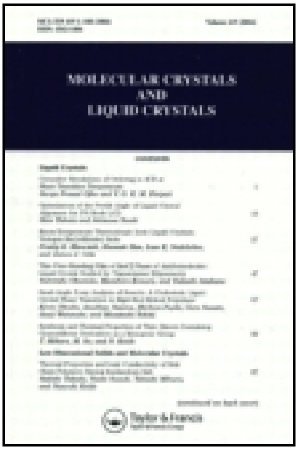

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Jerzy Kedzierski [a], Marek Andrzej Kojdecki [b], Zbigniew Raszewski [a], Paweł Perkowski [a], Jolanta Rutkowska [a], Wiktor Piecek [a], Ludwika Lipińska [c] & Emilia Miszczyk [d]

[a] Institute of Applied Physics, Military University of Technology, 00-908, Warsaw, 49, Poland

[b] Institute of Mathematics and Operations Research, Military University of Technology, 00-908, Warsaw, 49, Poland

[c] Institute of Electronic Materials Technology, 01-919, Warsaw, Poland

[d] Institute of Physics, Radom University of Technology, 26-600, Radom, Poland

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Composite Method for Determination of Liquid Crystal Material Parameters

JERZY KĘDZIERSKI[a], MAREK ANDRZEJ KOJDECKI[b], ZBIGNIEW RASZEWSKI[a], PAWEŁ PERKOWSKI[a], JOLANTA RUTKOWSKA[a], WIKTOR PIECEK[a], LUDWIKA LIPIŃSKA[c] and EMILIA MISZCZYK[d]

[a]*Institute of Applied Physics, Military University of Technology, 00–908 Warsaw 49, Poland,* [b]*Institute of Mathematics and Operations Research, Military University of Technology, 00–908 Warsaw 49, Poland,* [c]*Institute of Electronic Materials Technology, 01–919 Warsaw, Poland and* [d]*Institute of Physics, Radom University of Technology, 26–600 Radom, Poland*

A stable method for the determination of the nematic liquid crystal material parameters, such as the splay and bend elastic constants, the anisotropy of diamagnetic susceptibility, the electric permittivities and either the coupling between the nematic molecules and the substrate at the planar liquid crystal cell boundary (i.e. the director field boundary value), is presented in the work. The method consists of two stages: firstly the effective electric permittivity of planar nematics cell is measured as a function of external electric and magnetic fields, secondly the coefficient inverse problem is solved numerically using the experimental data to determine the values of material parameters. The coefficient inverse problem is posed in a variational way as a problem of nonlinear mean-square fit of the calculated nematics layer characteristics to the measured ones. The description of phenomena is based on Ericksen's – Leslie's theory. The unknown material parameters serve in this approach as the fit parameters, the best values of which corresponding to the best possible approximation of the experimental data by the refined mathematical model are to be found. The method was successfully used for the determination of the material parameters of PCB and can be applied to every nematics.

Keywords: nematics parameter identification; inverse problem

INTRODUCTION

It is well known that the Ericksen-Leslie [1] theory of nematics is a very adequate description of phenomena in them. It is applied successfully for the theoretical investigation of phenomena in continuous medium of such a kind as well as for the computer simulation of them. The simulation of physical phenomena is important for two reasons. Firstly, it is a valuable method for investigating phenomena and predicting their results (among them the physical fields, which can not be immediately observed) without making laborious experiments. Secondly, being compared with the results of experiments, it enables the verification of the theory as a quantitative description of physical reality. The most important procedure before the simulation is done is the precise determination of all physical and material constants appearing in the theory. This is the crucial moment – the simulation gives only qualitative description of phenomena until the constant values are determined sufficiently precisely. Looking for magnitudes of nematics material constants one has to overcome serious difficulties – some of them can not be measured immediately and some can be measured only in very sophisticated experiments. Those difficulties can be mastered by applying modern mathematical technique of treating such problems. The magnitudes of material parameters can be found as a solution of corresponding inverse problem. This is the main idea of the approach presented here.

For the flat liquid crystal cell of planar boundaries, which order the nematics parallel, the dependence of the effective dielectric permittivity of the cell (or nematics layer) on applied external electric or magnetic fields can be measured easily. Each of such characteristics can be treated as a function of unknown material parameters; this function can be defined by mathematical model of the phenomenon. So each of the measured characteristics can be either calculated when the magnitudes of material constants are known. This leads to the formulation of an inverse problem by defining the functional of material parameters as arguments and of suitable norm of difference between corresponding characteristics as values. Solving it one finds the required magnitudes of material parameters. This method can be applied for every nematics; some details are given below.

