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Core structure of a screw disclination in smectic-A liquid crystals

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The core structure of a screw dislocation in the smectic-A matrix is studied using the covariant form of the Landau–de Gennes free-energy density. Three qualitatively different core structures are found. In solution (i) the screw dislocation is singular only in the smectic component, while in solution (ii) the defect is also present in the nematic director field. In solution (iii) smectic layers bend significantly out of the undistorted reference plane and the core is singular in both components. In addition, it is shown that, if the smectic phase is composed of a mixture of conformers with opposing twist sense, the screw dislocation can cause spatial variation of individual mixture component concentrations. This can in turn influence the core structure itself.

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In ordered media competing ordering mechanisms often exist which force the system to form defects [1]. At a defect site some system-ordering properties are no longer uniquely defined. Recently there has been a growing interest in this field of research, not only because the defect classification depends in detail on the nature and topology of the order parameter manifold, but also because the defects can often mediate phase transitions between different phases, and can potentially play an important role in various applications.

Liquid crystals [2] (LC's) are particularly suitable as a probe of these phenomena. They form an extremely rich variety of different defects, known also as disclinations in this context, which can reach their equilibrium structure relatively easily, precisely because they are liquid. There have been numerous detailed [3–6] theoretical studies of defect core structures in nematic (N) LC's. However, there have been only preliminary studies of defect structures in the smectic phase [1,2,7–9]. Following the discovery of the twist grain boundary (TGB) phase [10–12] there has been renewed interest in the structure of the screw dislocation (Fig. 1) in the smectic-A (Sm-A) phase. This phase is the result of a frustrated compromise between the cholesteric and Sm-A phases. It consists of a lattice of screw dislocations in a Sm-A matrix, and was first predicted theoretically [10] on the basis of an analogy [13] between the Sm-A phase and superconductors. In this analogy the screw dislocations play the role of vortices in type-II superconductors.

To our knowledge there have been two studies concerned with the core structure of the screw dislocation [8,9]. Day, Lubensky, and McKane established [8] the connection between dislocation in liquid crystals and vortices in superconductors. They show that the structure of the nematic director field $\mathbf{n}(\mathbf{r})$ is similar to that of the magnetic vector potential within a vortex. Loginov and Terent'ev studied [9] the core structure using a harmonic elastic approach. But if the result of this theory is interpreted in the director-field representation, the resulting structure differs from the predictions of the model of Day, Lubensky, and McKane. In addition, the harmonic approach indicates that the director field is singular at the disclination axis, suggesting strong spatial variation of the nematic orientational order parameter.

The purpose of this paper is to extend these studies to the case where nematic order parameter variations are taken into account. In particular, we show that this inclusion enables the existence of new structures not seen in the theory of superconductivity. This complexity is further increased by including the case where the LC is composed of conformers with competing molecular chirality. Details will be published elsewhere.

The free-energy density of our model is expressed as [2,13,14]

$$f(\mathbf{r})=f_N^{\mathrm{loc}}(\mathbf{r})+f_N^{\mathrm{non}}(\mathbf{r})+f_{\mathrm{Sm}}^{\mathrm{loc}}(\mathbf{r})+f_{\mathrm{Sm}}^{\mathrm{non}}(\mathbf{r})+f_{\mathrm{coupl}}(\mathbf{r}) , \tag{1}$$

$$f_N^{\mathrm{loc}}=a_N(T-T_N)\frac{s^2}{2}-b_N\frac{s^3}{3}+c_N\frac{s^4}{4} , \tag{1a}$$

