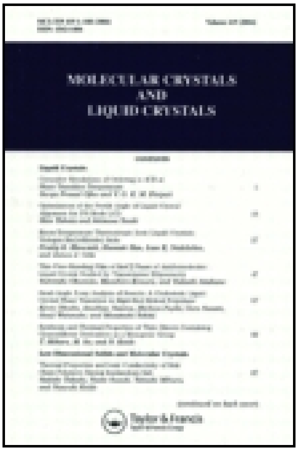

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Further Theoretical Proofs for the Existence of Relation Between $k_{11}'(k_{11})$, $k_{33}'(k_{33})$ and k_{13} in Hematics: Tensor Analysis

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FURTHER THEORETICAL PROOFS FOR THE EXISTENCE OF RELATION BETWEEN $k_{11}'(k_{11})$, $k_{33}'(k_{33})$ AND k_{13} IN NEMATICS: TENSOR ANALYSIS

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Abstract The smooth transformation of the anisotropic elastic energy of a nematic in an isotropic elastic energy requires either $k_{13} = 0$ and $k_{24} = 0$ or $2k_{13} = k_{33}' - k_{11}'$ and $k_{24} = k_{33}' - k_{22}$. Some physical interpretation of these relations are given.

INTRODUCTION

Recently we have found relation between the elastic constants of second-order splay-bend k_{13}, bend k_{33}' and splay k_{11}' as follows:[1, 2]

$$2k_{13} = k_{33}' - k_{11}' \quad (1)$$

On the other hand, from the relations[3, 4]

$$k_{11}' = k_{11} - 2k_{13} \text{ and } k_{33}' = k_{33} + 2k_{13} \quad (2)$$

and the relation (1) one can obtain relations between k_{11} and k_{33} on the one hand and k_{11}' and k_{33}' on other hand:

$$k_{11} = k_{33}' \text{ and } k_{33} = k_{11}' \quad (3)$$

Nehring and Saupe[3, 4] have obtained a relation between the elastic constants k_{24}, k_{11} and k_{22} in the following way:

$$2k_{24} = k_{11} - k_{22} \quad (4)$$

The same relation has been derived by Poniewierski and Stecki[5] and by Pleiner and Brand.[6] Replacing k_{11} with the really observable elastic constant of bend k_{33}', the relation (4) is transformed in the following way:

$$2k_{24} = k_{33}' - k_{22} \tag{5}$$

In this paper, using the tensor calculations performed by Vertogen et al[7] and including the k_{24} and k_{13} elastic terms we have confirmed the existence of the relation (1) and have corrected slightly the relation (5):

$$k_{24} = k_{33}' - k_{22} \tag{6}$$

THE EXPRESSION OF THE ELASTIC ENERGY FOR NEMATICS OBTAINED WITH THE AID OF TENSOR CALCULATIONS

The expression for the elastic energy of nematics including k_{24} and k_{13} terms can be easily obtained according to the procedure used by Vertogen et al:[7]

$$\begin{aligned}2f(r) = f_0 &+ 2(K_7-K_{12})n_i(r)n_j(r)n_{k,i}(r)n_{k,j}(r) \\ &+ 2(K_{10}-K_{13})n_{i,j}(r)n_{i,j}(r) + 2K_9 n_{i,i}(r)n_{j,j}(r) \\ &+ 2K_{11}n_{i,j}(r)n_{j,i}(r) + 2(K_{14} + K_{15})n_j(r)n_{i,ij}(r)\end{aligned} \tag{7}$$

On the other hand , the expression for the elastic energy of nematics including k_{24} and k_{13} terms proposed by Nehring and Saupe[3] is written in tensor notation:

$$\begin{aligned}2f(r) = f_0 &+ k_{22}n_{i,j}(r)n_{i,j}(r) + k_{24}n_{i,j}(r)n_{j,i}(r) \\ &+ (k_{11}' - k_{22} - k_{24} + 2k_{13})n_{i,i}(r)n_{j,j}(r) \\ &+ (k_{33}' - k_{22})n_i(r)n_j(r)n_{k,i}(r)n_{k,j}(r) \\ &+ 2k_{13}n_j(r)n_{i,ij}(r)\end{aligned} \tag{8}$$

The comparison of (7) and (8) leads to relations between the elastic constants of Frank-Oseen-Nehring-Saupe and the constants in the tensor notation by Vertogen et al[7] as follows:

$$k_{11}'-k_{22}-k_{24}+2k_{13}=2K_9;\ k_{22}=2(K_{10}-K_{13})$$
$$k_{33}'-k_{22}=2(K_7-K_{12});\ k_{24}=2K_{11};\ 2k_{13}=2(K_{14}+K_{15}) \quad (9)$$

One obtains finally the isotropic elastic energy for nematics:

$$2f(r) = f_0 + kn_{i,j}(r)n_{i,j}(r) \quad (10)$$

when $k_{33}' = k_{22}=k_{11}' = k,\ k_{13}=0,\ k_{24}=0$ (11)

or $k_{33}' = k_{22}= k_{11}' = k,\ 2k_{13}= k_{33}'-k_{11}',$
$k_{24}= k_{33}' - k_{22}$ (12)

The requirements (11) including $k_{13}= 0$ and $k_{24}= 0$ are too severe and in our opinion should be excluded. On the other hand, the inclusion of non-vanishing elastic constants k_{24} and k_{13} leads to decrease of the elastic energy.[2,8,9] Consequently at this stage of the knowledge on k_{24} and k_{13} we accept the relations (12). It is important to stress that the density of the elastic energy for nematics can be written in the following symmetric form:

$$2f = k_{11}'(\mathrm{div}\underline{n})^2 - k_{11}'\mathrm{div}(\underline{n}\,\mathrm{div}\underline{n}) + k_{33}'(\underline{n} \times \mathrm{rot}\underline{n})^2 - k_{33}'\mathrm{div}(\underline{n} \times \mathrm{rot}\underline{n}) + k_{22}(\underline{n}\cdot\mathrm{rot}\underline{n})^2 \quad (13)$$

