Mol. Cryst. Liq. Cryst., 1997, Vol. 299, pp. 301–306
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DISCLINATION LOOP IN MORI-NAKANISHI ANSATZ: ROLE OF THE DIVERGENCE ELASTICITY

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Abstract Energetic stability of loop defects in nematic liquid crystal is analyzed using Mori-Nakanishi ansatz and Frank-Oseen theory with non-zero K_{24} divergence term. The ratio of the bulk and divergence elastic constants defines a characteristic material length, which is the equilibrium radius a^* of the disclination ring. Positive K_{24} forces the ring to shrink.

Nematic liquid crystals show a rich variety of defects, including point ("hedgehog" or "monopole") and line ("disclination") singularities[1]. Important peculiarities of nematic defects are brought about by the identity $-\mathbf{n} \equiv \mathbf{n}$; $\mathbf{n}$ is the director that describes molecular orientation. The identity makes it topologically possible for a monopole to transform into a disclination ring of strength 1/2[2–7]. For a large volume the stability of the hedgehog vs. loop should be defined by intrinsic nematic parameters such as Frank elastic constants.

Mori and Nakanishi[2] considered how the hedgehog vs. loop stability depends on the splay and bend elastic constants. In this article we analyze how their results would be modified by the divergence elastic term K_{24}. Although the K_{24} term does not change the bulk equilibrium equations, it has to be taken into account when there are topological changes, such as transformation of the spherical-like core of the hedgehog into a torus-like core of the disclination ring with a macroscopic radius much larger than the nematic coherence length ξ.

The Frank-Oseen free elastic energy density[8]

$$f = \frac{1}{2}K\left((div\mathbf{n})^2 + (curl\mathbf{n})^2\right) + K_{13}\nabla(\mathbf{n}\,div\mathbf{n}) - K_{24}\nabla(\mathbf{n}\,div\mathbf{n} + [\mathbf{n}\times curl\mathbf{n}]) \quad (1)$$

contains the standard contribution with elastic constant K (represented here in the one-constant approximation[1]) as well as two divergence terms with constants K_{13} and K_{24}. We consider only K_{24} term, assuming $K_{13} = 0$.

The status of the K_{24} term as compared to that of the bulk K terms can be illustrated with an equilibrium radial hedgehog, $\mathbf{n} = \hat{\mathbf{r}}$ in spherical coordinates. To calculate the energy of the hedgehog, one needs to integrate f over $r_c \leq r \leq R$, where $R \gg \xi$ is the radius of the system and $r_c \sim \xi$ is the core radius of the defect; in the core, f does not represent the true energy density. Both K and K_{24} contributions to the hedgehog's energy are linear in R:

$$F_h = 8\pi(R - r_c)(K - K_{24}) + E_{c,h}{r_c}^3; \tag{2}$$

here $E_{c,h} \sim \tilde{K}/\xi^2$ is the hedgehog's core energy density with some effective elastic constant $\tilde{K} \sim K$. The r_c-terms are negligible as against R-terms. Eq.(2) shows that K_{24} should profoundly influence the stability of defects. The mechanism can be illustrated by differential geometry theorems[9]. If $\mathbf{n}$ is normal to a family of surfaces S, then the K_{24} distortion is nothing else but twice the Gauss curvature G of S ($G = \sigma_1\sigma_2$, where σ_1 and σ_2 are the two principal curvatures)[9]:

$$\nabla(\mathbf{n}\,div\mathbf{n} + [\mathbf{n} \times curl\mathbf{n}]) \equiv 2G. \tag{3}$$

For the radial hedgehog $G = 1/r^2$, and one immediately obtains the K_{24} energy in Eq.(2). The appearance of a loop would mean that G in the region enclosed by the loop is reduced. For example, $G = 0$ on the equatorial disc of radius a. The difference in elastic energy between the ring and the hedgehog would be $\sim aK_{24}$, forcing the ring to expand if $K_{24} < 0$, and to shrink if $K_{24} > 0$.