The planar nematics cell of thickness d can be treated with good accuracy as the layer infinitely extended in two dimensions (in Oxy plane) and placed between two parallel planes ($z=0$ and $z=d$). Moreover let the boundaries cause a homogeneous stationary state of the layer (described by a constant director field) and let the external fields act in the same plane Oxz. The static deformations of such cell caused by constant fields, electric $\vec{E}=\vec{E}(z)=(0,0,E(z))$ induced by a constant voltage U applied to the layer boundaries and magnetic induction $\vec{B}=\vec{B}(z)=(B\sin\psi,0,B\cos\psi)$, are planar and can be described in one-dimensional approximation by planar director field $\vec{n}=\vec{n}(z)=(\cos\vartheta(z),0,\sin\vartheta(z))$. Analysing the functional of free elastic energy of the nematics layer influenced by external fields, corresponding to such configuration, one obtains [2] the Euler equation for it in the following form:

$$\begin{gathered}(K_{11}\cos^2\vartheta+K_{33}\sin^2\vartheta)\vartheta''+(K_{33}-K_{11})\cdot\sin\vartheta\cdot\cos\vartheta\cdot\vartheta'^2\\+\frac{\varepsilon_0\varepsilon_a\varepsilon_e^2U^2\sin\vartheta\cos\vartheta}{d^2(\varepsilon_\perp\cos^2\vartheta+\varepsilon_\parallel\sin^2\vartheta)^2}+\frac{\chi_aB^2}{\mu_0}\sin(\vartheta+\psi)\cos(\vartheta+\psi)=0\\\varepsilon_e=\left\{\frac{1}{d}\int_0^d\frac{1}{[\varepsilon_\perp\cos^2\vartheta(z)+\varepsilon_\parallel\sin^2\vartheta(z)]}dz\right\}^{-1}\end{gathered}\tag{1}$$

where:

K_{11}, K_{33} are the splay and bend Frank elastic constants, $\varepsilon_\perp$, $\varepsilon_\parallel$ are the electric permittivities, $\varepsilon_a=\varepsilon_\parallel-\varepsilon_\perp$, χ_a is the anisotropy of diamagnetic susceptibility, ε_e is the effective electric permittivity of the layer.

In general the weak anchoring at the layer boundaries should be assumed. It can be characterised by suitable boundary condition for ϑ. The elastic torque density per unit area of layer boundary, transmitted from bulk, can be calculated [2,3,4] for function ϑ, satisfying the above equation, as

$$\begin{aligned}T_b&=\int_0^d\left[(K_{11}-K_{33})\cdot\sin\vartheta(z)\cdot\cos\vartheta(z)\cdot\vartheta'(z)^2\right]dz\\&+\int_0^d\left[\frac{\varepsilon_0\varepsilon_a\varepsilon_e^2U^2\sin\vartheta(z)\cos\vartheta(z)}{d^2\left[\varepsilon_\perp\cos^2\vartheta(z)+\varepsilon_\parallel\sin^2\vartheta(z)\right]^2}+\frac{\chi_aB^2}{\mu_0}\sin(\vartheta(z)+\psi)\cos(\vartheta(z)+\psi)\right]dz\end{aligned}\tag{2}$$

Since this torque causes the boundary orientation of the director different from the easy axis corresponding to nematics-substrate interaction, the boundary value of ϑ can be modelled by a certain function [2,3,4,5] (e.g. a polynomial of sufficiently large order):

$$\vartheta(0) = \vartheta(d) = \Theta(T_b). \tag{3}$$

In particular case of strong anchoring this function is constant: $\vartheta(0) = \vartheta(d) = \vartheta_0$.

Hence every stationary state of a planar deformation of the layer can be characterised by a solution $\vartheta = \vartheta(z)$ and ε_e of equations (1) with ϑ satisfying boundary condition (3), (2) and corresponding to the values of material parameters $K_{11}, K_{33}, \chi_a, \varepsilon_\perp, \varepsilon_\parallel, \Theta$ (where Θ is a function) and applied external forces $U, (B,\psi)$. On the other side the effective electric permittivity ε_e can be measured in experiment.

INVERSE PROBLEM

Every electric or magnetic characteristics of nematics cell as dielectrics, i.e. the dependence $\varepsilon_e = \varepsilon_e(U;B,\psi)$, contains the information about material constants $K_{11}, K_{33}, \chi_a, \varepsilon_\perp, \varepsilon_\parallel, \Theta$. Let Θ be a polynomial of coefficients $\Theta_0,\dots,\Theta_k$ and let $p = (K_{11}, K_{33}, \chi_a, \varepsilon_\perp, \varepsilon_\parallel, \Theta_0,\dots,\Theta_k)$ denote the set of unknown material parameters. For any sequence of measurements $(\varepsilon_{ee}(U^i;B^i,\psi^i))_{i=1}^n$ (i.e. points of experimental characteristics) one can calculate from (1), (2), (3) a corresponding sequence of values of effective electric permittivity $(\varepsilon_{ec}(U^i;B^i,\psi^i;p))_{i=1}^n$. These two sequences can be compared by the following similarity functional [6]:

$$S(p) = \sum_{i=1}^{n} \left[\varepsilon_{ee}(U^i;B^i,\psi^i) - \varepsilon_{ec}(U^i;B^i,\psi^i;p)\right]^2 \tag{4}$$

which has the unknown material parameters p as arguments.

