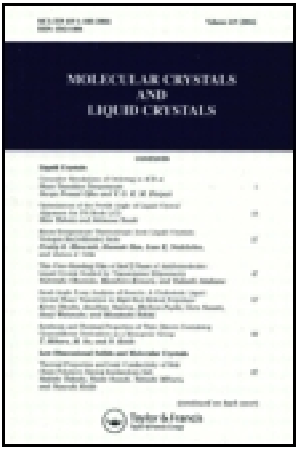

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Measurement of Disclination Energies in a Nematic Liquid Crystal

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Measurement of the equilibrium voltage for coexistence of disclination walls (Bloch walls) and pairs of singular disclination lines are presented. The temperature and the measuring-cell spacing have been varied. The results have been analysed to yield values for two characteristic quantities of the singular lines. While the elastic part agrees reasonably well with existing theories the temperature dependence of the core part shows no indication of features postulated in a recent blue-phase model.

1. INTRODUCTION

Singular lines in nematic liquid crystals have been of interest for some time.[1] Most of the previous investigations dealt with topological and qualitative aspects. Quantitative treatments are faced with a number of difficulties. The energy of line singularities is dependent and diverges with two cutoffs the lower or core cutoff and the upper cutoff which is determined by the experimental boundary conditions. For the most simple conditions the line tension T (energy per unit length) is given by [1]

$$T = \pi k m^2 \ln \frac{R}{a_{\text{eff}}} \tag{1.1}$$

where k is the curvature elastic constant in a one constant system ($k_{11} = k_{22} = k_{33} = k$), m is the disclination strength[2] ($m = \frac{1}{2}$ in our case) and R and a_{eff} are upper and lower cutoff. The most interesting quantity is a_{eff}. It contains information about the scale at which the continuum elastic theory with an order parameter of constant value starts to break down. Furthermore it contains an energy contribution from the disclination core.

In experimentally realizable systems a couple of complications arise. There seems to be no known substance with equal elastic constants. Continuously changing boundary conditions which are required for (1.1) in the case of $m = \frac{1}{2}$ can not be produced, not to speak of the unknown values of the boundary conditions for the case of differing elastic constants. For given fixed boundary conditions, calculating the director configuration is a formidable numerical task given the director arrangement in the neighbourhood of the disclination line. But this arrangement and its dependence on the elastic constant ratios is only known in a few simple model cases.[3]

In recent years the accurate structure and energy of disclination has become a subject of increased interest due to models for the blue phases of small-pitch cholesterics which postulate as structure a lattice of disclination-lines.[4,5]

Considering these points, experimental information on disclination lines seems to be of interest. An easy experimental access appears to be the observation of the equilibrium between Bloch-walls and pairs of disclination lines ('pincement'[1]) which has been observed by several authors[6,7] and from which an estimate for disclination line tension has been deduced.[7]

2. EXPERIMENTAL

We have utilized the liquid crystal PCH7 (trans-4-*n*-heptyl-(4'-cyanophenyl)-cyclohexane) which shows a fairly extended mesophase range including (metastably) room temperature. Elastic constants and dielectric properties are known.[8] Three sandwich cells of 8.98, 22.13 and 55.21 μm spacing have been used, the conducting surfaces of which were treated by evaporation of silicon oxide to induce homogeneous in-plane director-alignment. The cells were mounted such that the alignment directions of top and bottom substrates were parallel. Upon application of voltages above the Frederiks voltage

$$V_0 = \pi\sqrt{k_{11}/(\epsilon_0 \Delta\epsilon)} \tag{2.1}$$

the director in the middle of the cell rotates in either of two possible

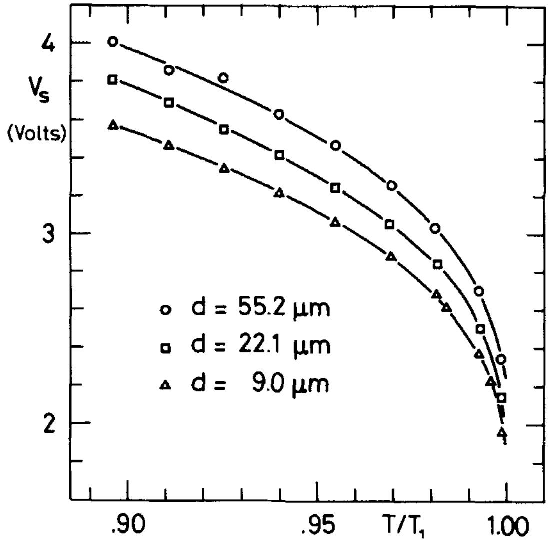

FIGURE 1 Measured voltages V_s for equilibrium between disclination wall and pair of singular disclination lines versus temperature for three different cell-spacings. Within the uncertainties of measurement no dependence on the orientation of the wall with respect to the surface-induced director-alignment direction could be observed. Temperature is in units of the clearing temperature T_1.

