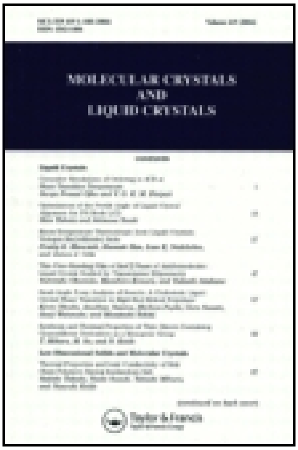

Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Annihilation Dynamics of the Disclination Loop in Bulk Nematic Liquid Crystals

M. A. Shahzamanian [a] & E. Kadivar [a]

[a] Department of Physics, Faculty of Sciences, University of Isfahan, Isfahan, Iran

Version of record first published: 31 Jan 2007

Mol. Cryst. Liq. Cryst., Vol. 457, pp. 83–91, 2006

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400500447280

Annihilation Dynamics of the Disclination Loop in Bulk Nematic Liquid Crystals

M. A. Shahzamanian
E. Kadivar
Department of Physics, Faculty of Sciences, University of Isfahan, Isfahan, Iran

We investigate the annihilation dynamics of the disclination loop in bulk nematic liquid crystals. This work is based on the Frank free energy and the nematodynamics equations. The dissipation of energy is calculated by two methods. In the first method, the dissipation of energy is obtained from the Frank free energy. In the second method, it is calculated by the nematodynamics equations. Finally, we obtain the equation of motion and annihilation velocity of the disclination loop.

Keywords: annihilation velocity; disclination loop; dissipation of energy; nematic liquid crystal

1. INTRODUCTION

The research of defects in order parameter fields corresponding to various condensed matter systems is driven by many motivations. Defects can be readily observed, either directly (e.g., by optical methods) or through other physical properties of the system that are crucially modified in the presence of defects. In many cases, defect-free structures are required, whereas in the others (e.g., in some liquid crystal displays), structures containing defects might be essential. In the latter cases, one must know something about the static or dynamic properties of defects. Theoretically, defects offer a rich playground for mathematically oriented excursions. Their topological properties can be very interesting and nontrivial, if only the order parameter has enough degrees of freedom. Defects play a decisive role in any phase transition, because in the late stages the ordering is governed

Address correspondence to E. Kadivar, Department of Physics, Faculty of Sciences, University of Isfahan, 81744 Isfahan, Iran. E-mail: e_kadivar@yahoo.com

exclusively by the dynamics of the defects created at the transition [1,2]. An important part of the motivation arises from the universality of defects; that is, they can occur in any system with a rich-enough order parameter. Their major properties are independent of the underlying physics, determined solely by symmetries and dimensionalities of the order parameter, the defect, and the system. Lately the aim toward the exploitation of this universality has motivated the research of laboratory-friendly condensed matter systems such as liquid crystals to yield knowledge in completely different realms of physics (e.g., the physics of the universe, elementary particles, and fields) [3,4].

To our knowledge, there have been only a few papers published on defect dynamics, including hydrodynamics. The effects of hydrodynamic flow on the kinetic of nematic–isotropic transition has been studied by Fukuda [5]. A similar topic, with a different method, the lattice Boltzmann algorithm, has been studied by Denniston *et al.* [6]. The hydrodynamics of topological defects have been studied by Toth *et al.* [7]. They studied the effect of backflow and elastic anisotropy on the pair annihilation of straight line defects with strengths of $\pm 1/2$, again using the lattice Boltzmann algorithm. Their treatment, however, is not based on the Ericksen–Leslie theory and involves only two viscous coefficients. The disclination dynamics in confined nematic liquid crystal has been studied by us [8]. We calculated an annihilation velocity of two parallel disclination lines with strengths of $\pm 1/2$ in the confined state.

The aim of our article is to present the solution to the disclination loop dynamics with strength m. In the first stage, we use the cylindrical polar coordinates for the Frank free energy. In section 2, the dissipation of energy is calculated from the Frank free energy. Another way to calculate dissipation of energy is nematodynamics equations. By this way, we calculate the dissipation of energy again. By using the two calculated dissipation of energies, we derive the annihilation velocity and the equation of motion.