For the quantitative consideration, we follow the Mori-Nakanishi ansatz[2] of the disclination loop: $\mathbf{n} = (1, 0, 0)$ in ellipsoidal coordinates $(\hat{\sigma}, \hat{\tau}, \hat{\phi})$ connected to the Cartesian ones by $x^2 = a^2(1+\sigma^2)(1-\tau^2)\cos^2\phi$; $y^2 = a^2(1+\sigma^2)(1-\tau^2)\sin^2\phi$; $z = a\sigma\tau$. The ansatz asymptotically satisfies boundary conditions $\mathbf{n} = \hat{\mathbf{r}}$ and the equilibrium condition $\nabla^2\mathbf{n} = 0$ as $R \to \infty$. The limit $a = 0$ is the radial hedgehog which satisfies exactly the two conditions above. With $a \neq 0$, the ansatz describes a circular wedge loop of radius a with $\mathbf{n}$ perpendicular to the surface of the oblate ellipsoids of revolution (Fig.1). Since with $a \neq 0$ the ansatz satisfies the equilibrium condition only asymptotically, the corresponding energy F_{loop} represents the upper limit of minimum energy of the loop[2].

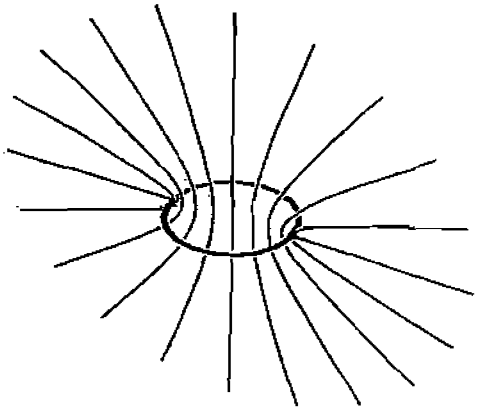

Fig.1 Loop of disclination 1/2

To find the equilibrium radius a^* of the loop, one has to find the integral F_{loop} of f and then minimize it. The volume of integration should not include the torus-like core of the loop with meridional radius $\sim r_c$, where deformations are large. The excluded volume can be chosen as[2] $0 \leq \sigma \leq p, 0 \leq |\tau| \leq q$, where $p = \sqrt{2r_c/a + r_c^2/a^2}$ and $q = \sqrt{2r_c/a - r_c^2/a^2}$. Any other geometry of the core cross-section changes the energy by $\sim r_c\tilde{K}$, which is negligible in comparison with terms $\sim a\tilde{K}$ and $R\tilde{K}$, when $a \gg r_c$; the last inequality sets the limit of validity of our consideration.

We first obtain the energy F_{24} caused by the divergence term:

$$F_{24} = -8\pi K_{24}R + 4\pi a K_{24}[\frac{\pi}{2} + pq - q^2\frac{\pi}{2} + (p^2 + q^2)\tan^{-1}\frac{q}{p}]. \tag{4}$$

As it was expected, the core p, q-terms bring only small corrections $r_c K_{24}$. The leading terms $(-8\pi K_{24}R)$ and $2\pi^2 a K_{24}$ are core-profile-independent and do not vanish even when $r_c/a \to 0$, their origin being purely topological, as discussed above. Of course, this topological argument holds only for $a \gg \xi$ when the region inside the ring is composed of uniaxial nematic phase.

