical texture, we have

$$u = \pm\sqrt{z^2 - x^2 - y^2} - z.$$

These functions are the solutions to the equation ($\delta a = 0$)

$$1 + \partial_z u = \frac{1}{\cos\varphi} = \sqrt{1 + (\partial_x u)^2 + (\partial_y u)^2}. \tag{14}$$

The specific features of the cylindrical and spherical textures considered above and the experience of solving small-angle approximation problems point to the strategy of solving problems beyond the limits of the small-angle approximation. To a first approximation, we may neglect curvature effects by assuming $\lambda = 0$. Then, the equilibrium equation is reduced to the equation

$$\begin{aligned} &\partial_\alpha \{(1 + \partial_z u)\cos^3\varphi[(1 + \partial_z u)\cos\varphi - 1]\partial_\alpha u\} \\ &\quad - \partial_z[(1 + \partial_z u)\cos^2\varphi - \cos\varphi] = 0. \end{aligned} \tag{15}$$

This equation should be solved in the region of smectic compression ($\delta a < 0$). A tension region ($\delta a > 0$) is absent because of the Helfrich instability, and a state with a zero stress ($\delta a = 0$) takes place in the other regions. When taking into account the effects of curvature proportional to λ^2 in the main portion of a smectic, we obtain small corrections for a layer profile. However, the curvature effects are substantial in twin boundaries and in the vicinity of disclination cores.

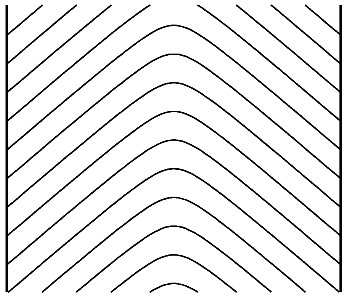

Fig. 2. Axially symmetric conical texture.

Twin boundaries of a molecular thickness with considerable angles or a certain dislocation distribution are likely to appear under certain boundary conditions in an equilibrium state [12].

Note that, if $\partial_z u = \varepsilon$ (where ε is a positive constant), we have

$$\cos\varphi = \frac{1}{1+\varepsilon}$$

according to Eq. (14). Thus, axially symmetric texture $u = r\tan\varphi$, which represents a stack of smectic layers having a cone shape, can exist (Fig. 2). Such a texture should appear in a cylindrical vessel if a tilted orientation of smectic layers is preferred at the walls. For a cone, we have

$$\mathcal{H} = -\frac{\sin\varphi}{r}, \quad \mathcal{K} = 0.$$

Correspondingly, the energy of a conical texture (conical disclination) in a first approximation is

$$E = \pi A\lambda^2 \sin^2\varphi \ln\frac{R}{\tilde{a}}, \qquad (16)$$

where R is the vessel radius and $\tilde{a} \sim a$.

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