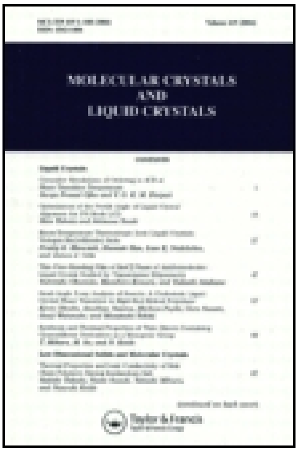


Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

# A Study of Defects in SSFLC Under a DC Electric Field

Setsuko Mukai [a] & Masahiro Nakagawa [a]
[a] Department of Electrical Engineering, Faculty of Engineering, Nagaoka University of Technology, Kamitomioka 1603-1, Nagaoka, Niigata, 940-21, Japan
Version of record first published: 23 Sep 2006.

To cite this article: Setsuko Mukai & Masahiro Nakagawa (1995): A Study of Defects in SSFLC Under a DC Electric Field, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 263:1, 179-187

To link to this article: http://dx.doi.org/10.1080/10587259508033582

*Mol. Cryst. Liq. Cryst.* 1995, Vol. 263, pp. 179–187
Reprints available directly from the publisher
Photocopying permitted by license only





# A STUDY OF DEFFECTS IN SSFLC UNDER A DC ELECTRIC FIELD

SETSUKO MUKAI AND MASAHIRO NAKAGAWA
Department of Electrical Engineering, Faculty of Engineering, Nagaoka
University of Technology, Kamitomioka 1603-1, Nagaoka, Niigata 940-21, Japan

**Abstract** On the basis of a continuum theory of compressive SmC*, we shall investigate a nucleation of disclinations, under a **DC** electric field, accompanied with the layer relaxation phenomenon between a couple of antiparallel chevrons. From the two-dimensional analyses of the layer structures and the c-director configuration with a screw disclination between a couple of anti-parallel chevrons, it is found that a screw disclination , which move depending on the applied electric field strength, may be produced under a certain electric field, and that such threshold field strengths critically depend on the molecular tilt angle, the cell thickness and an elastic constant. In addition one finds that there also exists a threshold for the layer reversal under a relatively high electric field.

## INTRODUCTION

The ferroelectric liquid crystalline materials have been investigated from the experimental to date because of their attractive potentiality for the application to the fast electro-optic display devices and the spatial light modulator [1-5]. According to the earlier pioneering works in this field, the material properties of the smectics have certainly blossomed, whereas most material properties of smectics have been still accompanied with many opened questions since the difficulty of the experiments to obtain a large mono-domain sample. Also the elastic properties of smectics have not been well clarified from a theoretical point of view.

From the above-mentioned point of views, the elastic free energy of SmC was first constructed by Orsay group in terms of an axial vector in a local coordinate system [6]. Later Rapini expressed it in a vector notation in the laboratory frame for the practical applications of the continuum theory [7]. Later a chiral energy was also involved in the elastic free energy for SmC* phase as seen in de Gennes' text book[8]. Another vector form of SmC* free energy was recently reported by Dahl and Lagerwall [9]. Recently Nakagawa deduced a generalised elastic free energy for compressible smectics to account for the layer compression or dilation[10] and analysed the chevron layer structure[11-13] which has been observed in the high resolution **X**-ray analyses[14-16]. The effect of the electric field in the chevron layer structure was investigated in the static deformations[12,13]. It was found therein that the electric field parallel to the spontaneous polarization vector $\mathbf{P}_s$ tends to make the layer tilt angle small in a chevron layer structure whereas the electric field opposite to $\mathbf{P}_s$ does to make it large [12]. Moreover it was also concluded that the c-director orientation can be easily distorted in comparison with the layer structure[13]. Then the present authors have analysed the double kink layer structures[17] as well as the anchoring effect[18] in **SSFLC**. Recently a hydrodynamic theory of incompressible SmC liquid crystals has been proposed by Leslie, Stewart and Nakagawa[19]. Very recently, based on the elastic free energy of compressible smectics, Nakagawa has reported a layer dynamics accompanied with the c-director motion with a weak anchoring at the bounding plates[20,21].

