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Short Communication

A New Method of Viscosity Determination from the Electro-Optical Response of a Nematic LCD

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Abstract. — We determine viscosity values of ZLI-2293 (Merck), to our knowledge for the first time, from a measured transmission *versus* time curve of a TN-cell with the "optical bounce" [1,2]. Our method combines the measurement of this transmission curve with the simulation of the corresponding director field and a suitable optimization process using Simulated Annealing [3] to obtain the viscosities. The advantage of our approach is the small experimental expense compared to that of a direct viscosimetric measurement while achieving nearly the accuracy of the direct method.

1. Introduction

Numerical simulation has become a powerful tool for the optimization of the optical and dynamical properties of liquid crystal displays (LCDs) [2,4–6]. It allows to vary the important display parameters in a wide range and to select the proper (suitable) configurations for further experimental investigations. This shortens development cycles and reduces costs.

Inclusion of flow effects into computer simulations leads to remarkably better agreement with measurements [6,7]. The Ericksen-Leslie theory [8,9] covers these flow effects and delivers equations of motion which contain six viscosity parameters, the "Leslie viscosities". The values of these parameters are only known for a few liquid crystal (LC) materials, *e.g.* MBBA (N-(4-methoxybenzylidene)-4-n-butyl-aniline) because the direct viscosimetric measurement is very difficult and expensive.

Several attempts have been made to determine Leslie viscosities in an easier way, for instance by introducing an effective rotational viscosity γ_1^* [10] or by determining viscoelastic coefficients through optical measurements [11]. Another possibility is to investigate the sensitivity of the optical response of a liquid crystal display due to changes of each viscosity parameter [12].

In [13] we introduced a new method, which to our knowledge for the first time allowed the extraction of the unknown viscosity values from a so-called reference curve which is the transmission time curve of a TN-cell with an "optical bounce". There we determined the viscosities of MBBA from a *calculated* reference curve with very good agreement to measured

(*) Author for correspondence (e-mail: cossalt@tem.etec.uni-karlsruhe.de) values. Furthermore we showed [14] that these values were reliably reproduced in a whole series of viscosity determinations applied to the same *calculated* reference curve of MBBA.

In this paper we apply our method to a *measured* transmission time curve of a TN-cell filled with ZLI-2293 (Merck) and compare the viscosity values obtained with those from viscosimetric measurements.

2. Preconditions

The preconditions of our method are:

a) We assume that each set of Leslie's viscosities leads to a unique transmission curve which differs from those obtained with different viscosity sets if the remaining material and liquid crystal cell parameters are held constant.

b) There are liquid crystal cells which show transmission time curves that depend sensitively on changes of Leslie's viscosities.

Remarks:

a) The assumption may be difficult to prove/disprove for the given nonlinear equations but is only required to be true within the chosen (possible) range of viscosity values. Our simulations and measurements support this assumption.
Furthermore if there were two different sets of viscosity values which give rise to the same transmission time curve then only one additional measurement of a second transmission time curve is required, for instance at a switch-off voltage different from that of the first one. Then it will be possible to decide which set is the searched one.

b) We choose a TN-cell and use it in the optical bounce case. The optical bounce is an oscillation in the transmission time curve of a TN-cell, which is induced by flow of liquid crystal material in the cell. This flow effect was measured and calculated [1,2,7] and depends strongly on the viscosity values [12].

3. Viscosity Determination

Our method to obtain good estimations of the unknown viscosities is summarized by the following steps (see also [13]):

1) Obtain a *reference curve* by measurement of the transmission time curve in the optical bounce case of a TN-cell.
2) Choose a legal set of values for Leslie's viscosities α_1-α_6.
3) Get a *test curve* of this TN-cell by calculation of the transmission time curve in the optical bounce case with the viscosity values chosen in step 2.
4) Determine the deviation between the reference and the test curve. This can be done by calculating the sum of the distance squares.
5) Repeat steps 2, 3 and 4 with changed viscosity values. These values are altered in such a manner that the deviation between the reference and the test curve vanishes or is minimized. The searched viscosity values are those for which this happens.

Remarks:

1) We used a factory made prebuilt TN-cell and determined its thickness of 7.9 μm with an interferometric method [15]. The boundary tilt of the liquid crystal molecules is estimated to be 3°. The experimental setup of the transmission measurement is shown in Figure 1.

