This article was downloaded by: [University of Haifa Library]
On: 14 August 2012, At: 09:08
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Three-Dimensional Modelling of Liquid Crystal Display Cells using Finite Elements

F. A. Fernandez [a], S. E. Day [a], P. Trwoga [a], H. F. Deng [a] & R. James [a]
[a] University College London

Version of record first published: 18 Oct 2010

To cite this article: F. A. Fernandez, S. E. Day, P. Trwoga, H. F. Deng & R. James (2002): Three-Dimensional Modelling of Liquid Crystal Display Cells using Finite Elements, Molecular Crystals and Liquid Crystals, 375:1, 291-299

To link to this article: http://dx.doi.org/10.1080/10587250210587

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.tandfonline.com/page/terms-and-conditions

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Mol. Cryst. Liq. Cryst., Vol. 375, pp. 291-299
Copyright © 2002 Taylor & Francis
1058-725X/02 $12.00 + .00

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

Three-Dimensional Modelling of Liquid Crystal Display Cells using Finite Elements

F. A. FERNANDEZ, S. E. DAY, P. TRWOGA,
H. F. DENG and R. JAMES

University College London

Abstract: A computer modelling method for the three-dimensional dynamic analysis of liquid crystal display cells is presented. The method is based on a variational approach to the Oseen-Frank free energy formulation considering three elastic constants and uses a vectorial representation of the director field. A simpler approximate form that uses only two elastic constants but is faster to operate is obtained as a by-product of the full three-constant model implementation. The modelling uses finite elements on a mesh of tetrahedral elements for the calculation of directors and electric potentials while finite differences in time are used in the time stepping process. Comparisons are made with results from a 2D dynamic program using a tensor model giving good agreement.

Keywords: Liquid Crystals; Computer Modelling; Finite Elements

INTRODUCTION

The accurate analysis and design of liquid crystal structures for displays is becoming increasingly more important as the specifications are becoming more demanding and the structures more complicated. While simpler and faster one-dimensional and two-dimensional models are adequate for the modelling of many liquid crystal structures [1,2], there are cases where they cannot provide a satisfactory representation of the behaviour of the structure. There are many features occurring in liquid crystal cells that are truly three-dimensional and a full 3D model is

required.

The model presented here is based on the Oseen-Frank energy formulation using a vectorial representation of the director field and consists of the calculation of the electric potential distribution and the associated directors within a time-stepping procedure. The nonlinear interdependence of the electric potential and directors is resolved by iterations within the time-stepping process until consistence is achieved. Both the director and potential distributions are modelled using finite elements over a mesh of tetrahedral elements. A variational approach to the energy formulation leads to the dynamic representation of the behaviour of the liquid crystal cell. Finite differences in the time domain are used as a base for the time stepping process.

The finite element representation of the director field leads to an expression containing third order powers of nodal values of director components. This causes difficulties for the numerical solution of the problem, which requires the linearization of this term. However, after some manipulation, the higher order terms can be modified into a form that becomes linear if the elastic coefficients K_{22} and K_{33} are considered equal. Thus, a simpler form of the method can be constructed using this approximation. Furthermore, this modification leads to a simpler implementation of the remaining nonlinear term. The full three constants implementation requires the inclusion of the nonlinear term, which is cubic in terms of director values. Linearization of this term for the numerical solution of the problem is performed by iterations partially using values of the directors at the previous time step.

Results of the analysis of practical liquid crystal cells show agreement with experimental results and with 2D analyses when these are applicable.

THEORY

Starting from the Oseen-Frank energy functional [3]:

$$\frac{1}{2}\int\Big\{K_{11}(\nabla\cdot\vec{n})^2+K_{22}(\vec{n}\cdot\nabla\times\vec{n}+q)^2+K_{33}(\vec{n}\times\nabla\times\vec{n})^2 - \varepsilon_0\Big[\Delta\varepsilon(\vec{n}\cdot\vec{E})^2+\varepsilon_l(\vec{E}\cdot\vec{E})\Big]\Big\}d\Omega \tag{1}$$

The last two terms of the elastic energy are of the order 4 on the values of the director $\vec{n}$. This will cause difficulties in a finite element

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

representation in terms of nodal values of directors, where we need to express this equation as a quadratic form in terms of the director values in order that the derived relaxation equation is linear in $\vec{n}$. Terms of order n^4 will give origin to cubic terms in the relaxation equation.

