Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

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O. Cossalter[a]; D. A. Mlynski[a]
[a] University of Karlsruhe, Institut für Theoretische Elektrotechnik und Meβtechnik, Karlsruhe, Germany

To cite this Article Cossalter, O. and Mlynski, D. A.(1995) 'Determination of Leslie's viscosities with high accuracy directly from the electro-optic response of a LCD', Liquid Crystals, 19: 4, 545 — 547
To link to this Article: DOI: 10.1080/02678299508032017
URL: http://dx.doi.org/10.1080/02678299508032017

LIQUID CRYSTALS, 1995, VOL. 19, NO. 4, 545–547

Determination of Leslie's viscosities with high accuracy directly from the electro-optic response of a LCD

by O. COSSALTER* and D. A. MLYNSKI
University of Karlsruhe, Institut für Theoretische Elektrotechnik und Meßtechnik, Kaiserstr.12, 76128 Karlsruhe, Germany

(*Received 6 April 1995; accepted 6 June 1995*)

For the accurate computer aided design of liquid crystal displays (LCDs) flow effects have to be considered which require knowledge of Leslie's viscosities. These values are hardly known for many liquid crystal materials. We have developed a new method which is capable of determining these viscosities directly from the electro-optic response curve. The viscosities are obtained by using a combination of a LC simulation program, which takes flow effects into account and a Simulated Annealing module which provides good estimates of the viscosity values. This module evaluates a measurable *reference* transmission versus time curve for a TN-cell in the 'optical bounce' case and a corresponding test curve. For our test example we chose MBBA as the liquid crystal material and determined its viscosity values α_3, α_4 and α_5 with only 0·2 to 2 per cent deviation from measured values.

To achieve better correspondence to measured values, flow effects have to be included in computer simulations. The Ericksen–Leslie theory [1, 2] covers these flow effects and delivers the equations of motion which contain six viscosity parameters, the 'Leslie viscosities'. The values of these parameters are hardly known for many liquid crystal (LC) materials with the exception, for instance, of MBBA(*N*-(4-methoxybenzylidene)-4-*n*-butyl-aniline).

Our approach allows for the first time, as far as we know, the direct extraction of the viscosity values from the transmission time curve of a TN-cell.

The basic idea is derived from the fact that in some cases the measured transmission of a LCD differs significantly from that obtained through calculations which *neglect* flow effects. One well known example is an oscillation in the transmission time curve of a TN-cell, the so called 'optical bounce', which has been measured and calculated [3–5]. This effect demonstrates the influence of Leslie's viscosities on the electro-optic response of a LCD.

One important conclusion from these observations is that the transmission time curve with the 'optical bounce' must contain information about the values of these additional viscosity parameters.

Our method of extracting good estimates of the unknown viscosities from this transmission time curve runs as follows:

(i) We assume that different sets of viscosity parameters correspond to different transmission time curves. Our simulation results support this assumption, which, however, might be difficult to prove/disprove for the given set of non-linear equations required to calculate the transmission. Figure 1 shows exemplarily the change in the transmission time curve for single variations of some viscosity parameters.

(ii) A *reference* transmission versus time curve of the optical bounce type is required. It can be obtained

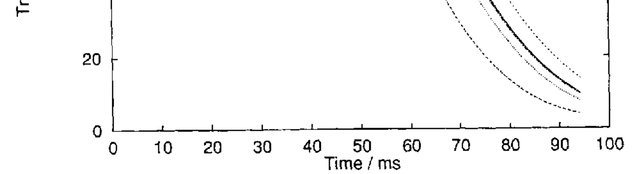

Figure 1. The transmission time curves in the optical bounce case for different sets of viscosity values. These sets differ only in a single parameter value from each other. The optical response depends differently on the viscosities. The parameter α_2 influences the transmission time curve much more than α_3 does. The cell thickness is about 8 μm and the switch-off voltage $6{*}U_{\rm fred}$.

* Author for correspondence.

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Table 1. Some results obtained with our method. The calculated values of the viscosities α_i^*, $i = 3, 4, 5$ are compared to measured values which are taken from [4]. The temperature T, the cooling rate f_T and the number of iterations i, while the temperature is constant, are the corresponding Simulated Annealing parameters. Rows with an asterisk/plus sign belong to calculations with slightly modified cost functions. Deviations in the central part of the optical bounce are punished with higher 'costs' in the Simulated Annealing part than in the other cases. The plus sign indicates that the transition between weighted/unweighted regions in the cost function is steady.

Calculated viscosities (and measured values)/Pas			Deviation/per cent					
α_3^*	α_4^*	α_5^*	$(1 - \alpha_i^*/\alpha_i) \cdot 100$ per cent, $i = 3, 4, 5$			T	f_T	i
−0·0025 (−0·0012)	0·0939 (0·0832)	0·0392 (0·0463)	108	13	15	1000	0·97	60
−0·0010 (−0·0012)	0·0816 (0·0832)	0·0473 (0·0463)	17	2	2	1000	0·97	100
−0·00114(−0·0012)	0·0828 (0·0832)	0·0465 (0·0463)	5	0·6	0·5	1000	0·97	150
−0·00140(−0·0012)	0·08473(0·0832)	0·04531(0·0463)	16·6	1·8	2·2	1000	0·97*	60
−0·00114(−0·0012)	0·08272(0·0832)	0·04663(0·0463)	5	0·6	0·7	1000	0·97*	100
−0·00139(−0·0012)	0·08481(0·0832)	0·04518(0·0463)	15·8	1·9	2·4	1000	0·95+	60
−0·00128(−0·0012)	0·08386(0·0832)	0·04584(0·0463)	6·7	0·8	1	1000	0·95+	100
−0·00122(−0·0012)	0·08334(0·0832)	0·04620(0·0463)	1·7	0·17	0·2	1000	0·95+	150

by measuring the optical transmission versus time curve of a TN-cell containing the LC material with the unknown viscosities.

