Thermomechanical effects in deformed nematics

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A number of specific effects peculiar to the director-distribution inhomogeneity in nematic liquid crystals are discussed. These include: 1) the onset of hydrodynamic flow due to the temperature gradient, 2) the onset of a temperature drop in an inhomogeneous flow, and 3) additional deflection of the director by the heat flow. An expression is obtained for the bulk rate of entropy generation, i.e., for the dissipation function divided by the temperature. Variation of this function permits a description of the foregoing effects and leads automatically to the Onsager relations between their constants. The constants are estimated and the possibility of experimentally recording the effects is discussed.

1. INTRODUCTION

Thermomechanical effects for cholesteric liquid crystals (CLC) were considered in Ref. 1 (see also the review by Stephen and Straley[2]). These effects are uniquely related to the chirality of the cholesterics, i.e., to the fact that they have no right-left symmetry. The thermomechanical effect in CLC was experimentally recorded in Refs. 3–5. Its gist is that application of a temperature gradient to a homeotropically oriented cell deflects the director by $\delta\mathbf{n}\approx\mathrm{const}\,[\mathbf{n}\times\nabla]T$. Contributing to the pseudoscalar constant were the thermomechanical effect proper, as well as the temperature dependence of the reciprocal pitch. The experiments were performed on a compensated CLC, i.e., on one in which q_0 vanished at a certain temperature.

In typical cholesterics, the chiral parameter $q_0\sim 10^4$ cm^{-1} is approximately 10^3 times smaller than the reciprocal size of the molecule $a^{-1}\sim 10^7$ cm^{-1}. The reason is the relatively weak influence of the chiral terms on the intermolecular interaction. Presumably, this is also the reason why the thermomechanical-effect constant, estimated experimentally in Ref. 5 at $\lambda\sim 10^{-3}$ dyn/cm·deg, is 10^3 times smaller than the natural estimate (see Sec. 3 below) $\lambda\sim(\eta\Lambda/T)^{1/2}$, where $\eta\sim 1$ is the orientational viscosity, $\Lambda\sim 10^4$ erg/cm·sec·deg is the thermal conductivity, and $T\approx 300$ K.

We discuss in this paper a number of thermomechanical effects for non-chiral LC, namely for nematics. It follows from space-symmetry considerations that for nematics to be produced the unperturbed distribution of the director must be spatially nonuniform.

In Sec. 2 are discussed some of the simplest thermomechanical effects in NLC and their observable manifestations. Estimates are given in Sec. 3 for the constants of the corresponding effects and in Sec. 4 for the possible values of the parameters that are observable under various experimental conditions. Possible manifestations of thermomechanical effects heretofore not discussed for cholesterics are briefly considered in Sec. 5. The Appendix contains the most general form of the rate of entropy production (i.e., the dissipation function divided by the temperature). This expression enables us to write down all the relevant thermomechanical terms of the NLC dynamics equations. The Onsager equations, which express the principle of symmetry of the kinetic coefficients, are automatically obtained by this approach.

2. PHENOMENOLOGICAL EXPRESSIONS FOR SOME SIMPLEST THERMOMECHANICAL EFFECTS

The invariance of the NLC dynamics equations to the rotation group does not prevent the existence of, e.g., the following corrections to the director rate of change $\partial n/\partial t$, to the stress tensor $\sigma_{ik}^{\mathrm{TM}}$, and to the het flow q_{TM}:

$$\sigma_{ik}{}^{\mathrm{TM}}=\xi'\nabla_i T[\mathbf{n}\times\mathrm{rot}\,\mathbf{n}]_k, \tag{1}$$

$$T^{-1}q_i{}^{\mathrm{TM}}=\xi''(\partial v_k/\partial x_i)\,[\mathbf{n}\times\mathrm{rot}\,\mathbf{n}]_k, \tag{2}$$

$$\beta_1\frac{\partial\mathbf{n}}{\partial t}=\xi'''(\mathbf{n}\,\mathrm{rot}\,\mathbf{n})\,[\mathbf{n}\times\nabla]T. \tag{3}$$

Here β_1 is the orientational viscosity, $\partial v_k/\partial x_i$ is the velocity gradient in the flow, and $\mathbf{n}$ is the director unit vector, with $\mathbf{n}$ and $-\mathbf{n}$ equivalent. We recall that the stress tensor $\sigma_{ik}^{\mathrm{TM}}$ in nematics need not be symmetric. All three constants (ξ', ξ'', and ξ''') have the dimension erg/cm deg. It is possible to set up for the corrections to $\partial\mathbf{n}/\partial t$, $\sigma_{ik}^{\mathrm{TM}}$, and q_{TM} many more phenomenological expressions that satisfy the space-invariance conditions and describe the thermomechanical effects of interest to us. We shall provide a complete list in the Appendix, and discuss at present the experimental results that can ensue from the indicated terms.