However, the last two terms of the elastic energy in (1) can be rewritten in the form:

$$K_{33}(\nabla\times\vec{n})^2 + 2qK_{22}(\vec{n}\cdot\nabla\times\vec{n}) + (K_{22}-K_{33})(\vec{n}\cdot\nabla\times\vec{n})^2 \qquad (2)$$

where the condition $\|\vec{n}\|^2 = 1$ has been used.

This new form has the advantage that only one of the terms is still expressed as a fourth order term in the director $\vec{n}$. Furthermore, it allows the use of an approximate functional using two elastic constants, corresponding to the case where $K_{22} = K_{33}$.

The remaining cubic term can be linearized within the time stepping process by expressing it as kn where k is proportional to the square of the values of $\vec{n}$ in the previous time step. Provided the time step is chosen sufficiently small, (a condition also necessary to achieve convergence in the time stepping process) $\vec{n}$ will not change abruptly between time steps and this approximation will be satisfactory. Furthermore, iterations within the same time step can be used if necessary to improve the accuracy of this approximation.

Discretization using Finite Elements

Writing the director in terms of finite element interpolation functions defined in tetrahedral elements as:

$$N_i(x,y,z) = \frac{1}{6V_e}(a_i + h_\alpha^i \alpha), \qquad (3)$$

gives: $\vec{n} = N_i(x,y,z)\vec{n}^i$ where $\alpha = x$, y and z, the coefficients a_i and h_α^i depend on the node coordinates, V_e is the element volume, and the repeated index $i = 1,..,4$ imply summation; $\vec{n}^i = (n_x^i, n_y^i, n_z^i)^T$ is the vector of component values of $\vec{n}$ at node i (T means transpose). With this the discretised form of curl $\vec{n}$ becomes: $(\vec{h}^i \times \vec{n}^i)/6V_e$ and the discretised expression for the total free energy will take the form:

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

$$\frac{K_{11}}{72V_e}h_\mu^i h_\nu^j n_\mu^i n_\nu^j + \frac{K_{33}}{72V_e}\left[h_\nu^i h_\nu^j n_\mu^i n_\mu^j - h_\mu^i h_\nu^j n_\mu^i n_\nu^j\right]$$
$$+ qK_{22}J_j\varepsilon_{\mu\nu\lambda}h_\mu^i n_\nu^i n_\lambda^j + \frac{K_{22}-K_{33}}{12V_e}\varepsilon_{\alpha\beta\gamma}\varepsilon_{\mu\nu\lambda}h_\alpha^i h_\mu^l n_\beta^i n_\gamma^j n_\nu^l n_\lambda^k J_{jk}$$
$$-\frac{\varepsilon_0\Delta\varepsilon}{12V_e}\phi^i\phi^j h_\alpha^i h_\beta^j n_\alpha^k n_\beta^l J_{kl} \qquad (4)$$

$\varepsilon_{\alpha\beta\gamma}$ is the Levi-Civita tensor, $J_j = 1/24$ and $J_{ik} = \frac{1}{120}\begin{cases}2 \text{ if } j=k\\ 1 \text{ if } j\neq k\end{cases}$ and the terms that will not contribute to the relaxation equation have been omitted.

The relaxation equation [4,5]: $\frac{\partial F}{\partial n_\delta^p} + \frac{\partial}{\partial \dot{n}_\delta^p}\left(\frac{\gamma}{2}\int \dot{n}_\mu \dot{n}_\mu d\Omega\right) = 0$ applied to the discretised representation of the energy F in (1) will now result in:

$$6V_e\gamma\dot{n}_\delta^i J_{ip} + \frac{K_{11}}{72V_e}h_\delta^p h_\mu^i n_\mu^i + \frac{K_{33}}{36V_e}\left\{h_\mu^i h_\mu^p n_\delta^i - h_\delta^i h_\mu^p n_\mu^i\right\}$$
$$+\frac{K_{22}-K_{33}}{6V_e}\varepsilon_{\alpha\beta\gamma}\varepsilon_{\mu\nu\delta}h_\alpha^i\left(J_{ip}h_\mu^k - h_\mu^p J_{kj}\right)n_\beta^i n_\gamma^j n_\nu^k$$
$$+qK_{22}\varepsilon_{\mu\delta\nu}\left\{h_\mu^p J_i - h_\mu^i J_p\right\}n_\nu^i - \frac{\varepsilon_0\Delta\varepsilon}{6V_e}\phi^i\phi^j h_\mu^i h_\delta^j J_{pk}n_\mu^k = 0 \qquad (5)$$

in each element, for $\delta = x$, y or z and $p = 1, \ldots, 4$, where γ is the rotational viscosity of the LC material.

