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Singularities in Nematics: The Effect of Elastic Constant Variations

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Singularities in Nematics

The Effect of Elastic Constant Variations

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In this paper we report typical calculations of the variations in the deformation energy, interaction energy and orientational pattern of $+1$, -1, $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities in the neighbourhood of a nematic–smectic transition in CBOOA. We find the interaction between $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities to increase much more rapidly than that between $+1$ and -1 as the smectic point is reached, indicating that the former have a greater probability of annihilating each other near the transition.

INTRODUCTION

It is well known that near a nematic–smectic phase transition the bend and the twist elastic constants of the nematic phase diverge rapidly, with the smectic phase accommodating only splay deformations.[1] Such an increase in elastic constants should affect to a considerable degree the structure and properties of the disclinations of the nematic phase. In this paper we report calculations of the variation of self energy (excluding the core), interaction energy and orientation patterns for $+1$, -1, $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities for a typical system (CBOOA). As is to be expected, it is found that the self energy of a -1 (or $+\frac{1}{2}$) disclination increases very rapidly as compared with that of a $+1$ (or $-\frac{1}{2}$) singularity. Additionally also it turns out that the interaction between $+\frac{1}{2}$ and $-\frac{1}{2}$ increases much more rapidly than that between $+1$ and -1, indicating that unlike half singularities have a greater possibility of annihilating one another.

THEORY

We consider only the schlieren texture. The director is assumed to be in the XY plane making an angle of ϕ with respect to X: $\mathbf{n} = (\cos\phi, \sin\phi, 0)$. The elastic deformation energy density is

$$F_0 = \tfrac{1}{2}[K_{11}(\nabla \cdot \mathbf{n})^2 + K_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2] \qquad (1)$$

with K_{11}, K_{22} and K_{33} as the splay, twist and bend elastic constants respectively.

The equation of equilibrium (in cylindrical polars) obtained by minimising F_0 is[2]

$$K\left[\frac{\partial^2\phi}{\partial r^2}+\frac{1}{r}\frac{\partial\phi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\phi}{\partial\alpha^2}\right]+\varepsilon K\left[\left\{\frac{\partial^2\phi}{\partial r^2}-\frac{1}{r}\frac{\partial\phi}{\partial r}\left(1-2\frac{\partial\phi}{\partial\alpha}\right)-\frac{1}{r^2}\frac{\partial^2\phi}{\partial\alpha^2}\right\}\cos 2(\phi-\alpha)+\left\{\frac{2}{r}\frac{\partial^2\phi}{\partial r\partial\alpha}-\left(\frac{\partial\phi}{\partial r}\right)^2-\frac{1}{r^2}\frac{\partial\phi}{\partial\alpha}\left(2-\frac{\partial\phi}{\partial\alpha}\right)\right\}\sin 2(\phi-\alpha)\right]=0 \quad (2)$$

Here $K=\frac{1}{2}(K_{11}+K_{33})$ and $\varepsilon=(K_{33}-K_{11})/(K_{33}+K_{11})$. We seek solutions which are independent of r. For this we set all the derivatives of r and sum of all the coefficients of r of the same power to zero. Then (2) becomes

$$\frac{\partial^2\phi}{\partial\alpha^2}-\varepsilon\left[\frac{\partial^2\phi}{\partial\alpha^2}\cos 2(\phi-\alpha)+\frac{\partial\phi}{\partial\alpha}\left(2-\frac{\partial\phi}{\partial\alpha}\right)\sin 2(\phi-\alpha)\right]=0 \quad (3)$$

When $K_{11}=K_{33}$, i.e., $\varepsilon=0$, we find

$$\frac{\partial^2\phi}{\partial\alpha^2}=0 \quad (4)$$

or

$$\phi=s\alpha+c \qquad (s=\pm\tfrac{1}{2}\text{ integer})$$

$$=s\tan^{-1}\frac{y}{x}+c. \quad (5)$$

These solutions describe the familiar structures of Frank–Oseen singularities. The properties of such singularities have been studied in detail by Frank[3] and Nehring and Saupe.[2]

When $\varepsilon\neq 0$ the only exact solutions are $\phi=\alpha$, $\alpha+\pi/2$ and $2\alpha+c$ (i.e., $s=1$ or 2). Singularities with $s=2$ have not been found to occur commonly and will not be discussed here. For general values of s, Eq. (3) has to be solved at every value of ε. This has been done numerically using the orthogonal collocation method.[4]

For a given value of s when $\varepsilon=0$ we have $\phi=s\alpha+c$ with $\alpha=0$ and 2π as boundary conditions. We start with these as the approximate solutions and proceed to solve Eq. (3) when $\varepsilon\neq 0$. The solution so obtained describes a singularity at $r=0$. Since this solution goes over to the neat solution Eq. (5) when $\varepsilon\to 0$, we shall continue to call s defined by Eq. (5) to be the strength of the disclination even when $\varepsilon\neq 0$.