Consider an NLC cell having the so-called hybrid orientation (Fig. 1). We direct the normal to the cell walls along the z axis and assume that the boundary condition on the wall specifies a hometropic orientation $\mathbf{n}(z=0)=\mathbf{e}_z$ at $z=0$ and a planar orientation $\mathbf{n}(z=L)=\mathbf{e}_x$ at $z=L$, where L is

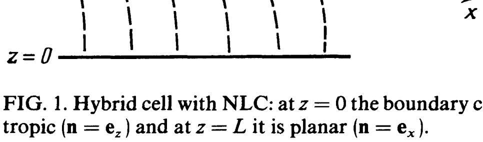

FIG. 1. Hybrid cell with NLC: at $z=0$ the boundary condition is homeotropic ($\mathbf{n}=\mathbf{e}_z$) and at $z=L$ it is planar ($\mathbf{n}=\mathbf{e}_x$).

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the cell thickness. Let the external heat sources maintain a temperature $T = T_0$ at the section $z = 0$ and a temperature $T = T_0 + \Delta T$ in the section $z = L$. The temperature gradient $dT/dz \sim \Delta T/L$ leads then, according to Eq. (1), to tangential stresses $\sigma_{zx}^{\mathrm{TM}} \simeq \xi' \Delta T/L^2$. The result is liquid flow in the x direction. The stationary velocity v in this flow can be roughly estimated by equating the thermomechanical and Navier-Stokes contributions to σ_{ik}. Assuming for the latter $\sigma'_{zx} \approx \eta v/L$, where η is the viscosity, we obtain

$$v \approx \xi' \Delta T/L\eta. \tag{4}$$

Introducing a specific liquid flow $Q = vL$ with dimension cm^2/sec, we obtain for it from (4) the estimate

$$Q \approx \xi' \Delta T/\eta. \tag{5}$$

In another possible experiment, external mechanical sources produce in an identical hybrid cell a nonuniform flow $\mathbf{v} = \mathbf{e}_x v(z)$. This can be Poiseuille flow if the walls are immobile or Couette flow if one wall moves relative to the other in the x direction. A z component of the heat flow $q_z \approx T_0 \xi'' v/L^2$ can then appear, according to (2). This flow produces a temperature difference $\Delta T_1 = T(L) - T(0)$ between the walls. A stationary value of ΔT_1 can be obtained by equating the obtained quantity qz to the counterflow $\Lambda \Delta T_1/L$ due to the thermal conductivity of the medium. As a result we get the estimate

$$\Delta T_1 \sim T_0 \xi'' v/\Lambda L. \tag{6}$$

To discuss the observed consequences of expression (3), we consider a planar twist-cell with a nematic (Fig. 2), in which the unperturbed distribution of the director is of the form

$$\mathbf{n}(z) = \mathbf{e}_x \cos\theta(z) + \mathbf{e}_y \sin\theta(z),$$
$$\theta(z) = \pi z/2L. \tag{7}$$

We assume that a temperature gradient $\Delta T/X$ is applied in the x direction, so that $T(x) = T_0 + x\Delta T/X$. It is easy to verify that even if account is taken of the dependence of the Frank constants K_1, K_2, and K_3 on the coordinate x (via their temperature dependence) a structure of the form (7) remains an exact solution of the usual equilibrium equations for a nematic. Inclusion of the term (3) produces a director deflection due exclusively to the thermomechanical effect. To estimate this deflection we can equate the force (3) to the elastic Frank force due to the additional deformation of the director. We can write also exact equilibrium relations. At $K_1 \approx K_2 \approx K_3$ we have in the stationary case $\partial \mathbf{n}/\partial t = 0$ and

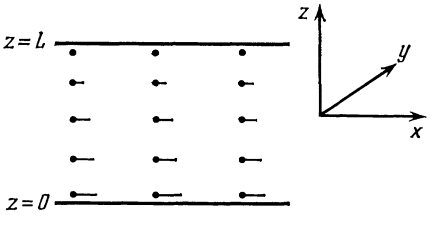

FIG. 2. Twist cell with NLC: planar orientation of the director is specified on both walls, with $\mathbf{n}(z=0) = \mathbf{e}_x$ and $\mathbf{n}(z=L) = \mathbf{e}_y$.

$$K\frac{d^2 n_z}{dz^2} - \frac{\pi}{2L}\xi''' \frac{\Delta T}{X} n_y = 0, \tag{8}$$

whence

$$n_z = \frac{2}{\pi}\frac{\xi'''}{K}\frac{L}{X}\Delta T\left(\frac{z}{L} - \sin\frac{\pi z}{2L}\right). \tag{9}$$

The maximum value of the expression in the parentheses in (9) is 0.21 and is reached at $z \approx 0.56L$.