(iii) Then, several transmission time test curves have to be calculated with a simulation program which includes flow effects. A program of this type needs the values of all Leslie's viscosities.

(iv) For each calculation of a transmission time test curve, a set of estimated viscosity values is passed to this program from a Simulated Annealing optimization part which creates consecutive sets of viscosities. The values of the parameters in the successive sets of viscosities are chosen by the Simulated Annealing module in such a way that the difference between the *reference* and the calculated transmission time curve decreases step by step. The viscosity values are determined when this difference vanishes (or is minimized).

A precondition that this method can work is that the simulation program required in (iii) gives results which are in good agreement with measured data.

Our flow simulation program calculates the time development of the director configuration and takes flow effects into account. It adapts the infinite extended layer cell model [4] and the corresponding equations of motion mentioned in [4, 6]. They are solved numerically with an implicit finite difference method using a Newton–Raphson algorithm which results in a stable and fast simulation program [6, 7].

The transmission time curve is then calculated with a Jones Matrix Method [8] for a wavelength of 632·8 nm.

The algorithm of the Simulated Annealing module is based on an idea of Kirkpatrick *et al.* [9], who introduced Simulated Annealing in 1983 as an optimization method. To deal with it you need a cost function which is a measure of the deviation of a configuration from the optimum. In our case, a configuration is a set of viscosity parameters and the cost function measures the difference between the calculated test curves and the *reference* transmission time curve. This is done by calculating the sum of the distance squares.

We tested our approach through the determination of the viscosity values of MBBA and compared them to measured values.

It should be noted that only three viscosities must be determined. 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 [7]. In general, the value of γ_1 is supplied by the liquid crystal manufacturer. We express α_2 which has the strongest influence on the electro-optical response [7] by γ_1 in our flow equations. Therefore only the viscosities α_3, α_4 and α_5 are left, which have to be determined by the Simulated Annealing part. (It is also possible to choose another set of viscosities which have to be determined, for instance α_2, α_4 and α_5.) So far the search interval contains two decades of viscosity values. We have taken the values of the additional material parameters from [4].

We used a TN-cell with a thickness of 10 μm and a boundary tilt of 3°. We obtained the measurable *reference* transmission time curve from a calculation using the measured viscosity values of MBBA.

The table shows the calculated viscosities compared to measured values, together with the corresponding parameters used for the Simulated Annealing part. The rows with an asterisk/plus sign indicate different choices of the cost function. It can be seen that in the end the main difference between these choices is the different number of iterations required to determine the viscosity values with a similar deviation from known values.

The determined viscosities deviate between 0·2 and

2 per cent (for the different viscosities) from measured values.

The sensitivity of our method differs for the different viscosity parameters as can be seen in figure 1. The sensitivity is very high for the viscosity α_2, whereas it is significantly smaller for the viscosity α_3. Therefore it is to be expected that the values for α_3 obtained with our method will only be in good correspondence with quoted literature values if the best test curve almost coincides with the reference transmission time curve.

The precondition concerning the flow simulation program also influences the accuracy of the method.

Our *reference* transmission versus time curve and the best test curve which corresponds to the first data set of the table is shown in figure 2.

Our next step is the measurement of *reference* curves and the determination of the viscosities from these curves. This is in progress and will soon be finished.

The authors thank C. Ball and H. G. Wolf from our CAD group of analog circuit design for helpful discussions about optimization methods and S. Dickmann for his Jones Matrix program.

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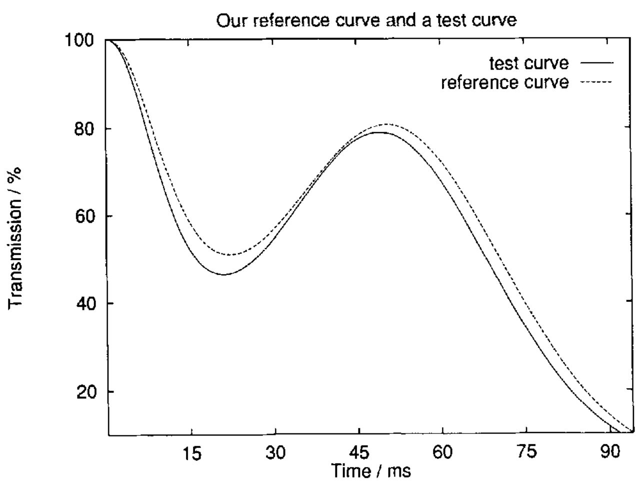

Figure 2. Transmission versus time for our reference curve and the corresponding best test curve. The reference curve is obtained from switching-off an applied voltage of $6{*}U_{\text{fred}}$ in the optical bounce case. We used a cell thickness of 10 µm. The boundary tilt is 3°.