2. DIRECTOR FIELD

Consider a disclination loop with a radius R, which lies in x–y plane. We use the coordinate frame which rests the center of loop. It is noted that in the annihilation dynamics of the disclination loop, the radius of the disclination loop is the function of time. We restrict our attention to the planar configuration. Consequently, the director field lies in planes parallel to the disclination loop. The elastic distortion is confined in the region inside the disclination loop. We call $\theta(r)$ the angle between the director field, n, and the y axis. This angle is a function of x', y', and z'. Far from the disclination loop, $\mathbf{n}$ is uniformly oriented along the y axis. Hence we may write the director field as

$$\mathbf{n} = (\sin\theta, \cos\theta, 0). \tag{2.1}$$

To keep our calculation as simple as possible, we will use the cylindrical polar coordinates (ρ, ϕ, z). In this coordinate, the director field may be written as

$$\mathbf{n} = (\sin(\theta + \phi), \cos(\theta + \phi), 0). \tag{2.2}$$

The energy of slowly varying spatial distortions of the director $\mathbf{n(r)}$ is determined by the Frank free energy [9]:

$$\mathcal{F} = \frac{1}{2}\int \left[K_1(\nabla\cdot n)^2 + K_2(n\cdot\nabla\times n)^2 + K_3(n\times\nabla\times n)^2\right]d^3r, \tag{2.3}$$

where K_1, K_2, and K_3 are the splay, twist, and bend elastic constants respectively. By inserting Equation(2.2) into Equation(2.3), we obtain

$$\mathcal{F} = \frac{1}{2}\int \Bigg[K_1\cos^2(\theta+\phi)\left(\frac{\partial\theta}{\partial\rho}\right)^2 + K_2\cos^2(2\theta+2\phi)\left(\frac{\partial\theta}{\partial z}\right)^2 + K_3\sin^2(\theta+\phi)\left(\frac{\partial\theta}{\partial\rho}\right)^2 + K_3\sin^2(2\theta+2\phi)\left(\frac{\partial\theta}{\partial z}\right)^2\Bigg]\rho\, d\rho\, d\phi\, dz. \tag{2.4}$$

To keep our calculation as simple as possible, we use the one-constant approximation, $K_1 = K_2 = K_3 = K$, of the Frank free energy:

$$\mathcal{F} = \frac{K}{2}\int \left[\left(\frac{\partial\theta}{\partial\rho}\right)^2 + \left(\frac{\partial\theta}{\partial z}\right)^2\right]\rho\, d\rho\, d\phi\, dz. \tag{2.5}$$

We can find θ by minimizing the Frank free energy. By using the Euler–Lagrange equations, we get

$$\frac{\partial^2\theta}{\partial\rho^2} + \frac{\partial^2\theta}{\partial z^2} = 0. \tag{2.6}$$

The director field inside and outside the disclination loop can be obtained from this equation by applying the boundary condition. As we already mentioned, the boundary condition is defined: far form disclination loop the director field must be along the y axis [i.e., $\mathbf{n}(\mathbf{r}) \rightarrow (0,1,0)$ as $\rho \rightarrow \infty$].

Hence, the solution of Equation (2.6) is

$$\theta = m \ \arctan\left(\frac{z}{R-\rho}\right), \tag{2.7}$$

where m is topological charge or strength. This angle, $\theta(r)$, has the following properties:

1. $\theta(r)$ satisfies Equation (2.6) and is regular except on the loop.
2. $\theta(r)$ does not diverge far from the loop.
3. $\theta(r)$ increases by $2\pi m$ if, starting from point $\mathbf{r}$, we make one turn around the line of loop and come back to $\mathbf{r}$.

By inserting Equation (2.7) into Equation (2.5) and doing some straightforward calculations, we get

$$\mathcal{F} = \frac{m^2 K}{2} \int_{-\infty}^{\infty} dz \int_0^{2\pi} d\phi \int_a^{R-a} \frac{\rho \, d\rho}{(R-\rho)^2 + z^2}, \tag{2.8}$$

where a is the core radius of disclination loop. By performing the integrals in this equation, we obtain the total Frank free energy:

$$\mathcal{F} = \pi^2 m^2 K \left[R \ln\left(\frac{R-a}{a}\right) + 2a - R \right]. \tag{2.9}$$

The core radius, a, is order angstrom, and the radius of disclination loop is order micrometer. In the case $R \gg a$, we can neglect the second term in Equation (2.9):

$$\mathcal{F} \approx \pi^2 m^2 K \left[R \ln\left(\frac{R}{ea}\right) \right], \tag{2.10}$$

where e is the Napierian number.