3. ESTIMATE OF THE CONSTANTS OF THE THERMOMECHANICAL EFFECTS

We consider some system described by two generalized velocities $\dot{x}$ and $\dot{y}$. The most general form of the dissipative function that describes the relaxation of x and y in the linear approximation is

$$R = {}^1/_2(a\dot{x}^2 + 2b\dot{x}\dot{y} + c\dot{y}^2). \tag{10}$$

It is easy to verify that the standard condition that the dissipative function not be negative yields $a > 0$ and $c > 0$. In addition, rewriting R of Eq. (10) in the form

$$R = (\dot{x}\sqrt{a} + b\dot{y}/\sqrt{a})^2 + (ac - b^2)\dot{y}^2/a,$$

we find that the requirement that R not be negative imposes one more condition:

$$b = \rho(ac)^{1/2}, \qquad |\rho| \leqslant 1. \tag{11}$$

In the absence of a coupling between the relaxations of x and y, the dimensionless parameter $\rho = 0$. If, however, there are no special reasons for the coupling between these relaxation processes to be small, we have generally speaking $|\rho| \sim 1$, and then the exact inequality $|\rho| \leqslant 1$ must hold.

Similar relations lead to the inequalities that are satisfied by the Leslie constants in nematodynamics problems (see Refs. 2, 6, and 7). Namely, we choose the following generalized velocities of the nematic:

$$\mathbf{N} = d\mathbf{n}/dt + {}^1/_2[\mathbf{n} \times \operatorname{rot} \mathbf{v}], \quad D_0 = n_i n_i d_{ij},$$
$$D_i = d_{ij} n_j - n_i D_0, \quad D_{ij} = d_{ij} - {}^1/_2(3n_i n_j - \delta_{ij}) D_0 - n_i D_j - n_j D_i. \tag{12}$$

Here

$$d_{ij} = ({}^1/_2)(\partial v_i/\partial x_j + \partial v_j/\partial x_i)$$

is the velocity-gradient tensor; we assume the nematic to be incompressible, so that $d_{ii} = \operatorname{Tr} d = 0$. The form (12) corresponds to an expansion, in irreducible representation of a one-parameter group, of rotation about an axis that coincides with the preferred direction $\mathbf{n}$ (cf. Ref. 8). The quantity D_0 is the scalar of this group, while N and D are two independent two-dimensional ($\mathbf{N} \cdot \mathbf{n} = 0$ and $\mathbf{D} \cdot \mathbf{n} = 0$) vectors of this group, while D_{ij} is a zero-trace tensor in a plane perpendicular to n. The most general dissipative function, which is bilinear in the indicated "velocities" and invariant to rotations about the $\mathbf{n}$ axis, is

$$R\,[\mathrm{erg/cm^3 \cdot sec}] = {}^1/_2(\beta_0 D_0{}^2 + \beta_1 \mathbf{N}^2 + \beta_2 \mathbf{D}^2 + 2\beta_{12}\mathbf{N}\mathbf{D} + \beta_3 D_{ik} D_{ki}). \tag{13}$$

In connection with all the foregoing it is obvious that the coefficients β from (13) satisfy the inequalities

$$\beta_0 \geqslant 0, \quad \beta_1 \geqslant 0, \quad \beta_2 \geqslant 0, \quad \beta_3 \geqslant 0,$$
$$\rho_{12} = \beta_{12}/(\beta_1+\beta_2)^{1/2}, \quad |\rho_{12}| \leqslant 1. \tag{14}$$

The standard symbols α_i for the Leslie coefficients are connected with our coefficients β_i by the relations

$$\beta_0 = \alpha_1 + {}^3/_2\alpha_4 + \alpha_5 + \alpha_6, \quad \beta_1 = \alpha_3 - \alpha_2,$$
$$\beta_{12} = \alpha_3 + \alpha_2, \quad \beta_2 = 2\alpha_4 + \alpha_5 + \alpha_6, \quad \beta_3 = \alpha_4. \tag{15}$$

Variation of R of Eq. (13) with respect to $\partial v_i/\partial x_k$ yields the viscous stress tensor σ'_{ki}, and variation of the same function with respect to N yields the "force" that reorients the director (see the Appendix). Equations (15) together with the conditions (14) were first obtained by Leslie[9] by a noticeably more complicated method (see also Refs. 2 and 6).

Substitution of the numerical values shows that $\rho_{12} \approx 0.7$ for the nematic MBBA. We wish to illustrate once more by means of this example the statement that the coefficient $|\rho|$ turns out to be of the order of unity in the absence of special factors that make the coupling weak.