2) The viscosities are chosen randomly from an interval of nearly two decades of viscosity values centered around those of MBBA. To obtain a legal set of viscosities we take into account

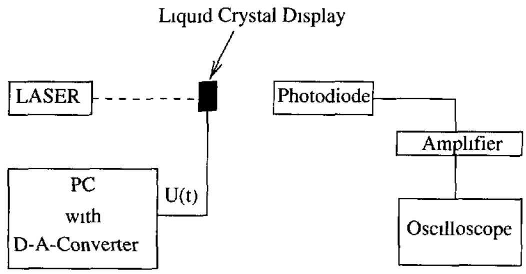

Fig. 1. — Measurement of the transmission time curve in the optical bounce case. Cell thickness is 7.9 μm, the boundary tilt is estimated to be 3° and the switching off-voltage is $6 \times U_{\text{fred}}$, where U_{fred} is the Fréedericksz-voltage.

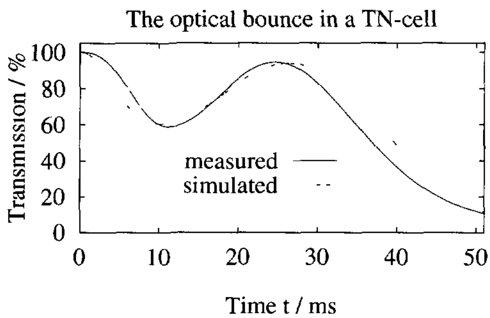

Fig. 2. — Comparison of a measured and a simulated transmission time curve of a TN-cell with a thickness of 7.9 μm and a switching-off voltage of $6 \times U_{\text{fred}}$.

the Parodi equation and the fact that the rotational viscosity γ_1 is always positive. Furthermore each Leslie viscosity keeps its sign.

3) We use a simulation program which takes into account the flow of liquid crystal material in the cell [4]. It will be described in next section and determines the time development of the director configuration which is required for the calculation of the transmission time curve. The transmission time curve is then calculated with the Jones Matrix Method [16] for a wavelength of 632.8 nm. Figure 2 shows a measured and a calculated transmission time curve of the prebuilt TN-cell.

Beside the viscosities the values of some additional material parameters are required for the simulation, *i.e.* Frank's elastic constants k_{ii}, the dielectric and the optical anisotropy $\Delta\varepsilon$ and Δn. These values were taken from [17].

5) For changing (optimizing) the viscosity values so that they minimize the deviation between the reference and test curve we use the classical Simulated Annealing algorithm. In 1983 Simulated Annealing was introduced by Kirkpatrick *et al.* as an optimization method [3]. In the terminology of optimization the cost or objective function in our context is the deviation between reference and test curve, and a configuration is one set of viscosity values. A start temperature of $T = 1000$, a cooling rate of $f_T = 0.95$ and a maximum of 150 iterations/temperature-step were our Simulated Annealing parameters.

The accuracy of our method depends on the measurement error of a) the reference curve, b) the liquid crystal parameters k_{ii}, $\Delta\varepsilon$ and Δn, which are held constant throughout the whole viscosity determination and are used in the simulation of the transmission time curve and c) the liquid crystal cell geometry (thickness and boundary tilt).

Additionally it depends on the accuracy of the simulation program and the specific viscosities to be determined because the sensitivity of the transmission time curve is different for each of the viscosity parameters. The viscosity α_2 has the largest influence on the optical response whereas that of α_1 can be neglected [14].

We should mention that only three Leslie viscosities need to be determined to obtain the full set of viscosities. We take into account the Parodi relation and neglect the value of α_1 which has no practical influence on the electro-optical response curve [12]. In general, the value of γ_1 is supplied by the liquid crystal manufacturer. Therefore only the viscosities α_3, α_4 and α_5 are left to be determined. (It is also possible to choose another set of viscosities, for instance α_2, α_4 and α_5).

4. Solving the Dynamic Equations of Nematic Liquid Crystals

For each cycle of our viscosity determination one has to calculate a complete time development of the director configuration for the TN-cell. We restrict our calculations to the one-dimensional liquid-crystal cell model [2], *i.e.* it is assumed that all quantities in this cell depend only on the coordinate perpendicular to the confining glass plates and the time. We apply strong anchoring conditions at the boundaries and assume that the flow-velocity vanishes there. Furthermore inertial effects are neglected. Then a set of five coupled PDEs has to be solved for each timestep.

We use the method of Finite Differences and choose an implicit discretization scheme. It is sufficient to determine the three components of the director **n** and two flow velocity components at 47 points of an equidistant grid between the boundaries.

