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DYNAMICS OF ANNIHILATION PROCESS OF DISCLINATION PAIRS IN NEMATIC LIQUID CRYSTALS

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Abstract We investigated the dynamics of annihilation process of a defect pair in the nematic phase which were generated as type-1 wedge disclinations by quenching the isotropic phase. We measured the time dependence of the distance between a defect pair with or without external electric field. The distance decreased linearly with time immediately after the defect pair was generated (the early stage) and then decreased to zero in proportion to the square root of the time to elapse before the defect pair was annihilated (the late stage). We also treated the annihilation dynamics by numerical simulation with a two-dimensional phenomenological equation of motion, and the simulation results were in good agreement with the experimental ones. The ratio of the coefficient of viscosity to that of elasticity and the strength of ordering field were evaluated from the comparison between the simulation and experimental results.

INTRODUCTION

When the system which can undergo the symmetry-breaking phase transition is quenched from the higher symmetry phase to the lower one, various kinds of topological defects such as walls, point defects and strings are generated depending on the symmetry of the system. Recently, the topological defects generated by the breaking of the continuous symmetry in the XY system, for example, have been intensively studied theoretically[1-6] and experimentally[7-10]. A typical example belonging to this category is the disclination which is a singular point of the molecular orientation in the liquid crystal.

Many researchers are interested in the dynamics of topological defects in the ordering process when the system is annealed in the lower symmetry phase after quenching[1,2,7,11].

The time evolution of the characteristic quantities such as the number density of defects and the correlation length or separation between defects are found to follow the dynamic scaling laws in the annihilation process of defects. Many direct observations of defects have been carried out on the uniaxial nematic liquid crystal where the symmetry O(3) of the isotropic phase is broken to $D_{\infty h}$ of the nematic phase[12,13]. The time evolutions of the number density of defects and the separation between defects were studied experimentally[2,14,15] at the thermal quenching or the pressure jump and discussed theoretically[16,17] including the computer simulations.

Recently, Pargellis *et al.*[2] found the region where the distance between a largely separated defect pair decreased linearly with time in the smectic-C' phase of a thin liquid crystal film, which was contrasted with the usual square root time dependence for a smaller separation. The linear time dependence behavior was also reported for a thin nematic liquid crystal by Lavrentovich *et al.*[11] In both the cases, the observed slender schlieren texture was quite different from the rounded one observed in the bulk system. To interpret this result, Pargellis *et al.*[2] phenomenologically introduced the "ordering field" which made the director align to the preferential direction by adding the coupling term between the ordering field and the director to the free energy density. Then it was found that the equation of motion, in which the constant line tension of the strings and the frictional force were balanced, well explained the time evolution of inter-defect distance.

In this paper, we observe the crossover behavior between the above two regions in a thermally quenched nematic liquid crystal. In the study by Lavrentovich *et al.*[11], only the linear time dependence of the distance between defects was observed in the whole time range of observation and did not discuss the crossover behavior was not discussed. We also apply the dc electric field with various strengths to the nematic sample during the annihilation process of defect pairs and investigate the effect of the electric field on the dynamics in the annihilation process. Further, we perform numerical simulations for this system to examine whether the static and dynamic behaviors can be explained in terms of the phenomenological equation of motion alone.

EXPERIMENTAL

The nematic liquid crystal 4-ciano-4'-n-pentylbiphenyl(5CB) was sandwiched between two glass plates. One of the cell surfaces was coated with homeotropic alignment material and the other was a clean surface. The aluminum foil 15μm thick was used as a spacer and an electrode for applying the dc electric field parallel to the glass plates. The sample cell was temperature-controlled within 50mK accuracy and was observed under the polarizing microscope. The image of the disclinations was recorded on a video tape through the CCD camera mounted to the microscope. The experiment was performed by quenching the liquid crystal sample from the isotropic phase at a temperature a little higher than the transition point to the nematic phase at a temperature about 0.5℃ below the transition point and then annealing it at this temperature.