To analyze two dimensional properties of the compressible smectics, the present authors have reported a few works on the two-dimensional layer structure with the chevron layer structures[22,23]. These analyses resort on an invariant layer structure along an axis parallel to the bounding plate and are assumed to be substantially two-dimensional in the plane perpendicular to it and parallel to the smectic layers. To date, however, there has been no report such a two-dimensional analysis accompanying with a layer dilation or compression as seen in the case of buckling instability under an externally driven layer dilation in smectic phases[24-26]. In the experimental observation[26], it has been found that a layer undulation occurs over a critical layer dilation in SmA phase. One may expect that such a layer undulation may be realized in the zig-zag defects which is accompanied with a couple of two opposite chevrons which has been observed in **SSFLC**[16].

In this paper, we shall investigate the electric field effect on the layer distortion as well as the c-director deformation of the compressible smectics, and also analyse the disclinations which result from a screw disclination located between a pair of anti-parallel chevrons. In the present framework a compressible elastic energy is involved together with the layer distortion and the c-director deformation energies based on the previously formulated continuum theory[10]. In section 2 a theoretical framework will be described in brief on the basis of the elastic free energy of the compressible smectics[10,13,22,23]. Then some numerical results will be given in section 3 to show the electric field effect on the disclinations as well as the chevron structures. Finally section 4 will address a few concluding remarks on the presently found numerical findings.

## THEORY

In similar to our previous works concerned with the compressible smectics[22,23], the elastic free energy density of compressible smectics can be simply given by

$$F=\frac{A}{2}a_{i,i}a_{j,j}+\frac{L}{2}(|\mathbf{a}|-a_0)^2+\frac{B}{2}c_{i,j}c_{i,j}-C a_{i,i}c_{j,j}+Dc_i\varepsilon_{ijk}c_{k,j}-\mathbf{P}_s\cdot\mathbf{E}\ , \tag{1}$$

where **a** and **c** are the wave vector and the **c**-director, respectively, A , B, C, D and L are the elastic constants for the splay distortion of the layer, the **c**-director distortion, the coupling effect between **a** and **c**, the chiral energy, and the layer compression, respectively, $\varepsilon_{ijk}$ is the Levi-Civita tensor, $\mathbf{P}_S$ is the spontaneous polarization vector, and **E** is the external electric field which is applied normal to the bounding plate. The wave vector is defined as a vector such that the direction is coincident with the layer normal and the magnitude is determined by

$$|\mathbf{a}|=d_A/d(\mathbf{r})\ , \tag{2}$$

where d(**r**) is the local layer spacing and $d_A$ is the layer spacing in SmA phase. Finally $a_0$ is the equilibrium value of |**a**| and given by

$$a_0=\frac{d_A}{d_C}=\frac{d_A}{d_A\cos\theta_m}\approx 1+\frac{\theta_m^2}{2}\ , \tag{3}$$

where $d_C$ is the layer spacing in SmC* phase and $\theta_m$ is the molecular tilt angle. Noting the restriction for the wave vector **a** such that $\nabla\times\mathbf{a}=0$ and introducing a scalar function $\phi=\phi(x,y)$ corresponding to the layer translation, one may put

$$a(x,y)=(-\phi_x,-\phi_y,a_z) \quad , \tag{4}$$

where $a_z$ must be a constant because of $a_{z,x}=a_{z,y}=0$ and simply can be put into 1 similar to the previous work[22,23] assuming that the layer spacing in SmA phase is conserved in SmC* phase at the bounding plates. It should be noted here that **a** represents a book-shelf type layer structure provided that $\phi=0$ or $\mathbf{a}=(0,0,1)$. Then assuming that the all variables depend only on x (parallel to the bounding plate ) and y ( perpendicular to the bounding plate and the layer normal) coordinates, one may rewrite F as

$$\begin{aligned} F= &\frac{A}{2}(\phi_{xx}{}^2+\phi_{yy}{}^2+2\phi_{xx}\phi_{yy})+\frac{L}{8}(\phi_x{}^2+\phi_y{}^2-\theta_m{}^2)^2 \\ &+\frac{B}{2}(c_{x,x}{}^2+c_{x,y}{}^2+c_{y,x}{}^2+c_{y,y}{}^2+c_{z,x}{}^2+c_{z,y}{}^2) \\ &+C\{(\phi_{xx}+\phi_{yy})(c_{x,x}+c_{y,y})\}+Dc_i\varepsilon_{ijk}c_{k,j}-P_sE(c_x+\phi_x c_z) \end{aligned} \tag{5}$$