directions to achieve alignment with the applied electric field. Domains of opposite rotation are separated by Bloch-type walls.[9,10] At fairly elevated voltages these walls split into a pair of disclination lines with the splitting point moving quickly along the wall. By reducing the voltage this splitting point can be made stationary. The voltage of stationary V_s has been measured as a function of temperature in the three differently spaced cells. Figure 1 shows these measurements. The thickness-dependence is small, considered the variation of spacing-values by a factor of six. For later comparison Figure 2 shows the temperature dependence of elastic properties as taken from Ref. 8.

3. DISCUSSION

A major problem in interpreting the above measurements is the rather difficult mathematical access from the measured quantities to the properties of disclination lines. The equilibrium condition states that at the given voltage V_s the free energy of a wall configuration as

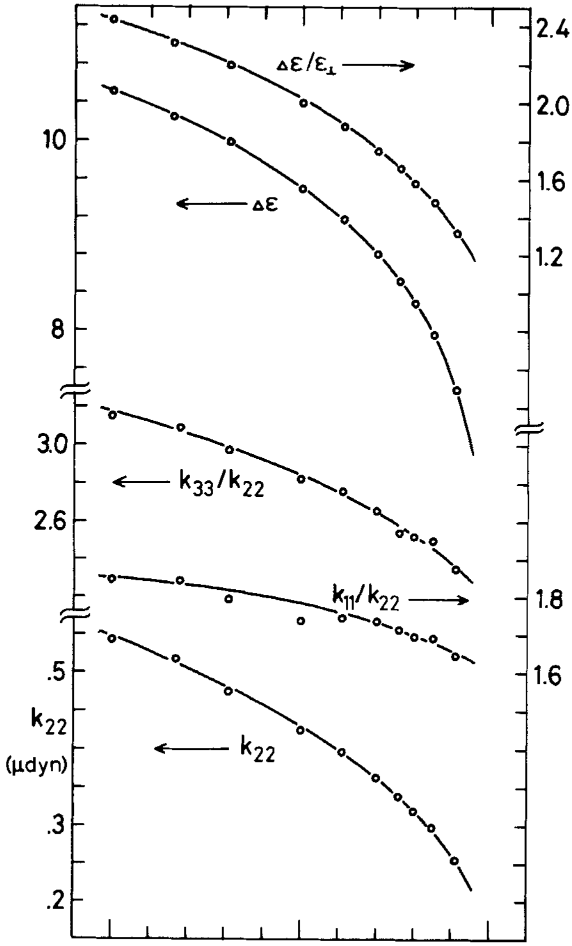

FIGURE 2 Elastic and dielectric properties of PCH7 versus temperature as taken from Ref. 8. (Abscissa as in Figure 1).

sketched in Figure 3a is equal to the free energy of the configuration of Figure 3b which includes two $m = \frac{1}{2}$ disclination lines. With the given material parameters, calculation of those requires heavy numerical work. We utilize here an approximate treatment.

The wall energy E_w per unit length is given in the limit of large spacing d by the bulk term[9]

$$\frac{1}{2}E_w \approx \pi k_{22}\frac{V_s}{V_2}, \qquad d \to \infty \tag{3.1}$$

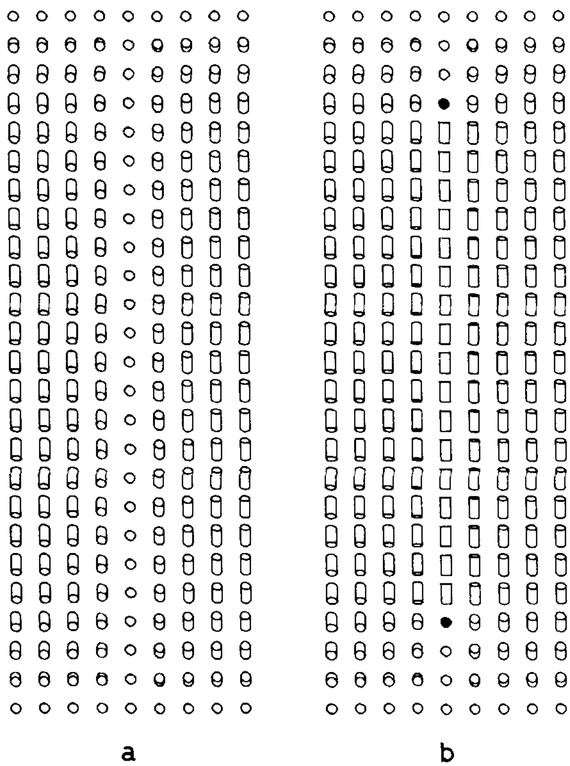

FIGURE 3 Qualitative pictures for director configurations for a twist-disclination wall (a) and a pair of disclination lines (b) (dark spots). The disclinations are drawn as pure $m = \frac{1}{2}$ twist lines.