This result is consistence with the de Gennes *et al*. result. They obtained the Frank free energy by another method. They supposed that this problem has a similar problem in electromagnetics. They interpreted $\nabla\theta(r)$ as the magnetic field due to a current loop. By using the magnetic energy, the distortion energy was obtained [10].

For an isothermal process, the dissipation of energy, $T\dot{S}$, is equal to the decrease in stored the Frank free energy [9]:

$$T\dot{S} = -\frac{d\mathcal{F}}{dt}. \tag{2.11}$$

As we mentioned previously, in disclination loop dynamics, R is the function of time. So, the annihilation velocity of disclination loop is along $\mathbf{u}_\rho$, where $\mathbf{u}_\rho$ is the unit vector along the ρ axis in the cylindrical polar coordinates. By using the Eulerian equation, we get

$$\frac{d\mathcal{F}}{dt} = \frac{\partial \mathcal{F}}{\partial t} + \frac{dR}{dt}\mathbf{u}_\rho \cdot \nabla \mathcal{F}. \tag{2.12}$$

The first term of this equation is zero. By performing some straightforward calculations, the dissipation of energy is obtained:

$$T\dot{S} = -\pi^2 m^2 K \ln\left(\frac{R}{a}\right)\frac{dR}{dt}. \tag{2.13}$$

On the other hand, the driving force, F_d, will be obtained from the Frank free energy:

$$F_d = -\frac{d\mathcal{F}}{dR}. \tag{2.14}$$

Hence, the driving force acting on the disclination loop is equal to

$$F_d = -\pi^2 m^2 K \ln\left(\frac{R}{a}\right). \tag{2.15}$$

It is noted that this force is an attractive force and a function of time.

3. SECOND ANSATZ FOR THE ENTROPY SOURCE

We intend to calculate the dissipation of energy another way. It is convenient at this stage to write the dissipation of energy by using nematodynamics equations. In the absence of fluid flow, $\mathbf{V} = 0$, the dissipation of energy that is created by the rotation of the director in nematic liquid crystal may written as [9]

$$T\dot{S} = \int \mathbf{h} \cdot \mathbf{N} d^3 r. \tag{3.1}$$

Dissipation of energy has another term that relates to the dissipation by shear flow. This term is zero in the absence of fluid flow.

In Equation (3.1) h and N are defined as follows: the molecular field, $\mathbf{h}$, may written as

$$h_\mu = \gamma_2 n_\alpha A_{\alpha\mu} + \gamma_1 N_\mu, \tag{3.2}$$

together with the relations

$$A_{\alpha\beta} = \frac{1}{2}\left[\frac{\partial V_\beta}{\partial x_a} + \frac{\partial V_\alpha}{\partial x_\beta}\right], \tag{3.3}$$

$$\gamma_1 = \alpha_3 - \alpha_2, \tag{3.4}$$

$$\gamma_2 = \alpha_2 + \alpha_3 = \alpha_6 - \alpha_5, \tag{3.5}$$

and the rate of change of the director with respect to the background fluid, $\mathbf{N}$, may written as [9]

$$\mathbf{N} = \dot{\mathbf{n}} - \omega \times \mathbf{n} \tag{3.6}$$

where $\omega = \frac{1}{2}\nabla \times V$ and $\dot{\mathbf{n}} = \frac{dn}{dt}$.

The coefficients α_i are usually called the Leslie coefficients [9].

In the absence of fluid flow, the second term of Equation (3.6) is zero. By inserting Equations (2.2) and (2.7) into (3.6), we get

$$\mathbf{N} = m\left[\cos(\theta + \phi)\mathbf{u}_\rho - \sin(\theta + \phi)\mathbf{u}_\phi\right]\frac{z}{(R-\rho)^2 + z^2}\frac{dR}{dt}, \tag{3.7}$$

where $\mathbf{u}_\rho$ and $\mathbf{u}_\phi$ are unit vectors in the cylindrical polar coordinates. In the absence of fluid flow, the first term in Equation (3.2) is zero and the molecular field, $\mathbf{h}$, is obtained by inserting Equation (3.7) into Equation (3.2).