RESULTS and DISCUSSION

When the sample is quenched from the isotropic phase to the nematic one, many wedge disclination pairs with strength of ±1 are generated and gradually disappear in pair. The defect pairs exhibit an ordinary schlieren texture with four white and black brushes under polarizing microscope as shown in Fig. 1. The typical time dependence of the separation D between a disclination pair is shown in Fig. 2(a). The annihilation process is found to be roughly divided into two time regions with different time dependence of D. At the early stage where the separation D is large, D decreases linearly with time and the defect pair is connected with line-shaped 2π walls. In contrast, at the late stage where D is small, D decreases in proportion to the square root of the time to elapse before the defect pair is annihilated.

We can calculate the time evolution of D from the equation in which the attractive and the frictional force are balanced. The attractive force between a defect pair is derived from the free energy.[7] According to the phenomenological model proposed by Pargellis *et al.* for the SmC film, the free energy density f is given as[2]

$$f = \frac{K}{2}(\nabla \Phi)^2 + \mu N_0(1 - \cos\Phi), \tag{1}$$

where Φ is the angle between the director $\boldsymbol{n}$ and the y-axis which is defined as the direction perpendicular to the line connecting a disclination pair, K the effective elastic constant (one constant approximation), and N_0 the ordering field. At the late stage with a smaller D the contribution of the ordering field is negligible, compared with the deformation energy $K(\nabla\Phi)^2$. Then, the equation of motion for D is approximately given as[2]

$$\pi\gamma \ln(\frac{D}{r_c}) \cdot \frac{\partial D}{\partial t} = -\frac{4\pi K}{D}, \tag{2}$$

where γ is friction constant. The solution of Eq. (2) is observed as[2]

$$D^2(\ln(\frac{D}{r_c}) - \frac{1}{2}) = \frac{4K}{\gamma}(t_0 - t), \tag{3}$$

where r_c is the core radius and t_0 is the time for the defect pair to be annihilated. In this equation, the attractive force of Coulomb-like nature ($\propto D^{-1}$) is balanced with the frictional force logarithmically dependent on D. Since $D >> r_c$ in the optically microscopic observations, the factor $\ln(D / r_c)$-1/2 on the lefthand side of Eq. (3) is regarded as nearly constant, and thus D decreases in proportion to the square root of the time to elapse before pair annihilation, that is, $D \propto (t_0 - t)^{1/2}$. At the early stage with a lager D, the contribution of the ordering field is not negligible compared with the deformation energy. In this case, the solution of the equation of motion for D is[2]

$$D = \frac{8K}{\pi\gamma w \ln(w / r_c)}(t_0 - t) \propto (t_0 - t), \tag{4}$$

where w is the wall width given by[2] $\sqrt{K / \mu N_0}$. The pattern of schlieren texture is slender at the early stage and is rounded at the late stage. A slender schlieren texture is not observed in the bulk system, which means that the contribution of the ordering field is negligible during all the stages in the bulk system where the deformation energy is larger than in a thin film.

Further we applied the dc electric field parallel to the cell surfaces as a controllable or external "ordering field" in order to estimate the elastic constant K and to observe any

change in the annihilation process due to the external electric field. The time dependence of D under various dc electric fields are shown in Figs. 2(b), (c) and (d). It is seen that the crossover between the two stages shifts to a later time and the period of the late stage becomes shorter as the strength of the dc electric field increases. We also find the applied dc electric field accelerates the annihilation process of the disclination pair at the early stage, which indicates that the dc field reinforces the intrinsic ordering field. Then we discuss the dependence of the 2π wall width w on the dc electric field by using Eq. (1). When the electric field E is applied, Eq. (1) is rewritten as[2]

$$f = \frac{K}{2}(\nabla \Phi)^2 + \mu N_0(1-\cos\Phi) + \frac{\Delta\varepsilon E^2}{2}\sin^2\Phi . \tag{5}$$