We know that heat flow through heat conduction can be obtained by varying the entropy production rate $\dot{S}$ [erg/cm^3 · sec · deg] = $2R/T$ over the temperature gradient:

$$q_i = -T\delta R/\delta(\nabla_i T). \tag{16}$$

In particular, the standard equation of thermal conductivity in a nematic is obtained by taking R in the form

$$R = {}^1/_2 T^{-1}[\Lambda_\parallel((\mathbf{n}\nabla)T)^2 + \Lambda_\perp(\nabla T - \mathbf{n}(\mathbf{n}\nabla)T)^2], \tag{17}$$

where $\Lambda_\parallel > 0$ and $\Lambda_\perp > 0$ are respectively the longitudinal and transverse components of the thermal conductivity tensor.

The thermomechanical effect in cholestrics is described by to terms in R:

$$R_{\mathrm{TM}}^{\mathrm{CLC}} = -\lambda'\mathbf{N}[\mathbf{n}\times\nabla]T - \lambda''\mathbf{D}[\mathbf{n}\times\nabla]T. \tag{18}$$

The constants λ' and λ'' have the dimensionality dyn/cm · deg. Combining (13), (17), and (18) and recognizing that

$$(\nabla T - \mathbf{n}(\mathbf{n}\nabla)T)^2 = ([\mathbf{n}\times\nabla]T)^2,$$

we can obtain from the non-negativity condition inequalities in the form

$$\rho'^2 + \rho''^2 + \rho_{12}{}^2 - 2\rho'\rho''\rho_{12} \leqslant 1,$$
$$\rho'^2 \leqslant 1, \quad \rho''^2 \leqslant 1, \quad \rho_{12}{}^2 \leqslant 1, \tag{19}$$

where ρ_{12} is defined in (14),

$$\rho' = \lambda'(\beta\Lambda_\perp/T)^{-1/2}, \quad \rho'' = \lambda''(\beta_2\Lambda_\perp/T)^{-1/2}.$$

Experiment yields for the parameters $|\rho'|$ and $|\rho''|$ estimates of the order of 10^{-3}. As already noted in the Introduction, there are special grounds for this result—smallness of the chiral contributions to the interaction between the molecules.

Our sought thermomechanical effects in nematics are given by R terms of the following approximate form:

$$R_{\mathrm{TM}} \approx \tilde{\xi}(\nabla T)(\nabla n)N + \tilde{\tilde{\xi}}(\nabla T)(\nabla n)(\partial v/\partial r). \tag{20}$$

We purposely do not specify here the tensor structure of the expressions in (20), relegating the details to the Appendix. The constants $\tilde{\xi}$ and $\tilde{\tilde{\xi}}$ in (20) have dimensionality erg/cm · deg and, apart from a change in the tensor notation, have the same meaning as the constants ξ', ξ'', and ξ''' introduced in Eqs. (1)–(3).

The term of type (20) in the dissipative function can be regarded as a cross term with respect to two "generalized velocities" ∇T and $(\partial n/\partial t)\nabla n$ or ∇T and $(\partial v/\partial r)\nabla n$. The square of the second of these "velocities" should have entered the dissipative function in the form

$$R_{\mathrm{mech}} \approx \mu[(\nabla n)\partial v/\partial r]^2. \tag{21}$$

The coefficient μ has the dimension P · cm^2. Since (22) contains two more differentiations with respect to the spatial coordinates than the expression (13) for R, it can be assumed that the corresponding estimate of μ contains two extra powers of the molecular dimension a compared with the viscosity constants β from (13): $\mu \sim \beta a^2$.

The hypothesis we wish to advance concerning the thermomechanical-effect constants is that the dimensionless parameters ρ corresponding to them have no special small quantity, $|\rho| \sim 1$. This yields the estimate $\xi \sim (\mu\Lambda/T)^{1/2}$ or

$$\xi \sim a(\eta\Lambda/T)^{1/2}, \tag{22}$$

where account is taken of the fact that the constants β are of the order of the viscosity coefficients η.

4. NUMERICAL ESTIMATES OF THE THERMOMECHANICAL EFFECTS IN NLC

We use in the estimates the coefficient values $\eta \sim 1$ P for the viscosity and $\Lambda \sim 10^4$ erg/cm · sec · deg for the thermal conductivity; we assume a temperature $T \sim 300$ K and a molecule size $a \sim 10^{-7}$ cm. We then obtain from (23) $\xi \sim 10^{-6}$ erg/cm deg.

For the hybrid cell of Sec. 2, with a wall-temperature difference $\Delta T \sim 10$ K, we obtain from (4) and (5) at a thickness $L \sim 10^{-3}$ cm a flow $Q \sim 10^{-5}$ cm^2/sec at a velocity $v_x \sim 10^{-2}$ cm/sec. In this case $v \propto L^{-1}$ and Q is independent of L. In our opinion such a flow and its velocity are easy to detect in experiment. One can therefore hope to observe the discussed thermomechanical effect even if the constant ξ is smaller by a factor 10^2–10^3 than the foregoing estimate.