This presentation of the elastic energy for nematics has several advantages:

<u>FIRST</u>, we can write the requirement for non-negative value of the distortional energy integrally:

$$k_{11}'\left\{\int_V(\mathrm{div}\underline{n})^2\,dv - \oint_S(\mathrm{div}\underline{n})\underline{n}\cdot\underline{\nu}\,ds\right\} + k_{22}\int_V(\underline{n}\cdot\mathrm{rot}\underline{n})^2\,dv + k_{33}'\left\{\int_V(\underline{n} \times \mathrm{rot}\underline{n})^2\,dv - \oint_S(\underline{n} \times \mathrm{rot}\underline{n})\cdot\underline{\nu}\,ds\right\} \geq 0 \quad (14)$$

It is apriori clear that this requirement is authomatically satisfied for constant solution div$\underline{n}$ = const and

$\underline{n}$ x rot$\underline{n}$ = const. Such deformations including singularities are discussed by Drzaic.[10] The more complicated case concerning bend-splay deformations[10] requires a separate discussion. SECONDLY it is clear that the presentation of the elastic energy for nematics expressed with the form (13) is consistent with the elastic behaviour of nematics near the nematic-smectic A transition.

PHYSICAL INTERPRETATION OF THE RELATIONS FOR k_{24} AND k_{13}

The elastic constants of splay and bend or twist and bend are not equal when:

a) there is an asymmetry in the molecular shape[11]:

$$k_{11}' : k_{22} : k_{33}' = 1 : 1 : (L/W)^2 \tag{15}$$

where $z_0/x_0 = z_0/y_0 \sim L/W$ and z_0 is the distance between the centers of neighbouring molecules in the direction of $\underline{n}$, and x_0 and y_0 are the distances between the centers of neighbouring molecules in all directions perpendicular to $\underline{n}$.

b) there is an asymmetry in the molecular interactions in direction of $\underline{n}$ and in any direction, perpendicular to $\underline{n}$:[5]

$$2k_{13} = k_{33}' - k_{11}' = (kT/2)\int (u_z^2 - u_x^2) C_0(\underline{u}, \underline{n}_1, \underline{n}_2) \rho_0'(\cos\theta_1) \times \rho_0'(\cos\theta_2) n_{1x} n_{2x} d\underline{n}_1 d\underline{n}_2 d\underline{u}$$

$$k_{24} = k_{33}' - k_{22} = (kT/2)\int (u_z^2 - u_x^2) C_0(\underline{u}, \underline{n}_1, \underline{n}_2) \rho_0'(\cos\theta_1) \times \rho_0'(\cos\theta_2) n_{1y} n_{2y} d\underline{n}_1 d\underline{n}_2 d\underline{u} \tag{16}$$

(these expressions are valid in the mean field approximations). Similar expressions can be found in other papers as well.

c) the second-order elastic constant k_{13} is proportional to the ratio of the order parameters $\langle P_4 \rangle$ and

$\langle P_2 \rangle$:[12-15]

$$2k_{13} = k_{33}' - k_{11}' = (7/3)(k_{11}' + k_{22} + k_{33}')\Delta'(\langle P_4 \rangle / \langle P_2 \rangle) \quad (17)$$

where $\Delta' = (e + fT)(a + bT)^{-1}$ and the constants a and e describe the attractive interactions between the molecules and the constant b describes the repulsive intermolecular interactions.[15]

CONCLUSION

The existence of relations between elastic constants of nematics is demonstrated and a physical interpretation is given.

REFERENCES

1. H. P. Hinov, Mol. Cryst. Liq. Cryst., 168, 7 (1989).
2. H. P. Hinov, "Further theoretical proofs for the existence of a relation between $k_{11}'(k_{11})$, $k_{33}'(k_{33})$ and k_{13} in nematics: one- and three- dimensional cases", submitted to Mol. Cryst. Liq.Cryst.
3. J. Nehring and A. Saupe, J. Chem. Phys., 54, 337 (1971).
4. J. Nehring and A. Saupe, J. Chem. Phys., 56, 5527 (1972).
5. A. Poniewierski and J. Stecki, Mol. Physics, 38, 1931 (1979).
6. H. Pleiner and H. Brand, Phys. Rev. A, 34, 2528 (1986).
7. G. Vertogen , S. D. P. Flapper and C. Dullemond, J. Chem. Phys., 76, 616 (1982).
8. S. Meiboom, J. Sethna, P. Anderson and W. Brinkman, Phys. Rev. Lett., 46, 1216 (1981).
9. S. Meiboom, M. Sammon and W. Brinkman, Phys. Rev.A 27, 438 (1983).
10. P. Drzaic, Mol. Cryst. Liq. Cryst., 154, 289(1988).
11. W. H. de Jeu, F. Leenhouts and F. Postma, in "Advances in Liquid Crystal Research and Applications", ed. L. Bata, Pergamon Press, Oxford - Akadémiai Kiado, 499 (1980).
12. J. P. Straley and R. G. Priest, Mol. Cryst. Liq. Cryst., 17, 129 (1972).
13. R. Priest, Phys. Rev. A, 7, 720 (1973).
14. H. Kimura, M. Hosino and H. Nakano, Mol. Cryst. Liq. Cryst., 74, 55 (1981).
15. S. D. P. Flapper, G. Vertogen and F. Leenhouts, J. Phys.(France), 42, 1647 (1981).