Minimizing the total free energy under the constraints, which correspond to $\mathbf{a}\cdot\mathbf{c}=0$ and $\mathbf{c}\cdot\mathbf{c}=1$, respectively,

$$-c_x\phi_x-c_y\phi_y+c_z=0 \quad , \tag{6a}$$

$$c_x{}^2+c_y{}^2+c_z{}^2=1 \quad , \tag{6b}$$

one finds the following the Euler-Lagrange equations for $\phi$ and **c**

$$\begin{aligned} &A(\phi_{xxxx}+\phi_{yyyy}+2\phi_{xxyy})-\frac{L}{2}\{\phi_{xx}(3\phi_x{}^2+\phi_y{}^2-\theta_m{}^2) \\ &+\phi_{yy}(\phi_x{}^2+3\phi_y{}^2-\theta_m{}^2)+4\phi_{xy}\phi_x\phi_y\} \\ &+C(c_{x,xxx}+c_{y,yxx}+c_{x,xyy}+c_{y,yyy})-P_sEc_{z,x} \\ &+(\mu_x c_x+\mu c_{x,x}+\mu_y c_y+\mu c_{y,y})=0 \end{aligned} \quad , \tag{7}$$

and

$$\begin{aligned} &\nu c_x-\mu\phi_x-B(c_{x,xx}+c_{x,yy})-C(\phi_{xxx}+\phi_{yyx})+2Dc_{z,y}-P_sE=0 \ , \\ &\nu c_y-\mu\phi_y-B(c_{y,xx}+c_{y,yy})-C(\phi_{xxy}+\phi_{yyy})-2Dc_{z,x}=0 \ , \\ &\nu c_z+\mu-B(c_{z,xx}+c_{z,yy})-P_sE\phi_x+2D(c_{y,x}-c_{x,y})=0 \ , \end{aligned} \tag{8}$$

respectively. Here $\mu$ and $\nu$ are the Lagrange multipliers concerned with equations (6a) and (6b), respectively, and have to be determined simultaneously. Hence we may analyse the layer structure as well as the **c**-director configurations by making use of equations (7) and (8) together with equations (6a) and (6b) under an appropriate boundary condition.

## PRELIMINARIES FOR PRACTICAL COMPUTATIONS AND BOUNDARY CONDITIONS

Before solving numerically equations (7) and (8) together with equations (6a) and (6b), we shall normalize some variables for convenience as follows.

$$
\begin{aligned}
\psi_{\xi\xi\xi\xi}+\psi_{\eta\eta\eta\eta}+2\psi_{\xi\xi\eta\eta} = \frac{1}{2}\{&\psi_{\xi\xi}(3\psi_{\xi}^{2}+\psi_{\eta}^{2}-\theta_{m}^{2})+\psi_{\eta\eta}(\psi_{\xi}^{2}+3\psi_{\eta}^{2}-\theta_{m}^{2}) \\
&+4\psi_{\xi\eta}\psi_{\xi}\psi_{\eta}\} \\
&-\frac{B^{*}C^{*}}{\lambda^{2}}(c_{x,\xi\xi\xi}+c_{y,\eta\xi\xi}+c_{x,\xi\eta\eta}+c_{y,\eta\eta\eta})-\frac{B^{*}}{\lambda^{2}}e^{*}c_{z,\xi} \\
&-\frac{1}{\lambda^{2}}\{\mu_{\xi}^{*}c_{x}+\mu^{*}c_{x,\xi}+\mu_{\eta}^{*}c_{y}+\mu^{*}c_{y,\eta}\}
\end{aligned}
\quad , \quad (9)
$$