We apply a procedure described by van Doorn [2] which reduces the numerical effort. The set of dynamic equations is divided in two equation blocks which are solved separately in a first step. Three equations (first block) (see [2]) describe mainly the director motion in place, and the remaining equations ([1])(second block)

$$\begin{aligned}
&\alpha_2 \dot{n}_x n_z + \alpha_3 \dot{n}_z n_x + (\frac{1}{2}\, n_x n_y\, (\alpha_3 + \alpha_6) + \alpha_1 n_x n_y n_z^2)\, v_{y,\,z} \\
&\qquad\qquad + \frac{1}{2}\, (2\alpha_1 n_x^2 n_z^2 + (\alpha_5 - \alpha_2)\, n_z^2 + \alpha_4 + (\alpha_3 + \alpha_6)\, n_x^2)\, v_{x,\,z} = C_1 \\
&\alpha_2 \dot{n}_y n_z + \alpha_3 \dot{n}_z n_y + (\frac{1}{2}\, n_x n_y\, (\alpha_3 + \alpha_6) + \alpha_1 n_x n_y n_z^2)\, v_{x,\,z} \\
&\qquad\qquad + \frac{1}{2}\, (2\alpha_1 n_y^2 n_z^2 + (\alpha_5 - \alpha_2)\, n_z^2 + \alpha_4 + (\alpha_3 + \alpha_6)\, n_y^2)\, v_{y,\,z} = C_2
\end{aligned}$$

where z is shortcut for spatial derivative with respect to z, α_i Leslie viscosity coefficients, n_j components of the nematic director, v_k components of the flow velocity, C_l constants of integration determined by the boundary conditions of the v_k, *i.e.*

$$\int_0^d v_{k,z}\, \mathrm{d}z = 0\,, \quad k = x, y, \quad d \text{ is the cell-thickness}$$

describe primarily the liquid crystal flow in the cell. A dotted symbol denotes the time derivative of this quantity.

Then we choose starting values for the five unknowns per grid point and solve the first block while holding the flow velocity constant. This yields improved values for the components of the director.

([1]) These equations differ slightly from those given in [2] which contains a minor sign-error in the definition of the vector **N**. Correctly it is $\mathbf{N} = \dot{n}_i - 0.5 * (v_{i,j} - v_{j,i})\, n_j$ [18,19].

Table I. — *Results of applying our procedure (40 runs) to the measured reference curve of Figure 2. The viscosities were compared to those obtained by direct viscosimetric measurement [20].*

	α_i^{ref} / Pa·s	$\overline{\alpha}_i$ / Pa·s	Error of $\overline{\alpha}_i$ / %	σ / Pa·s	n_{Sim}
ZLI-2293					40
α_4	0.08100	0.08971	10.8	0.0289	
α_5	0.10840	0.10379	4.2	0.0375	

Afterwards we solve the second block and treat the new values of the director components as constant parameters. This yields improved values of the flow velocity components.

Then, we solve again the first block of equations and treat these improved flow velocity values as constant parameters, and so on.

This procedure of outer iterations converges after 10-20 cycles. During each outer iteration the second equation block can be solved through an one-dimensional numerical integration because of the boundary conditions for the flow velocity. The first equation block gives rise to an nonlinear system of equations. This equation set is solved with the Newton-Raphson algorithm.

The calculation of the time development of the director needs approximately 50 s of computing time on our DEC-Alpha 200-4/166.

5. Results

Table I shows viscosity values for ZLI-2293(Merck) obtained by our method compared to those determined by viscosimetric measurements. Our results are the averages of a series of 40 viscosity determinations which we have applied on the measured reference curve shown in Figure 2.

The results show that the viscosities α_4 and α_5 were obtained with a accuray of 5% and 10%, resp., compared to the values obtained through viscosimetric measurements. In contrary to the results in [13] one could not obtain reliable values for the viscosity α_3 because their influence on the reference curve is too small compared to the measurement errors contained in the measured reference curve.

6. Summary and Outlook

We developed a new method for obtaining Leslie's viscosities whose experimental expense is remarkably smaller in comparison to that of viscosimetric determination because a measurement of the transmission time curve of a TN-cell and the cell thickness suffices completed by some computer calculations. Our method is capable to determine those viscosities of a nematic liquid crystal which influences the optical response and dynamical properties of a TN-cell primarily. The remaining viscosities α_1 and α_3 have only a negligible [12] respectively small influence on these properties of a liquid crystal cell.

We have started further investigations to decrease the computing time required for the viscosity determinations. This can be done by introducing a multi-grid algorithm in the director field simulation module and by replacing the Simulated Annealing algorithm with a different optimization algorithm, for instance Record-to-Record Travel [21], which needs a smaller number of optical bounce curve calculations and maintains the accuracy of the viscosity determination.

The new method should be applicable to similar problems of parameter determinations in other fields of research if the preconditions mentioned above hold, *i.e.*

- if each set of the unknown parameters give rise to a unique development curve of a measurable quantity (transmission *versus* time or applied voltage *versus* time or ..);
- if the sensitivity of this development curve is sufficient for changes of the parameters to be determined and;
- if the number of unknown parameters is small enough (< 10).

With these rather general preconditions the proposed method will prove useful for a more general class of problems.

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