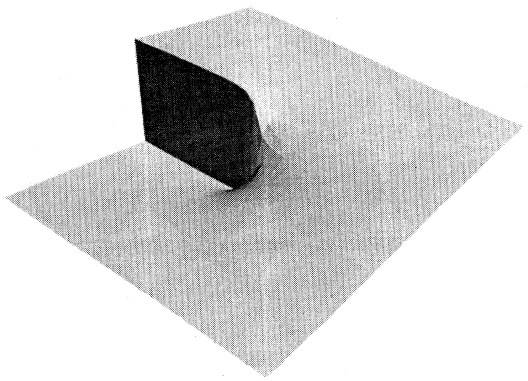

FIG. 1. Schematic presentation of the screw dislocation in a layer of the smectic-A matrix. The smectic layer rotates around the dislocation axis in a screw-staircase fashion. Far from the dislocation axis the nematic molecules tend to lie along the layer normal.

$$f_N^{\rm non}=\tfrac{1}{6}[k_\parallel(\mathbf{n}\cdot\nabla s)^2+k_\perp(\mathbf{n}\times\nabla s)^2]$$
$$+\frac{s^2}{2}[k_1(\nabla\cdot\mathbf{n})^2+k_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2+k_3(\mathbf{n}\times\nabla\times\mathbf{n})^2]\ , \tag{1b}$$

$$f_{\rm Sm}^{\rm loc}=a_{\rm Sm}(T-T_{\rm Sm})|\psi|^2+b_{\rm Sm}\frac{|\psi|^4}{2}+c_{\rm Sm}\frac{|\psi|^6}{3}\ , \tag{1c}$$

$$f_{\rm Sm}^{\rm non}=\gamma_\parallel|(\mathbf{n}\cdot\nabla-iq_0)\psi|^2+\gamma_\perp|\mathbf{n}\times\nabla\psi|^2\ , \tag{1d}$$

$$f_{\rm coupl}=-Ds|\psi|^2\ . \tag{1e}$$

In these equations $f_i^{\rm loc}$ denotes the local and $f_i^{\rm non}$ the nonlocal part of the free-energy density of the smectic ($i={\rm Sm}$) and nematic ($i=N$) phase contributions. The nematic orientational order parameter $s(\mathbf{r})$ describes the degree of orientational fluctuation around the average local orientation $\mathbf{n}(\mathbf{r})$. The smectic ordering is described by the one-dimensional density wave $\psi(\mathbf{r})=\epsilon(\mathbf{r})e^{i\phi(\mathbf{r})}$. The smectic translational order parameter $\epsilon(\mathbf{r})$ measures the amount of smectic ordering, and the phase factor $\phi(\mathbf{r})$ specifies the position of the smectic layers. The quantities γ_i ($i=\perp,\parallel$) and k_i ($i=1,2,3,\perp,\parallel$) are the smectic and nematic elastic constants; $\gamma_\parallel,\gamma_\perp$ are associated with smectic layer compression and bending, respectively. A positive value of $\gamma_\perp$ is crucial for the stability of the Sm-A phase: it tends to lock nematic molecules along the smectic layer normal. At $\gamma_\perp=0$ the Sm-A phase becomes unstable with respect to the smectic-C phase. s^2k_i corresponds to the splay ($i=1$), twist ($i=2$), and bend ($i=3$) Frank elastic nematic constant; and $k_\perp,k_\parallel$ determine the preferred director $\mathbf{n}(\mathbf{r})$ orientation at the nematic-isotropic interface. The quantity T is the temperature; $q_0=2\pi/d$ with d being the average separation between adjacent smectic layers. The values of T_N, $T_{\rm Sm}$, a_N, b_N, c_N, $a_{\rm Sm}$, $b_{\rm Sm}$, and $c_{\rm Sm}$ are given by the LC material properties. The term (1e) couples the smectic and nematic order parameters and is crucial if the Sm-A–N phase transition [2,15,16] is to be described correctly. For $D=0$, the Sm-A–N phase transition is continuous at $T=T_{\rm Sm}$, while the I–N transition (I denotes isotropic) is discontinuous at $T-T_N=2b_N^2/(9a_Nc_N)$. As D is increased, one reaches (a) a tricritical point at $D_{\rm crit}\sim\sqrt{b_{\rm Sm}(a_N(T-T_N)/2-b_Ns_b+3c_Ns_b^2/2)}$ and higher temperature T, satisfying the relation $a_{\rm Sm}^2(T-T_{\rm Sm})^2/b_{\rm Sm}=s_b^2(a_N(T-T_N)/2-b_Ns_b+3c_Ns_b^2/2)$, beyond which the N–Sm-A transition is first order, and (b) a triple point, beyond which the N phase no longer is stable and there is a direct I–Sm-A transition [16]. Here $s_b=s_b(T)$ denotes the bulk value of s.