Assume that Couette flow with a velocity difference $v \sim 0.1$ cm/sec is produced in the same hybrid cell by relative displacement of the walls. It is convenient here to use a thinner cell, $L \sim 10^{-4}$ cm. According to (6), the thermomechanical effect should produce then a temperature jump $\Delta T \sim 0.3 \cdot 10^{-4}$ K. This figure can quite reasonably expected to be observable in experiment. We note that we have taken the velocity v to be such that at the given cell thickness no orientational instability sets in as yet in the Couette flow in the nematic (see Ref. 10). Simple estimates show also that the temperature rise of the medium owing to energy dissipation in the viscous flow is, at the indicated parameter values, smaller by a factor 10^2–10^3 than the temperature drop to the thermomechanical effect of interest to us.

Finally, for the nematic twist cell discussed in Sec. 2 we have a temperature $\Delta T \approx 10$ K in the plane of the cell over a length $X \approx 10L$. Equation (9) yields then a director deflection angle $n_z \sim 0.1$ rad. Since n_z is independent of the cell thickness L at a fixed L/X, we can put $L \gtrsim 10^{-2}$ cm. At such a thickness it is not difficult to measure the indicated deflection by optical methods.

We have considered above phenomena that appear already in first-order perturbation theory in the thermomechanical-effect constants ξ. By the same token, the corresponding processes have a thresholdless dependence on the external action. The situation here is analogous to the Fréedericksz effect in an oblique (relative to the director) field. On the other hand, threshold Fréedericksz transitions are also known to be of great interest. Threshold phenomena due to the thermomechanical terms in the dynamic equations of nematics are similarly possible. We shall not discuss these threshold effects here.

We have considered above bulk effects in a liquid crystal, in which case the terms of interest to us contain an extra power of the molecular small parameter a. On the other hand, there is every reason for assuming that in the case of a layer of thickness a the usual hydrodynamic equations no longer hold near the interface of the liquid and the solid. In other words, one can expect corrections of first order in the parameter a to be added to the usual boundary conditions for the hydrodynamic variables (cf. the thermomechanical effect in gases[11]). We do not consider such "surface" contributions here. In addition, the quantities in the dynamic equations, such as entropy and pressure, should contain additional (relative to the equilibrium values) terms starting with second order in the velocity and temperature gradients. We disregarded these additional terms, too.

5. THERMOMECHANICAL EFFECTS IN CHOLESTERICS

Variation of the sum of (13), (17), and (18) yields expressions for the viscous-stress tensor, for the heat flow, and for the director-deflecting force. We write down here the terms corresponding to the thermomechanical effects in CLC:

$$\sigma_{ik}^{\mathrm{TM}} = -{}^1/_2(\lambda'+\lambda'')n_k[\mathbf{n}\times\nabla]_i T + {}^1/_2(\lambda'-\lambda'')n_i[\mathbf{n}\times\nabla]_k T, \tag{23}$$

$$\mathbf{q}^{\mathrm{TM}} = -T\lambda'[\mathbf{n}\times\mathbf{N}] - T\lambda''[\mathbf{n}\times\mathbf{D}], \tag{24}$$

$$\beta_1 \partial\mathbf{n}/\partial t = -\lambda'[\mathbf{n}\times\nabla]T. \tag{25}$$

By the same token, different thermomechanical effects in cholesterics turn out to be connected with one another by the Onsager symmetry relations.[12,2] In our treatment these relations are obtained extremely easily, namely, by merely varying a single dissipative function. We note that a factor, the absolute temperature, was left out of the expression corresponding to our (25) in the splendid review[2].

The thermomechanical deflection of the director, due according to (25) to the temperature gradient, was observed experimentally in Refs. 3–5. The quantity measured there was proportional to $\lambda' + K_2 dq_0/dT$, where K_2 is a Frank constant and $q_0 = 2\pi/h$ is the wave vector of the equilibrium cholesteric spiral. In this section we discuss possible measurements of the quantity $\lambda' - \lambda''$.