Here, $\Delta\varepsilon$ is the dielectric anisotropy and the direction of the ordering field is taken as the y-axis. By neglecting the y dependence of Φ to get a solution at $y = 0$ and solving the Euler-Lagrange equation derived from Eq.(5) under the boundary conditions $\partial\Phi/\partial x = 0$ and $\Phi = 2\pi$ for $x \to \infty$, we obtain,

$$x - x_0 = \frac{1}{\sqrt{Bp}}\ln\left(\frac{(p-4)(1-\cos\Phi)}{4p-(p+4)(1-\cos\Phi)-4\sqrt{p(1+\cos\Phi)(p/2-1+\cos\Phi)}}\right) \tag{6}$$

where $p = \frac{4\mu N_0}{\Delta\varepsilon E^2} + 4$. We can rewrite Eq.(6) by introducing the new parameter $t = \sqrt{\Delta\varepsilon E^2 p/K}(x - x_0)$ as

$$\Phi = 0 \quad (or\ 2\pi) \tag{7}$$

$$\Phi = \cos^{-1}\left\{\frac{(p-4)(1+e^{2t}) - 2(3p-4)e^t}{(p-4)(1+e^{2t}) + 2(p+4)e^t}\right\}. \tag{8}$$

Eq. (7) represents a uniform spatial distribution of directors. From Eq.(8), the wall width w defined as the distance with a phase change from $\pi/2$ to $3\pi/2$ is given by

$$w = \frac{1}{\sqrt{Bp}}\ln\left\{\frac{3p-4+2\sqrt{2p(p-2)}}{p-4}\right\}. \tag{9}$$

The electric field dependence of w is plotted in Fig. 3. The solid curve in this figure is the best-fitted one with the fitting parameters $\mu N_0/K = 4.11\times10^8$ [m^{-2}] and $\Delta\varepsilon/4K = 11.1$ [V^{-2}]. From the best-fitted value of $\Delta\varepsilon/4K$, the elastic constant K is evaluated

as 2.0×10^{-12} [N], which is smaller than that of the bulk, 1.0×10^{-11} [N].

Next we pursue the time evolution of the annihilation process by numerical simulation and compare the results with the experimental ones. In the simulation, we adopt a two-dimensional lattice model with directors on lattice points. First we calculate an initial configuration of directors by minimizing the free energy density f in the difference form obtained from Eq. (5) as

$$f_i = \frac{K}{4\Delta d^2}\sum_{j=1}^{4}(\Phi_j - \Phi_i)^2 + \mu N_0(1-\cos\Phi_i) + \frac{\Delta\varepsilon E^2}{2}\sin^2\Phi_i, \tag{10}$$

where Δd is a conversion coefficient from the length unit in the calculation to a real length, that is determined by comparing the calculated data with the experiment one for the electric field $E = 0$. Here, the subscripts i and j denote the nearest neighbor lattice sites. The simulation procedure is as follows: we change each Φ_i by a little amount. Then, if the free energy decreases, the change is approved. If not, the change is rejected and Φ_i keeps the same value. This routine is repeated until every Φ_i is settled down. We adopt the free boundary condition in this calculation.

The electric field dependence of 2π wall width w obtained from the numerical simulation is shown in Fig. 4 together with experimental ones. By the best-fitting procedure, we have $\Delta\varepsilon/4K \cong 25$, which leads to the elastic constant $K \sim 10^{-13}$ [N]. This value of K is smaller than that in the bulk.

Next we purse the change of Φ_i in the annihilation process of the defect pair step by step by numerical simulation. We employ the following phenomenological equation of motion for Φ derived from Eq.(5) by the Euler-Lagrange method.

$$\gamma\frac{\partial\Phi}{\partial t} = K\nabla^2\Phi - \mu N_0\sin\Phi - \frac{\Delta\varepsilon E^2}{2}\sin 2\Phi. \tag{11}$$

This equation is numerically solveed with the finite differential method as

$$\Phi_i(t+\Delta t) - \Phi_i(t) = \frac{K\Delta t}{\gamma}\left(\frac{1}{4\Delta d^2}\sum_{j=1}^{4}\{\Phi_j(t) - \Phi_i(t)\} - \mu N_0\sin\Phi_i(t) - \frac{\Delta\varepsilon E^2}{2}\sin 2\Phi_i(t)\right), \tag{12}$$

where Δt is also a conversion coefficient from a calculation step to real time and is determined by comparing the calculated data with the experiment one. Here, the

subscripts i and j denote nearest neighbor lattice sites. We adopt the free boundary conditions at the lattice edge again. We add an additional term to the righthand side of Eq. (12) in order to take into account the effect of the defects as singular points. The results for the time dependence of D obtained from the numerical simulation is shown in Figs. 5 and 6 which indicate a good agreement between the numerical results and experimental ones.