Now the inverse problem [7] can be posed: having the results of experiment $(\varepsilon_{ee}(U^i;B^i,\psi^i))_{i=1}^n$ given find the set of unknown parameters $p = (K_{11}, K_{33}, \chi_a, \varepsilon_\perp, \varepsilon_\parallel, \Theta_0,\dots,\Theta_k)$ minimising functional (4).

RESULTS OF EXPERIMENT

Two flat nematics cells filled with PCB have been studied: the first one ($d = 55 \mu m$) of planar nematics configuration (the orientation of easy axis parallel to the boundaries – with ϑ close to zero) and the second one ($d = 62{,}2 \mu m$) of homeotropic configuration (the orientation of easy axis perpendicular to the boundaries – with ϑ close to $\frac{1}{2}\pi$).

Three groups of characteristics were measured: first - the dependence of ε_e on voltage, parameterised by the constant magnetic induction stabilising the boundary-induced stationary state (i.e. parallel to the layer plane, $\psi = 1{,}5078$ rad), for planar cell – Figure 1; second - the dependence of ε_e on magnetic induction (perpendicular to the layer plane, $\psi = 0$ rad), parameterised by the constant voltage amplifying the deformations, for planar cell – Figure 2; third - the dependence of ε_e on magnetic induction (parallel to the layer plane, $\psi = 1{,}5078$ rad), parameterised by the constant voltage stabilising the boundary-induced stationary state, for homeotropic cell – Figure 3.

The inverse problem was solved using data from three characteristics; the other characteristics were calculated for confirming the precision of the determination of material parameters. It is also possible to find all unknown parameters using the data from only one characteristics. The electric permittivities $\varepsilon_\perp, \varepsilon_\parallel$ were determined after the observation maximal and minimal value of ε_e of cells influenced by stabilising field without deforming field. Then the elastic constants K_{11}, K_{33} and the coefficients $\Theta_0,...,\Theta_k$ of a polynomial approximating the nematics-substrate coupling were determined from the first purely electric characteristics of the planar cell and afterwards the anisotropy of diamagnetic susceptibility χ_a was determined from the first purely magnetic characteristics of the planar cell. Additionally the parameters of the nematics-substrate coupling for the homeotropic cell were determined from its first magnetic characteristics.

The following values of PCB material parameters were determined at 18° C (all in SI units): $\varepsilon_\perp = 6{,}23$; $\varepsilon_\parallel = 19{,}82$;

$$K_{11} = 6{,}82 \cdot 10^{-12}\,\mathrm{N}; \quad K_{33} = 9{,}89 \cdot 10^{-12}\,\mathrm{N}; \quad \chi_a = 1{,}297 \cdot 10^{-6}.$$

It was realised that the third-order polynomials were sufficiently accurate for approximating function $\Theta(T_h)$ - one of them (for the planar cell) is presented in Figure 4.

The error of approximation of the experimental characteristics by the calculated ones, defined by formula

$$R(\varepsilon_{ee},\varepsilon_{ec})=\left[\frac{1}{n}\sum_{i=1}^{n}\left(1-\left(\varepsilon_{ec}^{i}/\varepsilon_{ee}^{i}\right)\right)^{2}\right]^{\frac{1}{2}},$$

achieved values between 0,00138 and 0,0320; for majority of them it is equal about 0,01.

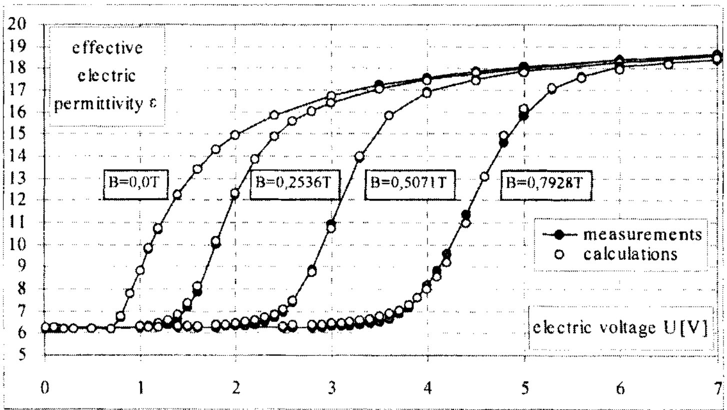

FIGURE 1. Characteristics $\varepsilon_e = \varepsilon_e(U)$ of planar PCB cell.