Consider a cholesteric cell whose two walls, $z = 0$ and $z = L$, maintain a homeotropic orientation (Fig. 3). At $q_0 L \leqslant \pi K_3/K_2$, the orientation is then known to be homeotropic in the entire volume of the cell. Assume that the cholesteric is bounded not only by walls $z = 0$ and $z = L$, but also by walls $x = 0$ and $x = X$ that maintain the same orientation. We specify the following temperature profile on these walls:

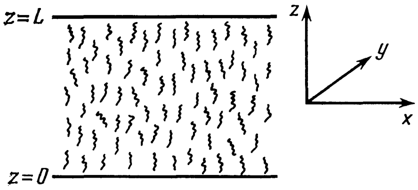

FIG. 3. Homeotropically oriented cholesteric liquid crystal with compensated pitch.

$$T(x, z=0) = T(x=0, z) = T_0, \quad T(x, z=L) = T_0 + \Delta T(x/X),$$
$$T(x=X, z) = T_0 + \Delta T(z/L). \tag{26}$$

The stationary solution of the heat-conduction equation yields then the temperature profile in the bulk:

$$T(x, z) = T_0 + \Delta T(x/X)(z/L). \tag{27}$$

The presence of a temperature gradient leads according to (23) to the onset of shear stresses $\sigma_{zy}^{\mathrm{TM}}$. Moreover, the force $f_i^{\mathrm{TM}} = \partial\sigma_{ki}^{\mathrm{TM}}/\partial x_k$ [dyn/cm^2] acting on a unit volume is likewise different from zero at the temperature profile (27)

$$f_y^{\mathrm{TM}} = {}^1/_2(\lambda'-\lambda'')\Delta T/LX. \tag{28}$$

Under the action of this force, the liquid begins to flow in the direction of the y axis. To determine the stationary flux, expression (28) must be equated to the viscous-friction forces:

$$\partial\sigma_{zy}'/\partial z = \eta_2 \partial^2 v_y/\partial z^2,$$

whence

$$v_y = \Delta T \frac{\lambda''-\lambda'}{16\eta_2}\frac{L}{X}\frac{4z(L-z)}{L^2}, \tag{29}$$

where $\eta_2 = (\alpha_4 + \alpha_5 - \alpha_2)/2$ is the Miesowicz viscosity coefficient. The total liquid flow W [cm$^{-3}\cdot$sec^{-1}] is equal to

$$W = \iint v_y\,dx\,dz = L^2\Delta T(\lambda''-\lambda')/24\eta_2. \tag{30}$$

Assuming by way of estimate $\Delta T = 10$ K, $L/X \sim 0.1$, $\eta_2 \sim 1$ poise and $\lambda'' - \lambda' \sim 10^{-3}$ erg/cm$^2\cdot$deg, we get $v_y \sim 10^{-4}$ cm/sec and for $L \sim 10^{-2}$ we obtain $W \sim 0.5 \cdot 10^{-7}$ cm^3/sec. In our opinion such flow velocities and rates are experimentally observable.

Another possibility is to orient the cholesteric homeotropically along the radius in a thin gap between two cylinders of radii R_0 and $R_0 + L$. We choose the x axis in the direction of the cylinder axis and specify a temperature gradient $dT/dx = \Delta T/X$. Then the shear stresses of type (23) lead to the appearance of a torque M [dyn $\cdot$ cm] with which one cylinder acts on the other:

$$M = 2\pi R_0^2 \sigma_{r\varphi} X = \pi R_0^2(\lambda''-\lambda')\Delta T. \tag{31}$$

If one of the cylinders is free, Couette flow corresponding to a linear velocity of the relative displacement of the walls should set in:

$$\Delta v = \frac{\lambda'' - \lambda'}{2\eta_2} \Delta T \frac{L}{X}. \tag{32}$$

At $L/X = 0.1$ and $\Delta T \sim 10$ K we get $\Delta v \sim 0.5 \cdot 10^{-3}$ cm/sec.

We discuss now the case when external forces produce Couette flow in a cell of the type shown in Fig. 3 with a homeotropically oriented cholesteric, or between the cylinders considered above (the flow is in the direction of the y axis for the cell and around the axis for the cylinder). The thermomechanical term (24) causes then heat flow. If the walls are thermally insulated, the stationary value of the temperature gradient is

$$\frac{dT}{dx} = \frac{v}{L} \frac{T(\lambda'' - \lambda')}{2\Lambda}. \tag{33}$$

Assuming $v \sim 0.1$ cm/sec and $X \sim 10L$, we obtain $\Delta T = XdT/dx \sim 10^{-4}$, which in our opinion is observable in experiment.

6. CONCLUSION

Our analysis and numerical estimates raise the hope of observing the predicted thermomechanical effects in liquid crystals. Investigation of these effects should, in our opinion, yield new important information on the molecular dynamics of the mesophase of liquid crystals. Besides the effects considered in this paper and connected with temperature gradients, a large number of diffusion-mechanical effects connected with density gradients of some component or of some impurity should occur in liquid crystals.