By substituting the expressions of $\mathbf{h}$ and $\mathbf{N}$ into Equation (3.1), we have

$$T\dot{S} = m^2\gamma_1\left(\frac{dR}{dt}\right)^2 \int_{-\infty}^{\infty} dz \int_0^{2\pi} d\phi \int_a^{R-a} \frac{z^2 \rho d\rho}{\left[(R-\rho)^2 + z^2\right]^{2.}}. \tag{3.8}$$

By performing the integrals in this equation, we obtain

$$T\dot{S} = m^2\pi^2\gamma_1\left(\frac{dR}{dt}\right)^2\left[R\ \ln\left(\frac{R-a}{a}\right) + 2a - R\right]. \tag{3.9}$$

In the case $R \gg a$, we can neglect the second term in this equation, and the dissipation of energy is equal to

$$T\dot{S} = m^2\pi^2\gamma_1\left(\frac{dR}{dt}\right)^2\left[R\ \ln\left(\frac{R}{a}\right) - R\right]. \tag{3.10}$$

4. EQUATION OF MOTION

Annihilation velocity of the disclination loop can be obtained by using Equations (2.13) and (3.10):

$$V_{ann} = \frac{dR}{dt} = \frac{-K}{\gamma_1} \frac{\ln(R/a)}{[R\ \ln(R/a) - R]}. \tag{4.1}$$

The negative sign indicates the loop tends to shrink and disappear. This velocity, hence, is called *annihilation velocity*. This relation describes the annihilation velocity with respect to the radius of disclination loop. The annihilation velocity is increasing with decreasing radius of the disclination loop. Figure 1 shows the annihilation velocity V_{ann} versus the radius of disclination loop R for nematic liquid crystal 5CB (pentylcyanobiphenyl). The constant parameters of this material are $K = 4.37 \times 10^{-12} N$ [11], $a = 10\,\text{nm}$ [12], $\alpha_6 = 0.184$ p, $\alpha_5 = 0.624$ p [13], and $\gamma = \gamma_2/\gamma_1 = 1$ [14].

By performing the integrals in this equation, we obtain the equation of motion for annihilation dynamics of the disclination loop:

$$R^2 \approx R_0^2 - \frac{2K}{\gamma_1} t, \tag{4.2}$$

where R_0 in Equation (4.2) is the initial radius of the disclination loop at $t = 0$. It is noted that we have ignored the term with a^2 coefficient in Equation (4.2). The total annihilation time is almost equal to $t = \gamma_1 R_0^2/2K$, which depends on the constant parameters of liquid crystal. In Figure 2, the radius of disclination loop $R(t)$ is drawn versus the annihilation time t.

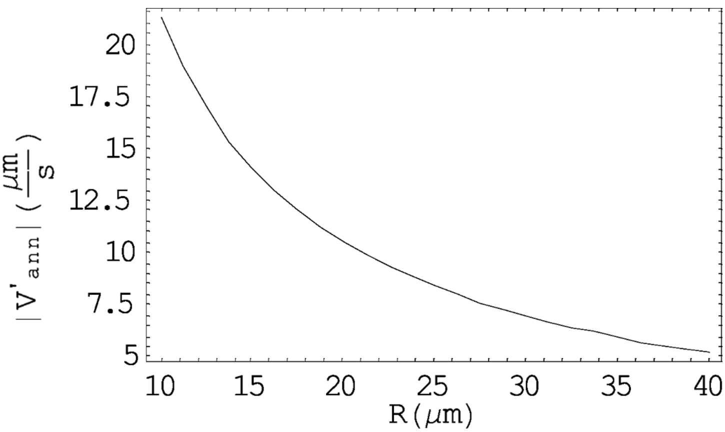

FIGURE 1 Annihilation velocity V_{ann} versus the radius of disclination loop R.