CONCLUSION

We observed the crossover behavior between two stages: the early stage where $D \propto (t_0 - t)$ and the late stage where $D \propto (t_0 - t)^{0.5}$. The dynamic behavior was found to be well explained by the phenomenological model proposed by Pargellis *et al.* We also applied to the sample the dc electric field as a controllable ordering field and revealed the field dependence of the wall width and the change of annihilation dynamics due to the dc field. These results showed that the static and dynamic behaviors of the defects were well explained by the phenomenological equation of motion alone.

REFERENCES

1. A. N. Pargellis, S. Green and B. Yurke, Phys. Rev. E 49, 4250 (1994).
2. A. N. Pargellis, P. Finn, J. W. Goodby, P. Panizza, B. Yurke and P. E. Cladis, Phys. Rev. A 46, 7765 (1992).
3. T. Nagaya, H. Hotta, H. Orihara and Y. Ishibashi, J. Phys. Soc. Jpn. 60, 1572 (1991).
4. I. Chuang, R. Durrer, N. Turok and B. Yurke, Science 251, 1336 (1991).
5. I. Chuang, N. Turok and B. Yurke, Phys. Rev. Lett. 66, 2472 (1991).
6. B. Yurke, A. N. Pargellis, I. Chuang and N. Turok, Physica B 178, 56 (1992).
7. H. Pleiner, Phys. Rev. A 37, 3986 (1988).
8. H. Toyoki and K.Honda, Prog. Theor. Phys. 78, 237 (1987).
9. H. Toyoki, Phys. Rev. A 42, 911 (1990).
10. H. Nishimori and T. Nukii, J. Phys. Soc. Jpn. 58, 563 (1988).
11. O. D. Lavrentovich and V. M. Pergamenshchik, Int. J. Mod. Phys. B 9, Nos. 18 & 19, 251 (1995).
12. L. Michel, Rev. Mod. Phys. 52, 617 (1980).
13. N. D. Mermin, Rev. Mod. Phys. 51, 591 (1979).

14. B. Yurke, A. N. Pargellis, T. Kovacs and D. A. Huse, Phys. Rev. E 47, 1525 (1993).
15. N. Mason, A. N. Pargellis and B. Yurke, Phys. Rev. Lett. 70, 190 (1993).
16. A. J. Bray and K. Humayan, J. Phys. A 25, 2191 (1992).
17. G. F. Mazenko, Phys. Rev. Lett. 63, 1605 (1989).