Using a forward difference approximation for the time derivative in the equation above and after linearization of the nonlinear term, gives a matrix problem that can be written in the form:

$$\mathrm{G}\mathrm{n}^{t+\delta t} = \mathrm{W}\mathrm{n}^t \qquad \text{or} \qquad \mathrm{n}^{t+\delta t} = \mathrm{G}^{-1}\mathrm{W}\mathrm{n}^t \qquad (6)$$

The matrix G is a simple matrix and its inverse can be calculated analytically and has the same sparsity characteristics of G. W is a sparse matrix formed by contributions of the terms in (5).

The nonlinear term in (5) can be linearized by considering in the triple product $n_\beta^i n_\gamma^j n_\nu^k$ two of the coefficients n to be the same from the

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

previous time step and so of known value. This approximation is satisfactory if time steps are small. In that case iterations to improve the degree of approximation within the time step have been found unnecessary.

A simpler and faster form of this procedure is obtained under the approximation $K_{22} = K_{33}$. This eliminates the nonlinear term and can provide a fast approximate answer.

Dirichlet boundary conditions for the directors (*i.e.* strong anchoring is assumed) and for the electric potentials are imposed directly on the resultant matrix equations, thus reducing the order of the systems. Neumann boundary conditions, required at the lateral edges of the cell, are implemented by defining auxiliary prismatic elements at the edges, and forcing the normal derivatives of potentials and/or directors to be zero there.

RESULTS

The study of two structures is presented here to validate this method. The first consists of a 5μm thick layer of nematic liquid crystal, with equal 40μm sides and electrodes at the top and bottom as shown in Fig. 1. The liquid crystal is untwisted and initially aligned parallel to the central section of electrode 2. Both top electrodes are connected at the same voltage and there is a ground electrode covering the complete bottom surface. The values of the elastic constants K_{11}, K_{22} and K_{33} are 10.87, 9.5 and 15.37 pN respectively, $\gamma = 0.1$Pas and the permittivity