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APPENDIX

Forms of the tensor structures for kinetic flows and for the dissipation function

To write down in the dissipative function all the terms of type (20) which cause thermomechanical effects in deformed liquid crystals, we expand the gradients of the temperature and of the director **n** in the irreducible representation of a one-parameter group of rotation about the **n** axis:

$$\mathbf{A} = \nabla T - \mathbf{n}(\mathbf{n}\nabla)T, \qquad A_0 = (\mathbf{n}\nabla)T, \tag{A.1}$$

$$\begin{gathered} P = (\mathbf{n}\,\mathrm{rot}\,\mathbf{n}), \quad M_0 = \mathrm{div}\,\mathbf{n} \equiv m_{kk}, \quad M_i = m_{ik} n_k, \\ M_{ik} = m_{ik} - {}^1/_2(\delta_{ik} - n_i n_k) M_0 - n_i M_k - n_k M_i. \end{gathered} \tag{A.2}$$

Here m_{ik} is the symmetric tensor of the director gradient:

$$m_{ik} = {}^1/_2(\partial n_i/\partial x_k + \partial n_k/\partial x_i). \tag{A.3}$$

P is a pseudoscalar, M_0 and A_0 are scalars, and **A** and **M** are vectors perpendicular to the director: $(\mathbf{A}\cdot\mathbf{n}) = (\mathbf{M}\cdot\mathbf{n}) = 0$; M_{ik} is a zero-trace symmetric tensor, all the components of which lie in a plane transverse to the director: $M_{ii} = 0$, $M_{ik} = M_{ki}$, $M_{ik} n_k = 0$. The quantities **N**, D_0, **D** and D_{ij}, which describe the rates of change of the director and the flow-velocity gradients, were introduced by Eq. (12) of Sec. 3. Let us show how these quantities behave under the substitution $\mathbf{n} \to -\mathbf{n}$. The quantities D_0, D_{ij}, **A**, P, and **M** are even with respect to these substitutions, while **N**, **D**, A_0, M_0, and M_{ij} are odd.

The most general form of the dissipation function, in which the velocity, the temperature gradient, and the director gradient are all of the same degree, and which satisfies the conditions of invariance to rotations about the **n** axis and simultaneously to the substitution $\mathbf{n} \to -\mathbf{n}$, is

$$\begin{aligned} R_{\text{TM}} = {} & \xi_1(\mathbf{NA})M_0 + \xi_2\mathbf{n}[\mathbf{NA}]P + \xi_3 N_i A_k M_{ik} \\ & + \xi_4(\mathbf{NM})A_0 + \xi_5(\mathbf{DA})M_0 + \xi_6\mathbf{n}[\mathbf{D}\times\mathbf{A}]P \\ & + \xi_7 D_i A_j M_{ij} + \xi_8(\mathbf{DM})A_0 + \xi_9(\mathbf{AM})D_0 \\ & + \xi_{10} D_0 A_0 M_0 + \xi_{11} A_i M_j D_{ij} + \xi_{12} A_0 D_{ij} M_{ji}. \end{aligned} \tag{A.4}$$

If we are dealing with a cholesteric, all the constants $\xi_1 - \xi_{12}$ are the same for right- and left-hand forms. In other words, the constants ξ_1 and ξ_{12} are scalars and not pseudoscalars. Variation of (A.4) with respect to the variables $\partial v_i/\partial x_k$ yields an expression for that part of the viscous-stress tensor which is due to the thermomechanical effect:

$$\begin{aligned} \sigma_{ki}^{\text{TM}} = {} & {}^1/_4(2\xi_1 - \xi_3 + 2\xi_5 - \xi_7) n_i \nabla_k T\, \mathrm{div}\,\mathbf{n} \\ & - {}^1/_4(2\xi_1 - \xi_3 - 2\xi_5 + \xi_7) n_k \nabla_i T\, \mathrm{div}\,\mathbf{n} \\ & - {}^1/_2(\xi_2 + \xi_6)(\mathbf{n}\,\mathrm{rot}\,\mathbf{n}) \\ & \quad n_i[\mathbf{n}\times\nabla]_k T + {}^1/_2(\xi_2 - \xi_6)(\mathbf{n}\,\mathrm{rot}\,\mathbf{n}) n_h[\mathbf{n}\times\nabla]_i T \\ & + {}^1/_2(\xi_3 + \xi_7) n_i m_{kj} \nabla_j T - {}^1/_2(\xi_3 - \xi_7) n_k m_{ij} \nabla_j T \\ & - {}^1/_2(\xi_3 - \xi_4 + \xi_7 - \xi_8 + \xi_{11} + 2\xi_{12}) n_i m_{kj} n_j (\mathbf{n}\nabla) T \\ & + {}^1/_2(\xi_3 - \xi_4 - \xi_7 + \xi_8 - \xi_{11} - 2\xi_{12}) n_k m_{ij} n_j (\mathbf{n}\nabla) T \\ & + {}^1/_2(-2\xi_5 + \xi_7 + 2\xi_{10} + \xi_{12}) n_i n_k\, \mathrm{div}\,\mathbf{n}\,(\mathbf{n}\nabla) T \\ & + {}^1/_2(-2\xi_7 + 2\xi_9 + \xi_{11}) n_i n_k n_j m_{jp} \nabla_p T \\ & + {}^1/_2\xi_{11} n_j (m_{jk}\nabla_i T + m_{ji}\nabla_k T) + \xi_{12} m_{ki}(\mathbf{n}\nabla) T. \end{aligned} \tag{A.5}$$