The total energy F_{loop} of the loop includes also the K-term and the core energy $\sim 2\pi a\mathcal{E}_{c,l}$ where $\mathcal{E}_{c,l} = E_{c,l}\xi^2/K$. In the limit $r_c/a \to 0$,

$$F_{loop} = 8\pi R(K - K_{24}) + 2\pi^2 a K_{24} + \frac{\pi^2}{2}aK[\ln(\frac{a}{2r_c}) - 5 + 4\mathcal{E}_{c,l}/\pi]. \tag{5}$$

Within the framework of Frank-Oseen theory, r_c should be estimated as $r_c \sim \xi$ and its scaled energy as $\mathcal{E}_{c,l} \sim 1$[1]. The same order of $\mathcal{E}_{c,l}$ follows from the models of biaxial core, where r_c is larger but $E_{c,l}$ is smaller[3,10,11]. Note that the usual bulk terms produce divergent factors such as $K \ln(a/r_c)$. In contrast, K_{24} integrals bring no divergence, Eq.(4); the same behavior was found for smectic focal conic defects[12]. This peculiarity brings rather strong exponential dependence of the loop radius on the ratio of elastic constants. Minimization of F_{loop} gives

$$a^* = 2r_c \exp\left[4 - 4K_{24}/K - 4\mathcal{E}_{c,l}/\pi\right] \approx 30\xi \exp[-4K_{24}/K]. \tag{6}$$

This value of a^* would be modified by the inclusion of different values of splay K_{11} and bend K_{33} elastic constants. In the first approximation of small anisotoropy $\alpha = (K_{11} - K_{33})/(K_{11} + K_{33})$ the factor is $\exp(1+\alpha)$, and thus $K_{33} > K_{11}$ favors a larger loop.

As recent experiments[13–15] and molecular theories[16] suggest, K_{24} can be of the order of K. According to the Ericksen's stability criteria, K_{24} should be positive[17]. Therefore the appearance of the loop instead of the radial hedgehog increases the elastic energy. We conclude that with positive K_{24}, the macroscopic loop is unlikely to be stable as against a radial hedgehog: in Eq.(6), the radius of the loop is the order of few tens of ξ when $K_{24} = 0$, but quickly decreases to $a^* \sim \xi$ when $K_{24} \to K$. Of course, for $a^* \sim \xi$ the Frank-Oseen approach gives only indicative results; a rigorous treatment should include the gradients of the degree of order and possibility of biaxial regions at the defect core.

The situation can be different for hyperbolic hedgehogs, $\mathbf{n} = (-x/r, -y/r, z/r)$, $r = \sqrt{x^2+y^2+z^2}$. It is easy to see that the elastic energy of the hyperbolic hedgehog contains K_{24} term with a sign opposite to that of radial hedgehogs:

$$F_{hh} = 8\pi R\left(\frac{K}{3} + \frac{K_{24}}{3}\right) + E_{c,hh} r_{c,h}^3. \tag{7}$$

The difference in the sign of the K_{24} term is because of predominantly negative Gaussian curvature of surfaces normal to $\mathbf{n}$; for the radial hedgehog these surfaces are spheres with a positive curvature. Transformation of the hyperbolic hedgehog into a loop of $m = -1/2$ and radius a should decrease the energy by a quantity $\sim aK_{24}$. Therefore, the increase of a positive constant K_{24} would increase the radius of the loop, $a^* \sim \mu\xi \exp(\lambda K_{24}/K)$; here $\mu \sim 10$ and $\lambda \sim 1$ are the two positive numerical coefficients with values that can be determined within the Frank-Oseen approach.

In summary, using the Mori-Nakanishi ansatz, we have shown that the saddle-splay elastic term in Frank-Oseen theory with a positive elastic constant K_{24} should force a loop $m = 1/2$ and large macroscopic radius (shown in Fig.1) to shrink into a radial-like structure with a microscopic core.

ACKNOWLEDGEMENTS

We benefit from the discussion with V.M. Pergamenshchik, T.J. Sluckin, J. Toner, H. Toyoki and H.R. Trebin. O.D.L. thanks NSF ALSOM Center for support under grant DMR-20147 as well as the organizers of the program "Topological Defects" at the Isaac Newton Institute for Mathematical Science for hospitality. E.M.T's research has been supported by Unilever PLC.

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