where

$$V_2 = \pi \sqrt{\frac{k_{22}}{\Delta\epsilon\epsilon_0}} \tag{3.2}$$

is written in analogy to Frederiks threshold voltage (2.1). The deformed regions near the substrates give corrections of the order of ζ_2/d where ζ_2 is a coherence length[10]

$$\zeta_2 = \frac{k_{22}}{\Delta\epsilon\epsilon_0} \cdot \frac{d}{V} = \frac{1}{\pi} \cdot \frac{V_2}{V} d. \tag{3.3}$$

Since the applied voltages in Figure 1 are well above the Frederiks threshold V_0 (2.1), we expect that the wall energy E_w can be written as a Taylor-expansion in increasing powers of V_2/V

$$\frac{E_w}{2\pi k_{22}} = \frac{V}{V_2} + A_0 + A_1\frac{V_2}{V} + \cdots, \tag{3.4}$$

in which, taken rigid boundary conditions for granted, the coefficients are independent of the cell spacing d. For the configuration of Figure 3b the situation is different due to the cutoff term of Eq. (1.1). Here it is appropriate to divide the energy into two contributions by a suitable choice of a cylindrical region of radius ρ_d about each disclination line. ρ_d is chosen proportional to d but small compared to the coherence length (3.3)

$$\rho_d \ll \zeta_2 \tag{3.5}$$

This choice ensures that the energy contribution from the core region is truly inherent to the nature of the singularity while the outer part now obeys true scaling and allows for an expansion analogous to (3.4). Thus the energy of the singular director configuration of Figure 3b E_s can be written as

$$\frac{E_s}{2\pi k_{22}} = B_0 + B_1\frac{V_2}{V} + \cdots + \kappa_s m^2 \ln\frac{\rho_d}{a_{\text{eff}}} \tag{3.6}$$

where obviously a term proportional to V/V_2 must be absent in the outer region-energy. In the last contribution the parameter κ_s describes the effective elastic constant in units of k_{22} which must be chosen to describe the singularity in a form similar to (1.1).

Equating (3.4) and (3.6) for the critical voltage V_s yields

$$\frac{1}{4}\kappa_s \ln\frac{\rho_d}{a_{\text{eff}}} = \frac{V_s}{V_2} + A_0 - B_0 + (A_1 - B_1)\frac{V_2}{V_s} + (A_2 - B_2)\left(\frac{V_2}{V_s}\right)^2 + \cdots \tag{3.7}$$

Figure 1 shows that the voltages V_s vary by only 10% when d changes by a factor of six. Thus, the correction terms in (3.7) may safely be neglected when evaluating the d-dependence, particularly so, because any possible corrections come in only in second order in V_2/V_s. Therefore, we have analysed V_s/V_2 in a form

$$V_s/V_2 = C_0 + \tfrac{1}{4}C_1 \ln d \tag{3.8}$$

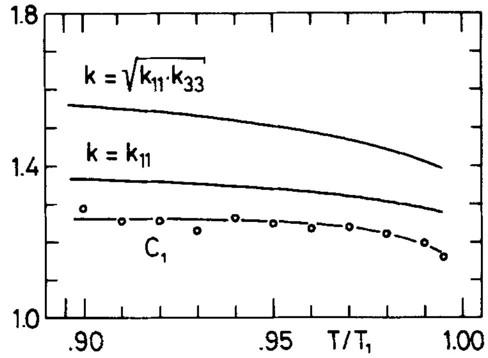

FIGURE 4 Temperature dependence of the values for the coefficient C_1 as fitted to the data of Figure 1 for the form (3.8). Also shown are values for κ_s (3.9) as calculated from the elastic data of Ref. 8 (Fig. 2) for $k = \sqrt{k_{11}k_{33}}$ and $k = k_{11}$.

where, remembering the proportionality between d and ρ_d, the coefficient C_1 represents a value for κ_s. Figures 4 and 5 show the coefficients C_1 and C_0 as determined from the measurements of Figures 1 and 2 as a function of temperature.