$$
\begin{aligned}
c_{x,\xi\xi}+c_{x,\eta\eta} &= -C^{*}(\psi_{\xi\xi\xi}+\psi_{\eta\eta\xi})+2D^{*}c_{z,\eta}-e^{*}+(\nu^{*}/B^{*})c_{x}-(\mu^{*}/B^{*})\psi_{\xi}, \\
c_{y,\xi\xi}+c_{y,\eta\eta} &= -C^{*}(\psi_{\xi\xi\eta}+\psi_{\eta\eta\eta})-2D^{*}c_{z,\xi}+(\nu^{*}/B^{*})c_{y}-(\mu^{*}/B^{*})c_{y}-(\mu^{*}/B^{*})\psi_{\eta}, \\
c_{z,\xi\xi}+c_{z,\eta\eta} &= -e^{*}\psi_{\xi}+(\nu^{*}/B^{*})c_{z}+2D^{*}(c_{y,\xi}-c_{x,\eta})+(\mu^{*}/B^{*}) .
\end{aligned}
\quad (10)
$$

Here the normalized variables are defined by

$$\xi=\frac{x}{\lambda}, \ \eta=\frac{y}{\lambda}, \ \zeta=\frac{z}{\lambda} \quad (11)$$

$$\psi=\frac{\phi}{\lambda} \ , \quad (12)$$

$$\lambda^{2}=\frac{A}{L} \ , \quad (13)$$

$$\mu^{*}=\frac{\mu\lambda^{2}}{L} \ , \quad (14)$$

$$\nu^{*}=\frac{\nu\lambda^{2}}{L} \ , \quad (15)$$

$$B^{*}=\frac{B}{L} \ , \quad (16)$$

$$C^{*}=\frac{C}{B} \ , \quad (17)$$

$$D^{*}=\frac{D}{B}\lambda \quad (18)$$

$$e^{*}=\frac{p_{s}E\lambda^{2}}{B} \ . \quad (19)$$

In the above definitions, the parameter $\lambda$ defined by equation (14) may be estimated as the order of the molecular length [8].

Then we have to numerically solve equations (7) and (8) to determine the layer structure as well as the c-director configuration, under such boundary conditions as a pair of antiparallel chevrons[11], expressed by

$$\psi(-W^*/2,\eta)=2\log\left(\frac{\cosh(\theta_m d^*/4)}{\cosh(\theta_m \eta/2)}\right) \quad , \tag{20a}$$

$$\psi(+W^*/2,\eta)=-2\log\left(\frac{\cosh(\theta_m d^*/4)}{\cosh(\theta_m \eta/2)}\right) \quad , \tag{20b}$$

and the wall-width W and the cell thickness d for the analysis (See Fig.1.) are normalized as

$$W^*=\frac{W}{\lambda} \quad , \tag{21}$$

and

$$d^*=\frac{d}{\lambda} \quad , \tag{22}$$

respectively. In addition the boundary conditions for the **c**-director are defined by

$$\begin{aligned} c_x(\varepsilon\cos,\varepsilon\sin\phi)&=-\sin\phi \\ c_y(\varepsilon\cos,\varepsilon\sin\phi)&=\cos\phi \quad (\varepsilon\rightarrow 0) \quad , \\ c_z(\varepsilon\cos,\varepsilon\sin\phi)&=0 \end{aligned} \tag{23}$$

where $\phi$ stands for the azimuthal angle in the polar coordinate. Here equation (23) represents to a screw disclination, with a strength $s=+1$[5,8], located at the origin in Fig.1. In addition the outer boundary conditions are given by

$$\begin{aligned} c_x(\xi,+/-d^*/2)&=-/+1 \,, \\ c_y(\xi,+/-d^*/2)&=0 \quad , \qquad \text{(Dirichlet type)} \\ c_z(\xi,+/-d^*/2)&=0 \quad , \end{aligned} \tag{24}$$

and

$$\begin{aligned} c_{x,\xi}(\pm W^*/2,\eta)&=0^* , \\ c_{y,\xi}(\pm W^*/2,\eta)&=0 \ , \qquad \text{(Neumann type)} \\ c_{z,\xi}(\pm W^*/2,\eta)&=0 \ . \end{aligned} \tag{25}$$

The boundary condition expressed by equation (24) corresponds to a couple of twisted configurations in **SSFLC** state.

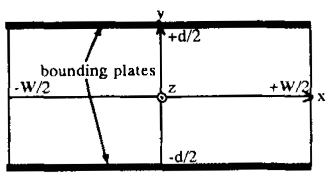



Fig.1 The coordinate system. Here z axis is taken as an axis parallel to the layer normal.