In order to study the structure of a screw dislocation in a Sm-A phase we describe the nematic director in terms of angles $\alpha(\mathbf{r})$ and $\vartheta(\mathbf{r})$ as

$$\mathbf{n}=\mathbf{e}_\rho\cos\alpha\sin\vartheta+\mathbf{e}_\varphi\sin\alpha\sin\vartheta+\mathbf{e}_z\cos\vartheta\ , \tag{2}$$

where $(\mathbf{e}_\rho,\mathbf{e}_\varphi,\mathbf{e}_z)$ denote the unit vector triad of the cylindrical coordinate system (ρ,φ,z).

The existence of the screw dislocation is enforced by the following form for ϕ:

$$\phi(\mathbf{r})=q_0(z-u(\rho))+M\varphi\ , \tag{3}$$

where $u(\mathbf{r})\to0$ as $\rho\to\infty$. Here the winding number M is the integer less than 0 measuring the strength of the screw dislocation whose axis is set along $\mathbf{e}_z$. The minimization of the free energy in terms of these parameters yields five coupled Euler-Lagrange equations for $s(\mathbf{r})$, $\vartheta(\mathbf{r})$, $\alpha(\mathbf{r})$, $u(\mathbf{r})$, and $\epsilon(\mathbf{r})$. We limit our interest to solutions preserving cylindrical symmetry, i.e., the parameters quoted depend solely on coordinate ρ, and for the case $D=0$ in which the Sm-A–N transition is continuous. The resulting set of coupled nonlinear differential equations is solved using standard relaxation techniques [17].

For conventional values of liquid-crystal material and elastic constants in the Sm-A phase ($k_2\sim k_3\gg k_1$), we find two qualitatively different ways in which the frustration along the dislocation core can be relieved. We denote these as the "double-twist" [8,10] (DT) and "classical" (CL) solutions. The spatial variation of variables describing these structures is presented in Figs. 2 and 3 in units of smectic correlation length $\xi_\perp=\sqrt{\gamma_\perp/[2a_{\rm Sm}(T_{\rm Sm}-T)]}$. In these solutions $\alpha(\rho)$ and $u(\rho)$ have constant values: $\alpha(\rho)=\pi/2$ and $u(\rho)=0$.

In the DT structure (see Fig. 2) the Sm-A phase avoids a smectic layer discontinuity by forming a semidefect [18], i.e., the singularity is only in the smectic order parameter; the nematic ordering remains continuous. The core is nematic. Within it the director tends to lie along the disclination axis [$\vartheta(\rho<1)\propto\rho$] and twists in a reverse sense to its sense in the asymptotic (and elastic) limit far from the core: $\mathbf{n}(\rho\gg1)\sim\mathbf{e}_\varphi\sin\vartheta_b+\mathbf{e}_z\cos\vartheta_b$, $\vartheta_b(\rho)=\arctan[M/(q_0\rho)]$, $\alpha_b(\rho)=\pi/2$. This director-field variation is predicted by the analogy with the theory of superconductivity [8]. The extent of nematic fluid surrounding the defect is progressively enhanced with increased winding number M which plays a role similar to the centrifugal force. In the neighborhood of the defect

