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Numerical Simulation of the TGB Phase of Chiral Liquid Crystals

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We numerically minimized the Landau-de Gennes free energy to investigate the layer structure of the twist-grain boundary (TGB) phase of chiral liquid crystals. We compare the obtained structure with Scherk's minimial surface. For large twist angles, an unlocking of the director and the layer orientation reduces the effective layer bending rigidity, which causes a large deviation of the mean curvature from zero. At temperatures close to the TGB-cholesteric transition, we find a melting of the smectic layers in the whole grain boundary.

Keywords: chiral liquid crystal; defect structure; minimal surface; twist-grain-boundary

Chiral liquid crystals exhibit a wide variety of frustrated phases. Frustration between the smectic layer order and helical orientational order causes the TGB phase, in which smectic slabs (grains) of a certain length are separated by planes containing arrays of screw dislocations [1]. Detailed understanding of this one-dimensionally twisted structure is a key step to understand more complex chiral phases, such as the chiral line and the smectic blue. Theoretically, the TGB layer structure is well approximated by Scherk's minimal surface for small twist angles [2]. In this paper, we study the frustration mechanism at larger twist angles, focusing on the local structure of a single grain boundary [3].

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Our method is direct numerical minimization of the Landau-de Gennes free energy,

$$F = F_{D.W.} + F_{int} + F_{Frank}, \tag{1}$$

$$F_{D.W.} = \int d\boldsymbol{r} \frac{g}{4}\left(\frac{\tau}{g} + |\Psi|^2\right)^2, \tag{2}$$

$$F_{int} = \int d\boldsymbol{r} \frac{B}{2}|(\nabla - iq_0\boldsymbol{n})\Psi|^2, \tag{3}$$

$$F_{Frank} = \int d\boldsymbol{r}\left\{\frac{K_1}{2}(\nabla\cdot\boldsymbol{n})^2 + \frac{K_2}{2}(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n} - k_0)^2 + \frac{K_3}{2}(\boldsymbol{n}\times\nabla\times\boldsymbol{n})^2\right\}. \tag{4}$$

Here Ψ is the complex order parameter and $\boldsymbol{n}$ is the director, with the layer compression modulus B and the Frank elastic constants K_i. We simulated one grain boundary with two adjacent smectic slabs, which are twisted by an angle α from each other. In this geometry we can exploit the 2D crystalline symmetry of the two slabs, and impose the periodic boundary condition in the plane perpendicular to the twist axis. We use the parameter set $\tau = -0.02$, $g = 1.0$, $B = 0.2$ and $K_1 = K_2 = K_3 = 0.002$ unless otherwise stated. Then the Ginzburg parameter κ equals $1.80 > 1/\sqrt{2}$, and the TGB phase is stable according to the mean field theory [1]. The box boundaries in the direction along the twist axis are connected by reflection so that the two smectic slabs are tilted by $\pm\alpha/2$ from the horizontal plane. The chirality k_0 is obtained as a function of α as we minimize the free energy.

The resultant layer structure, as shown in Figure 1, is compared with Scherk's minimal surface. The deviation from the minimal surface is measured by squared mean curvature of the layers, averaged over the sample $\langle H^2\rangle$. The deviation grows faster than linearly as a function of the twist angle. This significant deviation is found to originate from an unlocking of the layer normal from the director. To see this, we decompose the coupling energy F_{int} as follows.

$$F_{int} = \frac{B}{2}\int d\boldsymbol{r}|i\nabla|\Psi| - |\Psi||\nabla\Phi|(\boldsymbol{m} - \boldsymbol{n}) - |\Psi|(|\nabla\Phi| - q_0)\boldsymbol{n}|^2, \tag{5}$$

Here Φ is the phase of Ψ and $\boldsymbol{m} = \nabla\Phi/|\nabla\Phi|$ is the layer normal. The second term in the integrand gives what we shall call the locking free energy, $f_\ell \propto |\boldsymbol{m} - \boldsymbol{n}|^2$, while the third term gives a layer compression energy $f_c \propto |\nabla\Phi - q_0|^2$. The twist-angle dependence of f_ℓ can be estimated by treating it as a small perturbation. If it is small, the smectic

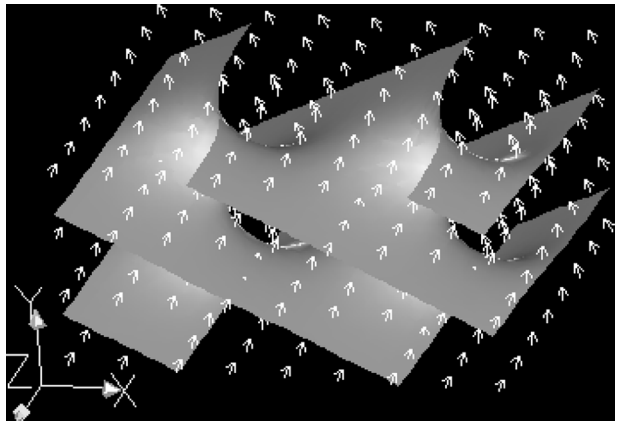

FIGURE 1 Snapshot of the TGB layer structure at $\alpha = 50^{\circ}$. Shown are the isosurface $\mathrm{Re}(\Psi) = 0$ and the director in arrows.