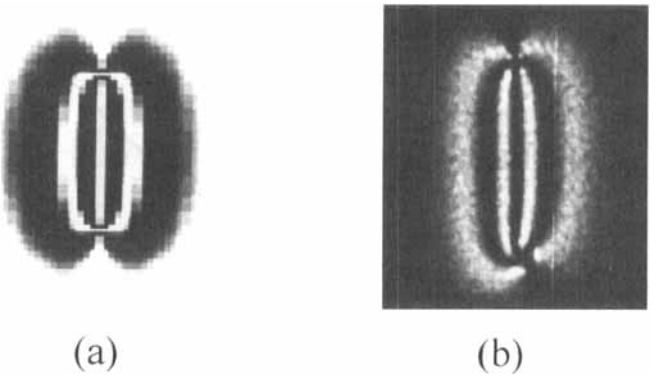

Figure 1 The pictures of "schlieren texture"
(a) simulation vs. (b) experiment

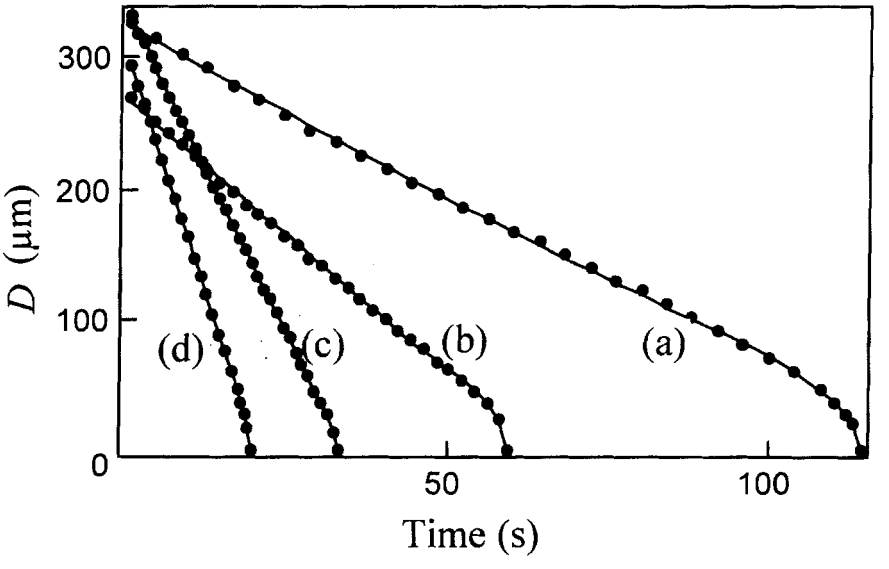

Figure 2 The time dependence of the separation D between a defect pair under a dc electric field of
(a) 0 kV/m, (b) 2 kV/m, (c) 6 kV/m and (d) 10 kV/m.

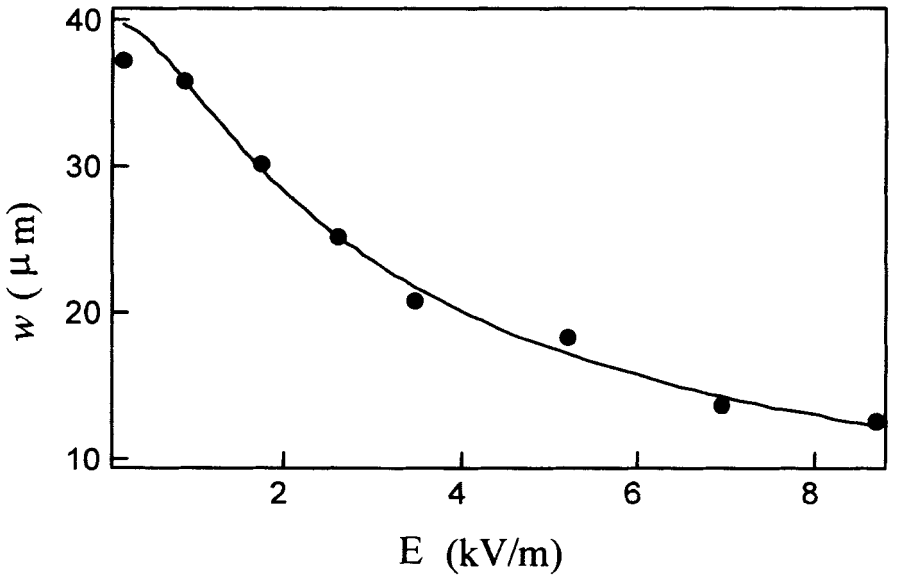

Figure 3 The dependence of the width w of the 2π wall on the dc electric field E.

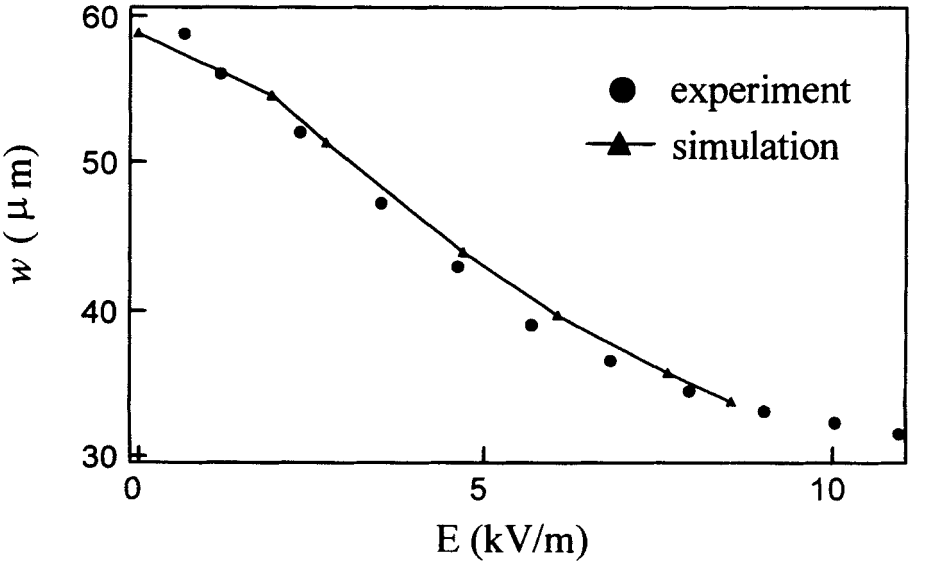

Figure 4 The dependence of the width w of the 2π wall on the dc electric field E.