When more than one singularity is present, we solve locally the equilibrium equation for each singularity and then add the solutions due to the others to obtain the orientation at any point. This superposition principle is strictly valid for $\varepsilon = 0$ and completely fails for $\varepsilon = 1$ (the maximum value of ε). Therefore the superposed solution is very good at smaller values of ε and is only approximate at higher values of ε.

In principle, the core energy may also depend on ε, but we ignore it in these calculations as we do not have a precise knowledge of its structure.

RESULTS

Calculations have been made for a 50 μm $\times$ 50 μm sample of unit thickness and with singularities of strengths $+s$ and $-s$ (both with $c = 0$) placed symmetrically about the centre on a line running (through the centre) parallel to one of its edges. The distance between the two singularities was never allowed to exceed 10 μm or fall below 2.5 μm, and the core region was taken to be 0.5 μm $\times$ 0.5 μm. We have used the data of Cheung *et al.*[1] on the elastic constant variation of CBOOA.

The deformation energy (per unit thickness) of a singularity is given by $W_T = W + W_c$ with

$$W = \int_{-a/2}^{+a/2} \int_{-a/2}^{+a/2} F_0(x, y)\mathrm{d}x\, \mathrm{d}y \qquad (6)$$

(a = edge length)

and W_c being the energy corresponding to the core. As mentioned earlier, in the absence of detailed knowledge of the core structure this quantity cannot be calculated. When more than one singularity is present, a similar expression holds for W_T with this difference that F_0 is calculated from the orientation obtained from the superposition principle and W_c includes the core energies of all the singularities. We define the interaction energy W_{INT} between $+s$ and $-s$ singularities by (neglecting the core contribution)

$$W_{\mathrm{INT}} = W(+s) + W(-s) - W(+s, -s). \qquad (7)$$

Here $W(s)$ and $W(-s)$ are values of W as given by Eq. (6) for $+s$ at d/2 and $-s$ at $-$d/2 singularities respectively and $W(+s, -s)$ is the value of W when both the singularities are present.

In Figure 1 we give W as a function of ε for $+1$, -1, $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities. (The individual energies varied very little when the singularity was moved from d/2 = 5 μm to d/2 = 0.) For $s = +1$ and $s = -\frac{1}{2}$, W does not change much with ε. This is so because a structure with a predominantly

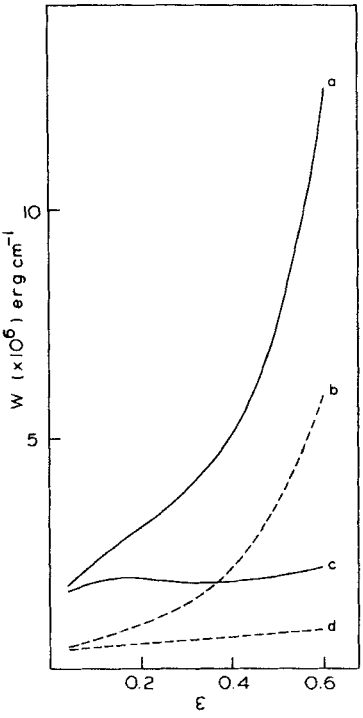

FIGURE 1 Deformation energies of (a) -1, (b) $\frac{1}{2}$, (c) 1 and (d) $-\frac{1}{2}$ singularities as functions of ε.

splay deformation (involving K_{11}) will not be much affected. On the other hand $s = -1$ or $s = \frac{1}{2}$ singularities involve a considerable amount of bend when $\varepsilon = 0$ and hence show large increase in their energies as ε increases.

Figure 2 gives W_{INT} for a pair of unlike $(+1, -1)$ and $(+\frac{1}{2}, -\frac{1}{2})$ singularities, as a function of ε for a few values of d, the distance between the singularities. It is seen that the interaction energy increases with ε. Figure 3 gives dependence of W_{INT} on d for a given value of ε. From these two figures it will be clear that with increase of ε unlike singularities prefer to come closer together. However, what is more interesting is that the W_{INT} for $(+1, -1)$ and $(+\frac{1}{2}, -\frac{1}{2})$ do not increase at the same rate with ε. This fact is illustrated in Figure 4. For any given value of d we find that the ratio

$$F = \frac{W_{INT}(+1, -1)}{W_{INT}(+\frac{1}{2}, -\frac{1}{2})}$$

decreases with ε, implying that unlike singularities of half strength have a greater chance of annihilating one another than those of unit strength.