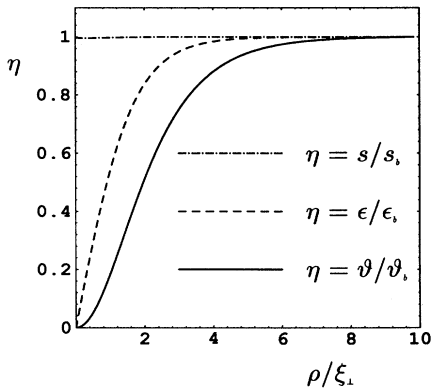

FIG. 2. The normalized ϑ/ϑ_b and order parameter s/s_b, ϵ/ϵ_b spatial variation of the DT solution. ϑ is scaled with respect to ϑ_b to demonstrate departures from the elastic continuum theory solution. In the calculations we set $k_1q_0^2c_N/b_N^2=b_{\rm Sm}c_N^3q_0^2\gamma_\parallel/(c_{\rm Sm}b_N^4)=100$, $b_{\rm Sm}^3c_N^3/(c_{\rm Sm}^2b_N^4)=1$, $\gamma_\perp/\gamma_\parallel=1$, $k_2/k_1=k_3/k_1=30$, $k_\perp/k_1=k_\parallel/k_1=1$, $(T-T_N)/T_N=-0.02$, $T_{\rm Sm}/T_N=0.97$, $c_{\rm Sm}a_{\rm Sm}T_{\rm Sm}/b_{\rm Sm}^2=c_Na_NT_N/b_N^2=50$.

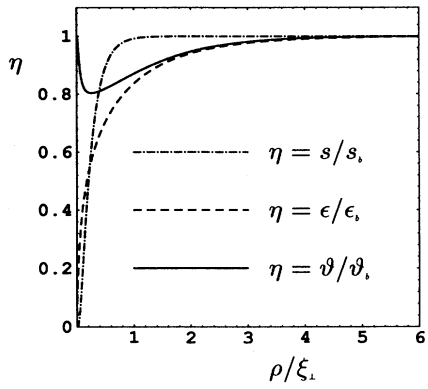

FIG. 3. The spatial dependence of the normalized order parameters ϑ/ϑ_b, s/s_b, ϵ/ϵ_b for the CL solution. The values of material constants and temperature are the same as in Fig. 2.

the smectic order parameter behaves as $\epsilon \propto \rho^M$ and approaches its bulk value ϵ_b as $\delta\epsilon=\epsilon-\epsilon_b \propto -1/(\epsilon_b\rho^4)$. In the CL solution (Fig. 3) the director field is similar to the result [9] of the classical elastic continuum approach, i.e., $\vartheta(\rho)\sim\vartheta_b(\rho)$. In this case the screw dislocation is singular in both the smectic and nematic order parameter (a so-called [18] "full defect"). The core is isotropic, and the core region is an "unescaped" nematic disclination of index 1. This defect is topologically unstable in that the nematic director field can avoid singularity by escape along the screw dislocation axis. Escape can be achieved in a uniaxial [3] way or via intermediate biaxiality [4], which is here not taken into account. Nevertheless, under specific circumstances this solution can be stable in the "physical" sense. To estimate the core radius of the isotropic ($\rho_c^{(i)}$) and nematic liquid ($\rho_c^{(n)}$) surrounding the screw dislocation, we discard the ∇s and $\nabla\epsilon$ terms in Eqs. (1b) and (1d), set $\vartheta(\rho)=\vartheta_b(\rho)$, and define $\rho_c^{(\text{phase})}$ as a maximal value of ρ where the corresponding higher-temperature phase is locally still stable, yielding $\rho_c^{(i)}\sim M^{2/3}(-k_3/(q_0^4(a_N(T-T_N)-2/3b_{\text{Sm}}s_b+c_{\text{Sm}}s_b^2/2)))^{1/6}$, $\rho_c^{(n)}\sim M(\gamma_\perp/(2a_{\text{Sm}}\epsilon_b^2q_0^2))^{1/4}$. For the parameters given in Fig. 2 we get $\rho_c^{(i)}/\xi_\perp\sim 0.3M^{2/3}$ and $\rho_c^{(n)}/\xi_\perp\sim 0.3M$, which is in good agreement with more accurate numerical calculations. Note that $\epsilon_b\to 0$ on approaching the N–Sm-A transition, providing $D<D_{\text{crit}}$. Therefore the value of $\rho_c^{(n)}$ diverges at this temperature. The core radius of the CL solution is apparently smaller than in the DT case. This is because the structure of the CL solution is more consistent with a layered structure; the smectic order in the CL case thus persists closer to the defect axis. The nematic bulk ordering relaxes much more quickly than the smectic ordering. We find $s-s_b \propto -1/\rho^6$, while $\epsilon-\epsilon_b \propto 1/\rho^4$, just as in the case of the DT solution.