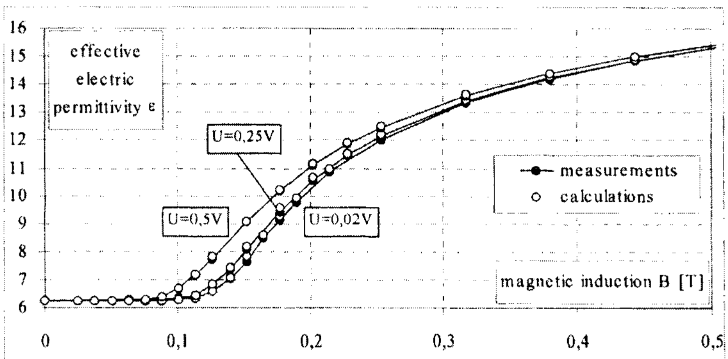

FIGURE 2. Characteristics $\varepsilon_e = \varepsilon_e(B)$ of planar PCB cell.

It is interesting to compare the magnitudes of the material parameters given above with known from another works.
The Frank elastic constant magnitudes can be found in books [8,9]: by L.M.Blinov and V.G.Chigrinov $K_{11} = 6{,}4 \cdot 10^{-12}$ N, $K_{33} = 10{,}0 \cdot 10^{-12}$ N at 25° C; by G.Ahlers $K_{11} = 5{,}95 \cdot 10^{-12}$ N, $K_{33} = 7{,}86 \cdot 10^{-12}$ N at 26° C.

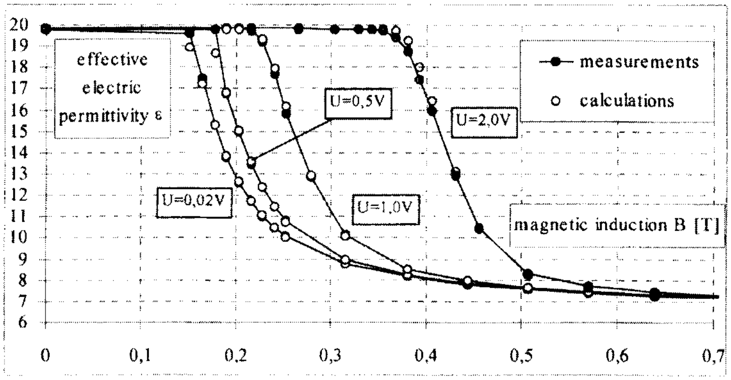

FIGURE 3. Characteristics $\varepsilon_e = \varepsilon_e(B)$ of homeotropic PCB cell.

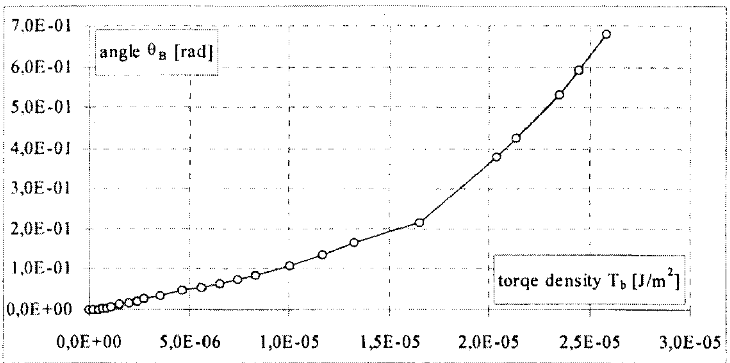

FIGURE 4. The director boundary value as a function of torque density $\vartheta_B = \Theta(T_b)$ – the approximate characterisation of coupling between nematics (PCB) and substrate material (polyimide) at the boundaries of the planar cell.

The anisotropy of diamagnetic susceptibility can be found in works[8,10]: by G.Ahlers $\chi_a = 1{,}40 \cdot 10^{-6}$ at $26^\circ C$; by A.Buka and W.H. de Jeu, $\chi_a = 2{,}136 \cdot 10^{-6}$ at $25^\circ C$.

CONCLUSION

The method of determining the material parameters of nematic liquid crystal presented above seems to be reliable. It enables quite precise computing their magnitudes (with relative error of order 0,01). The nematics layer characteristics, calculated (for PCB) with the determined parameters, are very close to the experimental ones. This confirms both the adequacy of the applied theory and the usefulness of the method. It can be adapted either for the determination of the magnitudes of another parameters.

Acknowledgements

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