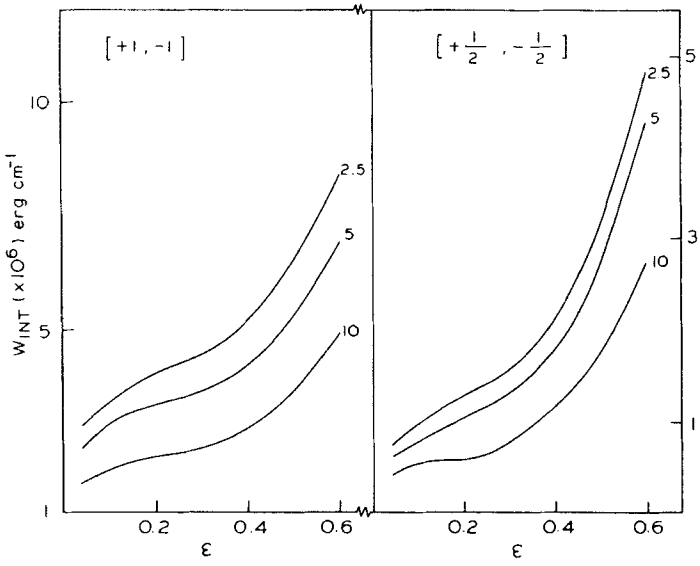

FIGURE 2 Interaction energies between 1 and -1 and that between $\frac{1}{2}$ and $-\frac{1}{2}$ singularities as functions of ε. Distances between singularities 2.5 μm, 5 μm and 10 μm.

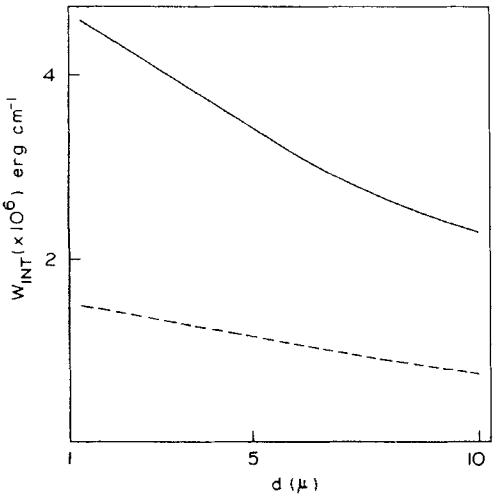

FIGURE 3 Interaction energy between 1 and -1 (full line) and that between $\frac{1}{2}$ and $-\frac{1}{2}$ (dashed line) as functions of d, the distance between the singularities. $\varepsilon = 0.2424$.

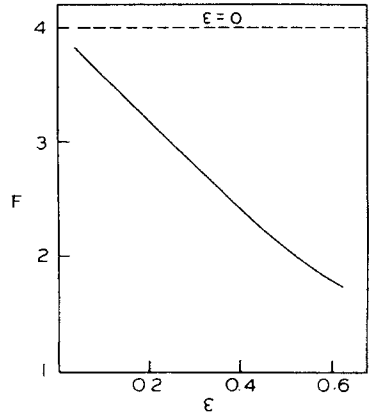

FIGURE 4 The variation of F the ratio of interaction energies between $(1, -1)$ and $(\frac{1}{2}, -\frac{1}{2})$ with ε. The calculations have been presented for d = 10 μm.

In Figure 5 we give the orientation of the director as a function of ε at few collocation points. Orientation varies monotonically with ε, emphasizing the fact that any change in the schlieren texture will be gradual.

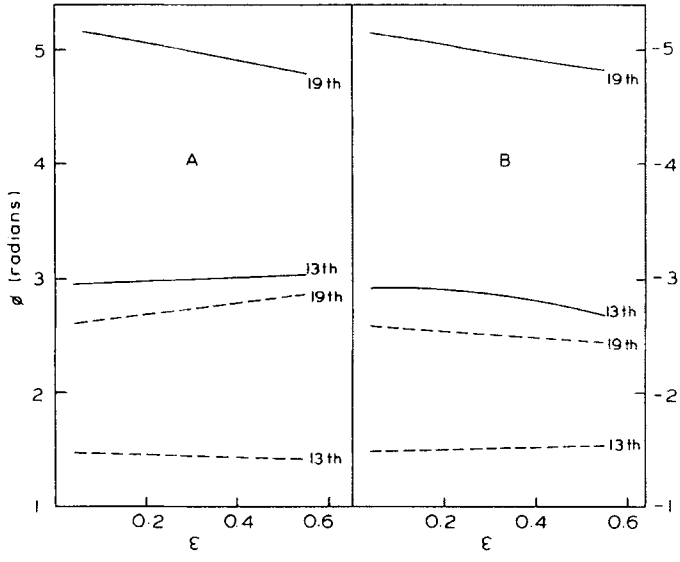

FIGURE 5 Director orientation ϕ as a function of ε at the 13th and 19th collocation points for (A) $1, \frac{1}{2}$ and (B) $-1, -\frac{1}{2}$ singularities.

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