## NUMERICAL RESULTS

Solving equations (9) and (10) under the boundary conditions, equations (20a), (20b), (23)-(25), we have found the following results. Since we have no available data for the elastic constants, $B^*$, $C^*$, $D^*$, $\lambda$, $\theta_m$ and $W^*$ were assumed to be 0.001, 0.1, 0, 0.1, 0.4 and $2d^*$, respectively, if not mentioned. Here the chiral coefficient $D^*$ was put into 0 since its effect is not so appreciable in SSFLC geometry as has been previously noted[11-13]. The basic equations were solved in the conventional difference and the iteration schemes in similar to the previous works[22,23].

Several examples of the layer distortions and the c-director configuration for the pair of chevrons are given in Figs.2(a)-(d) for various molecular tilt angles $\theta_m$. Therein the c-director is depicted as a projection onto the $\xi-\eta$ plane along the z or $\zeta$ axis. Here it should be noted that a new screw disclination appear under a certain electric field, and that two possible directions, $+\xi$ and $-\xi$, are energetically equivalent from symmetry consideration. On the contrary the other possible directions, $+\eta$ and $-\eta$, are not energetically equivalent but must depend on the polarity of $e^*$. That is, if $e^*>0$ (<0), then $\eta>0$ (<0) provided that $P_S>0$. The dependence of the coordinates $(x^*,y^*)=(|x/\lambda|, y/\lambda)$ of the produced disclinations on the electric field strength $e^*$ is summarized in Fig.3. From these one may see that there exists certain critical electric field for the nucleation of a new screw disclination, and that $x^*$ values critically depend on the molecular tilt angle, whereas $y^*$ values are almost same for various values of it.

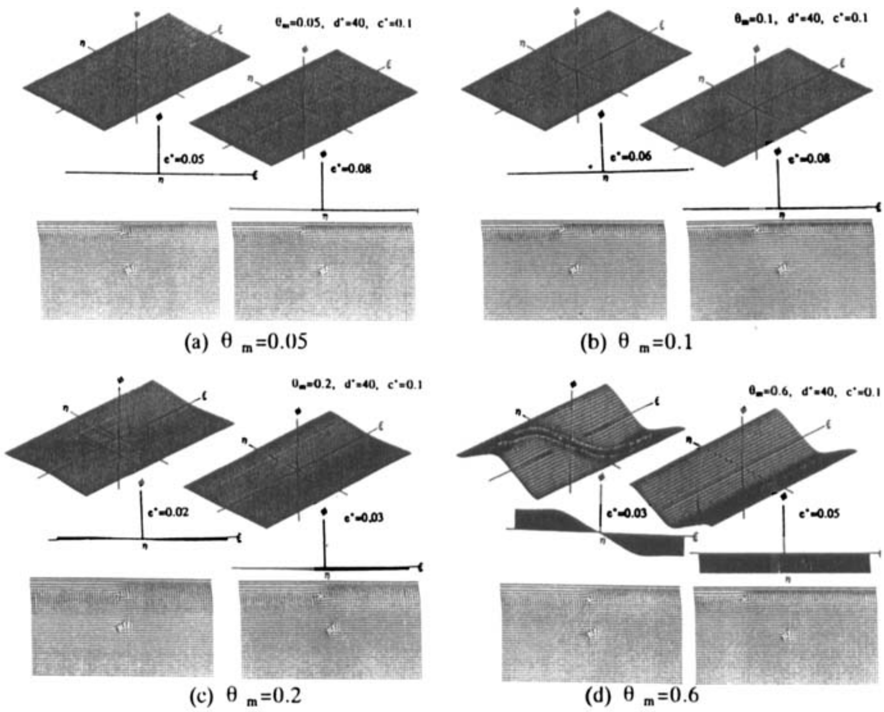



Fig.2 Several examles of the dependence of the layer structure and the c-director configuration on the molecular tilt angle, $\theta_m$. Here $d^*=40$, $C^*=0.1$.