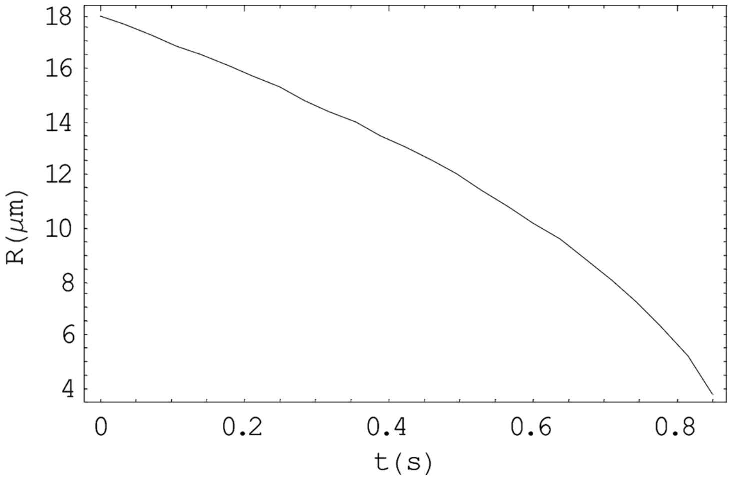

FIGURE 2 Radius of disclination loop R versus the annihilation time for $R_O = 18\,\mu m$.

By differentiating the equation of motion, Equation (4.2), with respect to time t we can find the annihilation velocity versus the annihilation time:

$$V_{ann} \approx \frac{-K}{\gamma_1 [R_0^2 - (2K/\gamma_1)t]^{1/2}}. \tag{4.3}$$

It is noted that in bulk nematic liquid crystals, the annihilation velocity of the disclination loop and equation of motion are independent of the topological charge m, whereas the driving and viscous forces depend on it.

5. CONCLUSION

The equations of motion describing hydrodynamics of defects in nematic liquid crystals are complex. The Frank free energy is one of the ways to investigate the annihilation dynamics of the disclination loop. By taking the cylindrical polar coordinates, the Frank free energy is calculated. The director field is obtained by minimizing the Frank free energy. This director field indicates discontinuity on the loop in nematic liquid crystals, whereas the radius of the loop is a function of time. The dissipation of energy is calculated from the Frank free energy. We also obtain the driving force acting on the disclination loop. The dissipation of energy and driving force depend on topological charge. By another way, nematodynamics equations, the dissipation of energy is obtained again. The annihilation velocity is calculated from the two calculated dissipation of energies. The negative sign of annihilation velocity shows that the loop tends to shrink and disappear. The annihilation velocity is increasing with decreasing the radius of disclination loop. We also find the radius of disclination loop follows a square-root time law. The annihilation velocity and equation of motion are independent of the topological charge in bulk nematic liquid crystals.

REFERENCES

[1] Blatter, G. (1994). *Rev. Mod. Phys.*, *66*, 1125.
[2] Renn, S. & Lubensky, T. (1988). *Phys. Rev. A.*, *38*, 2132.
[3] Zurek, W. H. (1985). *Nature (London)*, *317*, 505.
[4] Pismen, L. M. (1999). *Vortices in Nonlinear Fields*, Clarendon Press: Oxford.
[5] Fukuda, J. I. (1998). *Eur. Phys. J. B.*, *1*, 173.
[6] Denniston, C., Orlandini, E., & Yeomans, J. M. (2001). *Phys. Rev. E*, *63*, 056702.
[7] Tóth, G., Denniston, C., & Yeomans, J. M. (2002). *Phys. Rev. Lett.*, *88*, 105504.
[8] Shahzamanian, M. A. & Kadivar, E. (Unpublished).
[9] de Gennes, P. G. & Prost, J. (1995). *The Physics of Liquid Crystals*, Clarendon Press: Oxford.
[10] Friedel, J. & de Gennes, P. G. (1969). *C. R. Acad. Sci. Paris*, *258*, 257.
[11] Tóth, G., Denniston, C., & Yeomans, J. M. (2002). *Phys. Rev. Lett.*, *88*, 105504.
[12] Bogi, A., Martinot-Lagarde, P., Dozov, I., & Nobili, M. (2002). *Phys. Rev. Lett.*, *89*, 225501.
[13] Stark, H. (2001). *Physics Reports*, *351*, 387.
[14] Ryskin, G. & Kremenetsky, M. (1991). *Phys. Rev. Lett.*, *67*, 1574.