The vector of the heat flow due to the thermomechanical effect is given by

$$\begin{aligned} -T^{-1} q_i^{\text{TM}} = {} & \frac{\delta R_{\text{TM}}}{\delta(\partial T/\partial x_i)} = {}^1/_2(2\xi_1 - \xi_3) N_1\, \mathrm{div}\,\mathbf{n} + \xi_2(\mathbf{n}\,\mathrm{rot}\,\mathbf{n}) \\ & \times[\mathbf{nN}]_i + \xi_3 m_{ik} N_k - (\xi_3 - \xi_4) n_i N_j n_k m_{kj} + {}^1/_2(2\xi_5 - \xi_7) d_{ij} n_j\, \mathrm{div}\,\mathbf{n} \\ & - {}^1/_2(2\xi_5 - \xi_7 - 2\xi_{10} - \xi_{12}) n_i n_j n_k d_{jk}\, \mathrm{div}\,\mathbf{n} - \xi_6(\mathbf{n}\,\mathrm{rot}\,\mathbf{n}) e_{ijk} n_k n_p d_{pj} \\ & \xi_7 m_{ik} d_{kj} n_j + \xi_{11} d_{ik} m_{kj} n_j + \xi_{12} n_i d_{kj} m_{jk} \\ & + {}^1/_2(-2\xi_7 + 2\xi_9 + \xi_{11}) m_{ij} n_j n_k n_p d_{kp} \\ & - (\xi_7 - \xi_8 + \xi_{11} + 2\xi_{12}) n_i n_p d_{pj} m_{jk} n_k. \end{aligned} \tag{A.6}$$

Finally, the contribution of the thermomechanical effect to the "force" acting on the director is

$$\begin{aligned} f_i^{\text{TM}} & = \frac{\delta R_{\text{TM}}}{\delta(\partial n_i/\partial t)} \\ & = \frac{1}{2}(2\xi_1 - \xi_3)\nabla_i T\, \mathrm{div}\,\mathbf{n} - \xi_2(\mathbf{n}\,\mathrm{rot}\,\mathbf{n})[\mathbf{n}\times\nabla]_i T \\ & \quad + \xi_3 m_{ik}\nabla_k T - (\xi_3 - \xi_4) m_{ik} n_k (\mathbf{n}\nabla) T. \end{aligned} \tag{A.7}$$

The exceedingly complicated form of expressions (A.4)–(A.7) notwithstanding, when simple specific problems are considered a large number of terms of one type or another drop out and the results turn out in general to be quite compact. The nematodynamics equations with allowance for all the considered effects are

$$\Pi_{ji}\left[\frac{\delta R}{\delta(\partial n_i/\partial t)}-\frac{\partial}{\partial x_k}\frac{\delta R}{\delta(\partial^2 n_i/\partial x_k\,\partial t)}+\frac{\delta F}{\delta n_i}-\frac{\partial}{\partial x_k}\frac{\delta F}{\delta(\partial n_i/\partial x_k)}\right]=0, \qquad (A.8)$$

where $\Pi_{ij}=\delta_{ji}-n_j n_i$ is the operator of projection on a plane perpendicular to the local value of the vector $\mathbf{n}(\mathbf{r}, t)$. Here F [erg/cm^3] is the free-energy density in its usual Frank form. The equations for the velocity $\mathbf{v}(\mathbf{r}, t)$ of the liquid are of the form

$$\rho\left(\frac{\partial v_i}{\partial t}+(\mathbf{v}\nabla)v_i\right)=\frac{\partial\sigma_{ki}}{\partial x_k},$$
$$\sigma_{ki}=-p\delta_{ki}+\sigma_{ki}'+\sigma_{ki}^{\text{TM}}, \quad \operatorname{div}\mathbf{v}=0, \qquad (A.9)$$

where ρ is the density and $p(\mathbf{r}, t)$ is the pressure determined from the same system (A.9) and from the boundary conditions. Finally the thermal-conductivity equation takes in this approximation the form

$$\rho c_p=(\partial T/\partial t+\mathbf{v}\nabla T)-\operatorname{div}\mathbf{q}=U, \qquad (A.10)$$

where U [erg/cm^3 · sec] is the density of the energy release due to extraneous forces, and c_p is the specific heat at constant pressure.

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