slabs are discontinuously twisted at the center of the grain boundary, while the director is twisted continuously. Then the angle between $\boldsymbol{m}$ and $\boldsymbol{n}$ reaches $\pm\alpha/2$ near the grain boundary center, leading to the estimate $f_\ell \propto \cos^2(\alpha/2)$. On the other hand, the layer width at the grain boundary center is dilated by a factor of $1/\cos(\alpha/2)$, which gives the estimate of the compression term $f_c \propto (\cos(\alpha/2) - 1)^2$. The ratio between these geometric factors are shown in Figure 2. For small twist

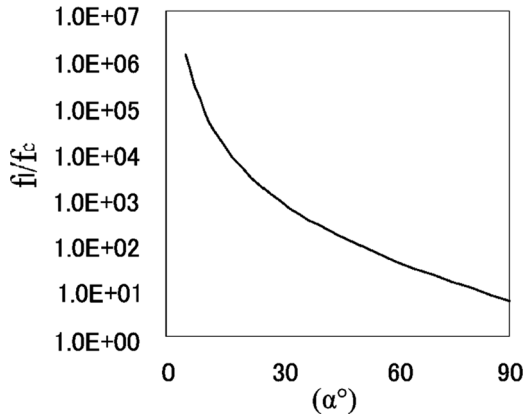

FIGURE 2 Twist angle dependence of the ratio between the locking and layer compression terms, $f_\ell/f_c \simeq \{\cos(\alpha/2)/(\cos(\alpha/2) - 1)\}^2$, estimated at the center of the grain boundary (see text).

angles, the locking term is dominant over the layer compression term, and $\boldsymbol{m}$ is close to $\boldsymbol{n}$. This converts the splay term of the Frank energy into effective layer bending energy. As the twist angle grows, on the other hand, the locking term becomes comparable to the layer compression term. As a result, the average angle between $\boldsymbol{m}$ and $\boldsymbol{n}$ increased and reached as much as 20° at $\alpha = 90^\circ$. This unlocking reduces the effective layer bending rigidity and causes a large mean curvature.

To confirm this, we investigated the following two cases. First, we turn off the Frank elasticity and confirmed that the variance of the

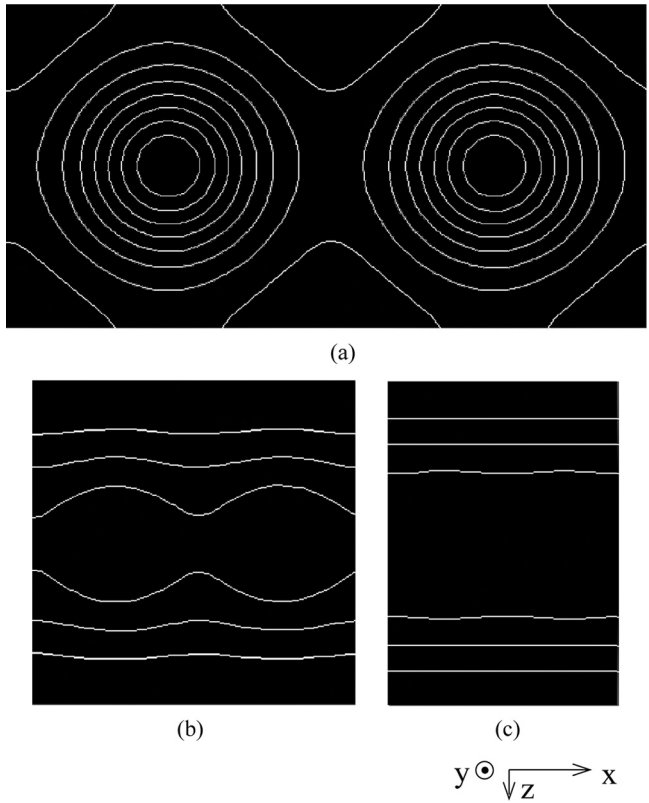

FIGURE 3 Plots of renormalized smectic modulation $|\Psi/\Psi_0|^2$ in the plane perpendicular to the screw dislocations at (a) $\alpha = 30^\circ$, (b) $\alpha = 60^\circ$ and (c) $\alpha = 90^\circ$ near the TGB-cholesteric transition $\tau = -0.005$, where $\Psi_0 = \sqrt{|\tau|/g}$. Here, we set y- and z-axis along the screw dislocation and twist axis respectively, and the contour lines are drawn at $|\Psi/\Psi_0|^2 = 0.1, 0.2, \ldots, 1.0$. The smectic layer melts not only at the defect core but at the whole grain boundary.

mean curvature $\langle H^2 \rangle$ increases by five times. Second, an extra locking term $D(\boldsymbol{m} - \boldsymbol{n})^2$ is added to the Landau-de Gennes free energy density. As we increase D, the variance of $\langle H^2 \rangle$ decreased faster than $\langle (\boldsymbol{m} - \boldsymbol{n})^2 \rangle$, which shows that the locking surely contributes to the effective bending rigidity.

We also study the temperature dependence of the grain boundary structure. At high temperature close to the TGB-cholesteric transition and for large twist angles, the smectic order melts in the whole grain boundary, not only near the dislocation cores (see Fig. 3).

In summary, we simulated the TGB phase of chiral liquid crystals by numerically minimizing the Landau-de Gennes free energy. For small twist angles, the layer structure is close to Scherk's minimal surface, in agreement with the previous analysis [2]. For large twist angles, the layer structure strongly deviates from the minimal surface because of the unlocking of the director and the layer orientation, which reduces the effective layer bending rigidity. The layer structure also melts at temperatures close to the TGB-cholesteric transition.

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