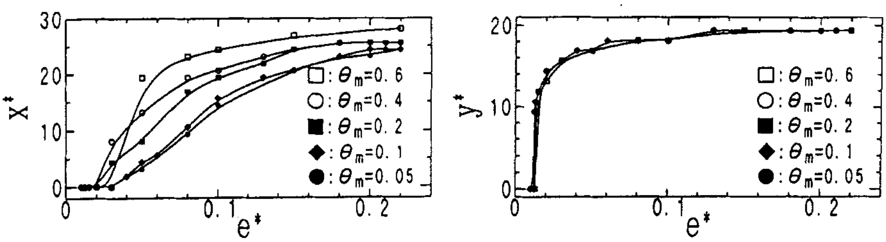
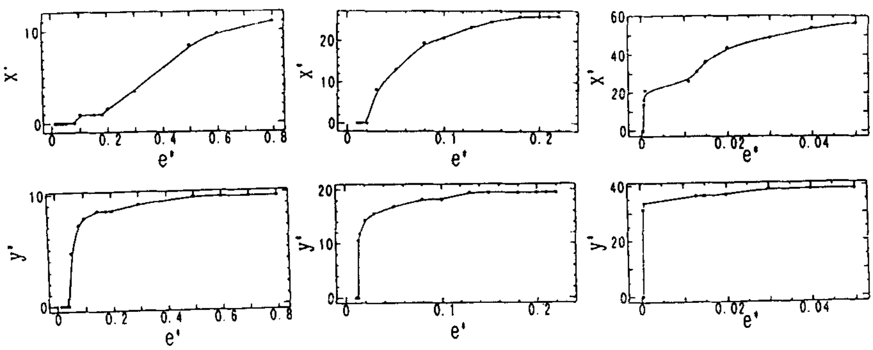



Fig.3 The dependence of the coordinates (x*,y*) of the created screw singularity on the electric field strength e*. Here d*=40, C*=0.1.

Next the dependence of the above-mentioned critical behaviour on the cell thickness d* is summarized in Fig.4(a)-(c). From these results, one may see that the new disclination has a tendency to move more quickly upward, or +η direction, with a relatively low electric field as the




(a) d*=20 (b) d*=40 (c) d*=80

Fig.4 The dependence of the coordinates (x*,y*) on the cell thickness, d*. Here $\theta_m$=0.4 and C*=0.1.

Finally the dependence on the coupling parameter C* is summarized in Fig.5. From them, one may find that the new disclination has a tendency to move more quickly -ξ direction as C* increases.

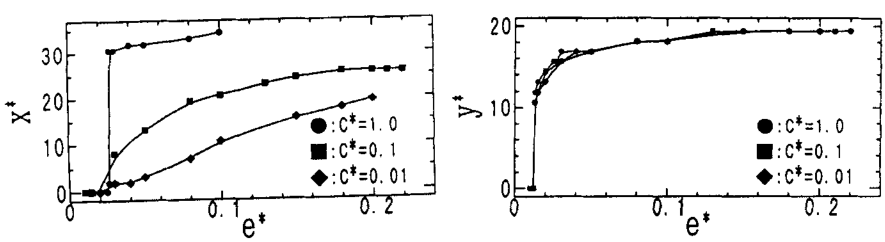



Fig.5 The dependence of the coordinates (x*,y*) on the coupling parameter, C*.

## CONCLUDING REMARKS

In this work we have presented layer distortion and the **c**-director configuration accompanied with a production of screw disclination. From numerical computations, one has found that there exists a certain critical electric field for the nucleation of such a screw singularity. We also have found that the disclination moves quickly towards $+\xi$ or $-\xi$ direction as the coupling energy between the layer and the **c**-director increases, *i.e.* as $\theta_m$ or C* does. On the contrary, it has been found that the disclination moves quickly towards $+\eta$ (e*>0) direction to reduce the elastic energy concerned with the **c**-director configuration as the cell thickness d* increases.

To the end of this work, let us confirm the conservation of the disclination strength s. Initially the total strength equals to +1 corresponding to the initially located screw disclination at the origin in Fig.1. Then, as the field strength increases, a new screw disclination with the strength +1 may be produced as was found in the previous section. At the same time, it should be noted that a pair of disclinations, with -1/2, have to be also produced to align the spontaneous polarization vector towards the electric field as seen in Fig.6. Consequently the total strength is found to be substantially conserved in whole system.