We now discuss the stability of the DT and CL defect structures. Under normal circumstances the CL solution is considerably more costly in the nematic free-energy contribution. The isotropic core is highly energetic. But this cost can be substantially reduced near a first-order I–Sm-A phase transition. This can be achieved with strong nematic-smectic order parameter coupling [Eq. (1e)]. In addition, the stability of structures can be considerably influenced by the ratio k_2/k_3 of the twist to bend nematic elastic constant. The nematic free-energy contribution of the DT solution comes almost entirely from the twist contribution, but in the CL case the bend deformation dominates. Therefore for $k_2/k_3>1$ the CL solution is preferred. The CL solution can be also stabilized by a high $\gamma_\perp/\gamma_\parallel$ ratio, which tends to lock nematic molecules perpendicular to smectic layers. Normally, however [2], $\gamma_\perp/\gamma_\parallel<0.2$.

We have also found a solution which breaks the polar symmetry of the system (Fig. 4). In this configuration—the "broken polar" (BP) solution—the smectic layers near the dislocation axis bend significantly out of their asymptotic plane, in which the layer normals are perpendicular to the axis. The core forms a full defect with the director field emerging radially from the disclination axis. However, this configuration is only stable in a rather unphysical regime of the Sm-A phase ($k_2\sim k_1$, $k_3\gg k_1$). For larger k_2/k_1 or smaller k_3/k_1 ratios the region corresponding to $\alpha=0$ rapidly shrinks, ruling out the escape of smectic layers. This structure is stable, however, if $k_\perp/k_\parallel\gg 1$. In this regime it is the existence of a nematic-isotropic interface which favors a radial nematic director.

Finally we have investigated the behavior of the core of the DT solution consisting of a mixture of molecules of opposite chirality. In this case the core may have a composition significantly different from that of the asymptotic regime; the resulting difference may even affect the size of the core itself. To estimate this effect we introduce into the free-energy density expression [Eq. (1)] the entropy term $\rho_0(-kTc_l\ln(c_l)-kTc_r\ln(c_r))$ and add to f_N^{non} [Eq. (1b)] a chiral term $-k_2s^2\gamma(c_l-c_r)\mathbf{n}\cdot\nabla\times\mathbf{n}$. Here the constant γ describes the molecular twisting power, which is assumed to be equal for both conformers and ρ_0 the molecular density. The concentration of left- and right-handed chiral molecules is denoted by c_l, c_r, respectively. The effect is demonstrated in Fig. 5 for the DT

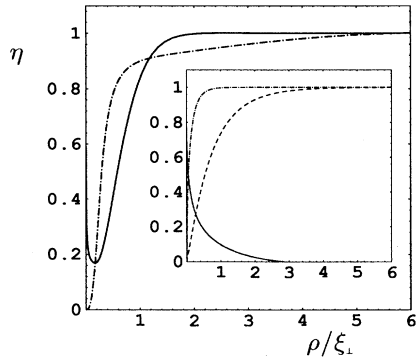

FIG. 4. The spatial dependence of $\eta=\vartheta/\vartheta_b$ (full line) and $\eta=\alpha/\alpha_b$ (dash-dotted line) of the BP solution. In the inset the dependence of $\eta=u(\rho)q_0$ (full line), normalized nematic $\eta=s/s_b$ (dash-dotted line), and smectic order parameter $\eta=\epsilon/\epsilon_b$ (dashed line) is shown. The values of material constants and temperature are the same as in Fig. 2, except $k_2/k_1=1$.