Ranganath[3] has considered twist disclinations and arrived at a result for the case $k_{11} = k_{33} = k$, k_{22} arbitrary, which may be applied approximately to our situation. His result is

$$\kappa_s = \sqrt{k/k_{22}}\,. \tag{3.9}$$

Figure 4 shows the corresponding values as calculated from the data of Figure 2 by setting $k = \sqrt{k_{11} \cdot k_{33}}$ and, as the most favourable case, by setting $k = k_{11}$. Considering the uncertainties in the evaluation procedure, there is fair agreement though the calculated values are somewhat high.

To get lower values than the $(k = k_{11})$-case probably requires relaxation of the condition of planar director-configuration which was made in Ref. 3.

The discussion of the coefficient C_0 must be on a more speculative footing. Let us assume that the energy contributions of the surface region are similar for the two configurations of Figures 3a and 3b. Thus setting $\rho_d = \bar{\zeta} = \zeta_2\sqrt{k/k_{22}}$, $k = \sqrt{k_{11}k_{33}}$ we may approximately equalize $A_i = B_i$ in equation (3.7) and arrive at

$$\tfrac{1}{4}\kappa_s \ln(\bar{\zeta}/a_{\text{eff}}) \cong C_0 + \tfrac{1}{4}C_1 \ln d \tag{3.10}$$

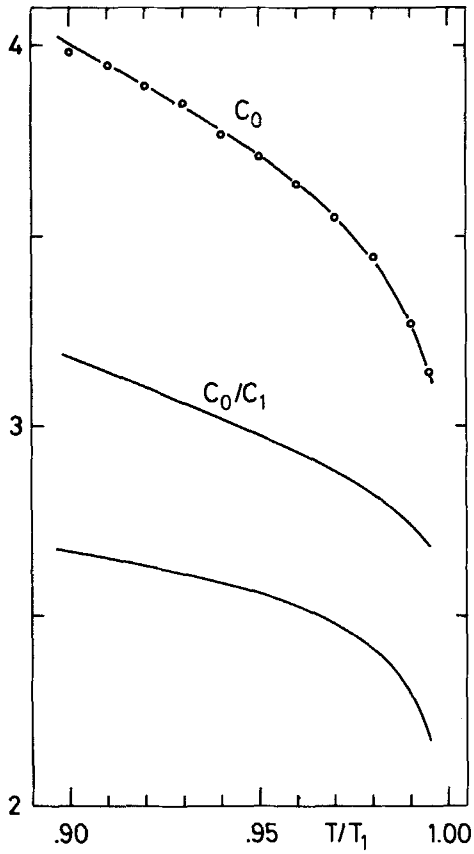

FIGURE 5 Temperature dependence of the fitted parameter C_0 (3.8). Also shown is the ratio C_0/C_1 as obtained from the smoothed curves. In addition the values predicted by Ref. 5 are shown as calculated from (3.12) with $k = \sqrt{k_{11}k_{33}}$ and $a = 8 \cdot 10^4$ erg cm^{-3} K^{-1} (bottom curve). The measurements do not indicate the postulated logarithmic singularity.

which, with $C_1 = \kappa_s$ and (3.3), leads to

$$-\frac{1}{4}\ln a_{\text{eff}} \cong \frac{C_0}{C_1} + \frac{1}{4}\ln\frac{d}{\xi} \cong \frac{C_0}{C_1} + \frac{9}{16}. \tag{3.11}$$

Figure 5 shows the quantity C_0/C_1 as calculated from the smoothed values of C_0 and C_1. It characterizes the core energy as a function of temperature.

In the theory of Meiboom *et al.*[4,5] the corresponding quantity would read

$$-\frac{1}{4}\ln a_{\text{eff}} - \frac{9}{16} = -\frac{7}{16} - \frac{1}{4}\ln\frac{k}{8a(T_1 - T)} \tag{3.12}$$

where T_1 is the first order isotropic–mesophase transition temperature and a is the entropy of transition. For comparison we have also drawn the graph of the right hand side of (3.12) taking $k = k_{22} \cdot C_1^2$ (see 3.9) and a value of $8 \cdot 10^4$ erg cm^{-3} K^{-1} for a.[5] Since the average elastic constant k approaches a finite limit, this model predicts a logarithmic divergence at T_1. It is evident from Figure 4 that our measurements show no indication of such a divergence but rather seem to reach a finite value of roughly $C_0/C_1 \sim 2.5$.

In conclusion, we have measured the equilibrium voltage for coexistence of inversion walls and pairs of singular disclination lines as a function of temperature and for widely varying cell spacings. The results led to values for the coefficient of the logarithmic term and to an estimate for the effective lower cutoff radius in the expression for the disclination energy. The result of the former agrees reasonably with existing theories while the latter misses features postulated in recent models.

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