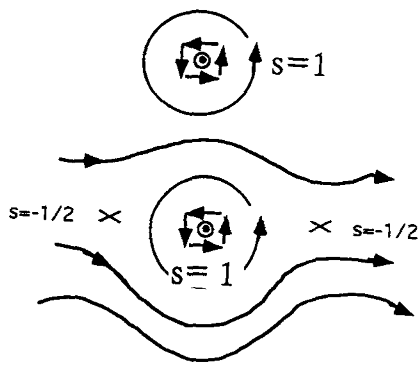



Fig.6 The conservation of the disclination strengths. Here the upper screw disclination with the strength +1 corresponds to a new one produced under a certain electric field. In addition a couple of disclinations, +1/2 and -1/2, are also produced to attain the overall upward orientation of the spontaneous polarization to reduce the interaction energy, $-\mathbf{P}_s \cdot \mathbf{E}$.

As a future problem, it seems to be interesting to analyse, as a three-dimensional problem, a layer structure accompanied with a possible dispiration related to the dislocation as seen in the zig-zag domains in **SSFLC** cells[15,16]. Furthermore it may be worthwhile to analyse the dynamics of such a singularities under an alternative electric field.

## REFERENCES

1. R.B.Meyer, L. Liebert, L. Strzelecki and P.Keller:J.Phys.(France) **36**,L69(1975)
2. R.B.Meyer: Mol.Cryst.&Liq.Cryst.,**40**,33(1977).
3. N.A.Clark and S.T.Lagerwall : Appl. Phys. Lett.,**36**,**899(1980).**
4. L.A.Beresnev, L.M.Blinov, M.A.Psipov, S.A.Pikin: Mol. Cryst.& Liq. Cryst.,**158A**,3 (1988).
5. M.Kleman: *"Points, Lines and Walls"*,(John Wiley & Sons, 1983).

6. Orsay group: Solid State Commun.,**9**,653(1971).
7. A.Rapini:J.Phys.(France)**33**,237(1972).
8. P.G. de Gennes :*" The Physics of Liquid Crystals"*,(Oxford, 1975)Chap.7.
9. I. Dahl and S.T.Lagerwall:Ferroelectrics,**58**,215(1984).
10. M.Nakagawa:Liq.Cryst.,**8**,651(1990).
11. M.Nakagawa:Mol.Cryst.&Liq.Cryst.,**174**,65(1989).
12. M.Nakagawa:*Displays*,67(Scientific Butterworth, April,1990).
13. M.Nakagawa:J. Phys. Soc. Jpn.,**59**,1995(1990).
14. N.A. Clark and S.T. Lagerwall: Proc. 6th International Display Research Conf. Tokyo, Japan,456(1986).
15. T.R.Rieker, N.A.Clark, G.S.Smith, D.S.Parmer,E.B.Sirota and Safinia:Phys.Rev.Lett.,**59** 2658(1987).
16. Y.Ouchi, Ji Lee, H.Takezoe, A.Fukuda, K.Kondo, T.Kitamura and A.Mukoh: Jpn.J. Appl.Phys.,**27**,L725(1988).
17. S. Mukai and M.Nakagawa:J.Phys.Soc.Jpn.,**61**,1516(1992).
18. S. Mukai and M. Nakagawa:J.Phys.Soc.Jpn.,**59**,112(1992).
19. F.M. Leslie , I.W. Stewart and M.Nakagawa: Mol.Cryst.&Liq.Cryst.,**198**,443(1991).
20. M. Nakagawa: J.Phys.Soc.Jpn.,**61**,4390(1992).
21. M. Nakagawa: Liq.Cryst.,**14**,1763(1993).
22. S.Mukai and M.Nakagawa:J.Phys.Soc.Jpn.,**62**,1984(1993).
23. S.Mukai and M. Nakagawa:Liq.Cryst.,**14**,1409(1993).
24. W.Helfrich: Appl.Phys.Lett.,**17**,531(1970).
25. J. Hurault: J.Chem.Phys.,**59**,2068(1973).
26. J.Yamamoto and K. Okano:Jpn.J.Appl.Phys.,**30**,754(1991)754.