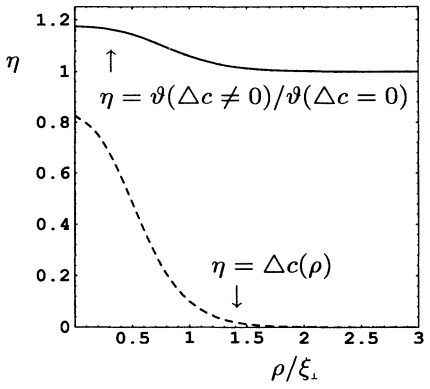

FIG. 5. The effect of the DT structure of the screw dislocation on the concentration profile. The feedback of the $\Delta c(\rho)$ variation on $\vartheta(\rho)$ is also shown. $\Delta c = c_l - c_r$, $\Delta c(\rho \to \infty) = 0$, $k_2 \gamma q_0/(\rho_0 kT) = 10$, $k_{2\gamma}/(k_{1q_0}) = 0.01$. the values of other parameters are the same as in Fig. 2.

solution, in which the twist deformation plays a dominant role. Close to the disclination there is a significant interaction between the twist direction and the concentration of the component with the same molecular chirality. The director-field distortion at the core boundary is enhanced but the core size is not significantly increased in this case.

In conclusion, we have studied the structure of a smectic screw dislocation within Landau–de Gennes theory, taking into account spatial variation of both nematic and smectic order parameters. The major weak point of our model concerns the behavior of $f_{\mathrm{Sm}}^{\mathrm{non}}$ in the presence of a varying nematic order parameter. This term explicitly depends on the director $\mathbf{n}(\mathbf{r})$. However, if $s(\mathbf{r})$ vanishes, $f_{\mathrm{Sm}}^{\mathrm{non}}$ should lose its $\mathbf{n}(\mathbf{r})$ dependence. Unfortunately there seems to be no easy cure for this pathological feature in the model. A better model would have to use the Saupe tensor $Q_{ij} = s/2(3n_i n_j - \delta_{ij})$, but then other problems emerge. We shall return to this problem elsewhere.

For conventional values of material constants in the Sm-A phase we find two possible solutions, both having constant $\alpha(\rho)$ and $u(\rho)$ values. We also find a symmetry-breaking solution, but for values of nematic elastic constants apparently incompatible with the smectic-A phase. In addition, we have studied the case in which the LC is composed of conformers of different chirality. The twist character of the screw dislocation can induce spatial concentration variations of mixture components, which can weakly influence the core structure itself. This effect may play an important role at the cholesteric–Sm-A transition.

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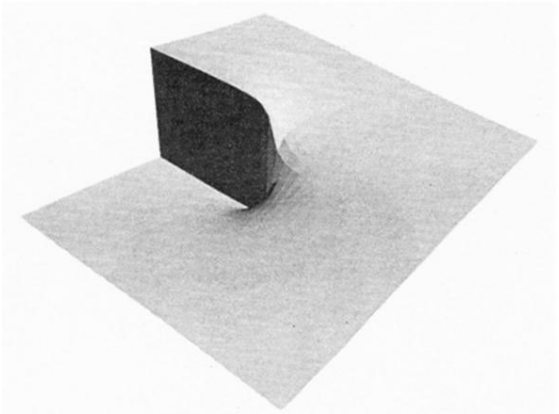

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