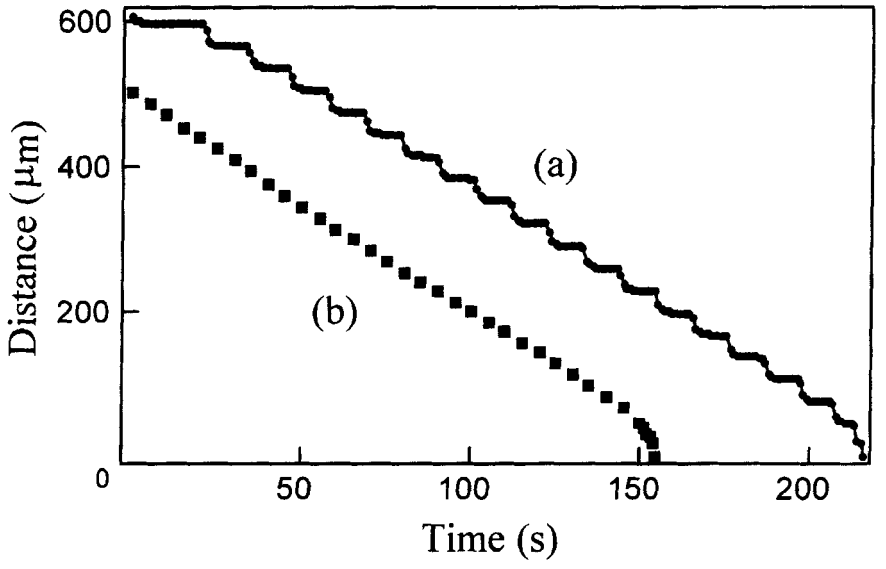

Figure 5 The time dependence of the separation between defectspair D undervarious dc electric field. (a) simulation vs (b) experiment

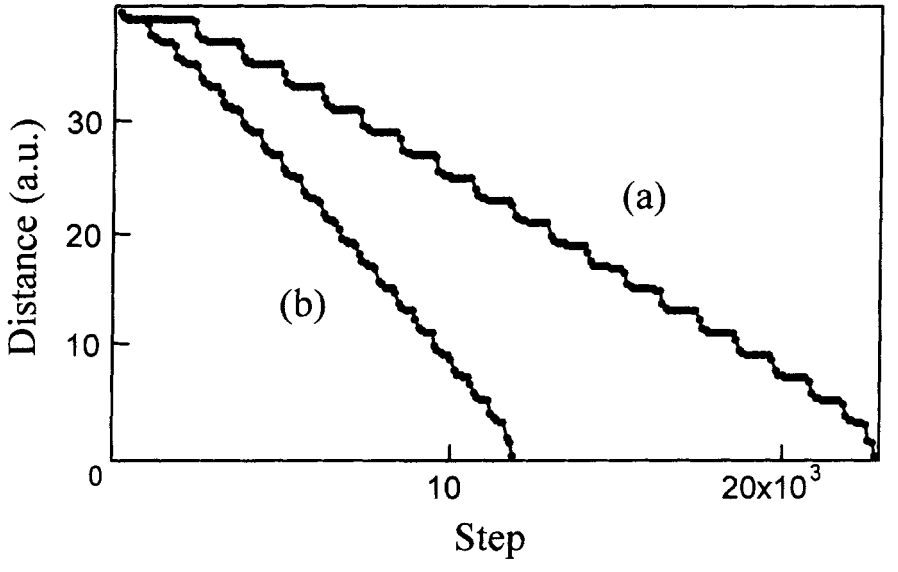

Figure 6 The time dependence of the separation D between a defect pair obtained by simulation. (a) without and (b) with the dc electric field.