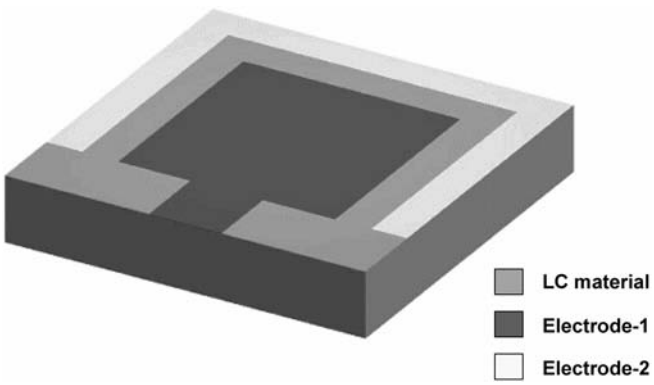

FIGURE 1 Diagram of test cell geometry

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

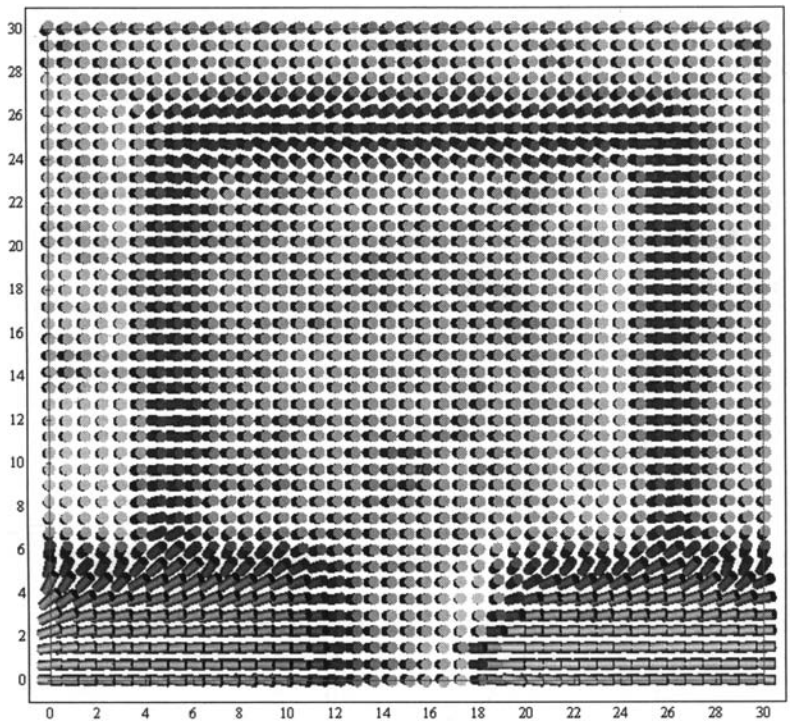

FIGURE 2 Director distribution in a horizontal cross-section.

is characterised by ε_l = 3.1 and $\Delta\varepsilon$ = 5. The calculated director distribution plotted over a horizontal cross-section 0.5 μm below the top surface is shown in Fig. 2. The director can be seen to be tilting under the two top electrodes and twisting along the edges parallel to the alignment direction. The director is tending to align with the electric field as expected for a positive $\Delta\varepsilon$ LC material. This is also observed experimentally as shown in Fig. 3. The experimental results were obtained with parallel polarisers aligned along the rubbing direction. The dark areas correspond to regions where the director is twisted. The Jones matrix method was used to calculate the optical transmittance through the cell from the modelled director distribution and is shown as the left hand side picture in Fig. 3.

The second case consists of an In-Plane-Switching (IPS) cell with strip electrodes as shown in Fig. 4. The light coloured electrodes are at ground potential and a voltage is applied to both of the two dark

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

electrodes. The directors are initially aligned forming an angle of 10° to the strip electrodes. This configuration is used in order to provide switching of the directors in the plane of the device following the in-plane fields between the electrodes on the same surface so as to improve the viewing angle characteristics of the cell [6,7].

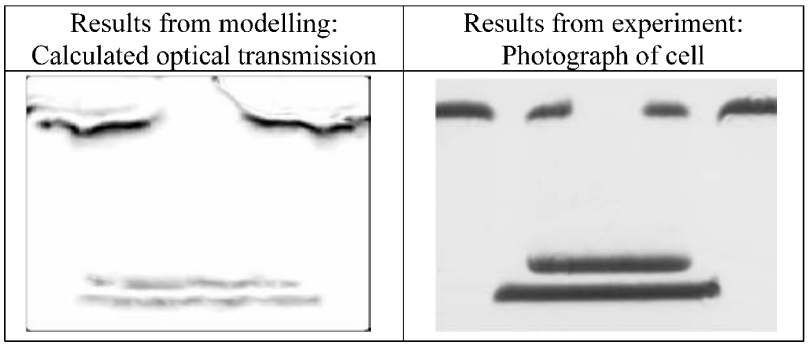

FIGURE 3 Comparison of calculated and experimental transmittance.

Fig. 5 shows the director distribution on a vertical cross-section and the optical transmittance calculated for the same section. It can be observed from this figure how the directors align with the electric field between the electrodes. The rapid variation of the director orientation under the strip electrodes corresponds to a rapid change of transmittance that can be seen as a double peak under the three central electrodes.

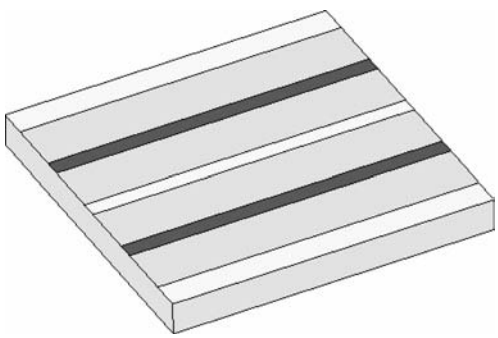

FIGURE 4 In-Plane-Switching structure

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

CONCLUSIONS

A computer modelling method has been described in detail for the three dimensional analysis of the dynamic evolution of the behaviour of liquid crystal cells driven by time-varying voltages applied at electrodes. The method uses three elastic constants and a vectorial representation of the director. The numerical procedure uses the finite element method in space and finite differences in time to produce a highly accurate description of the cell's operation.

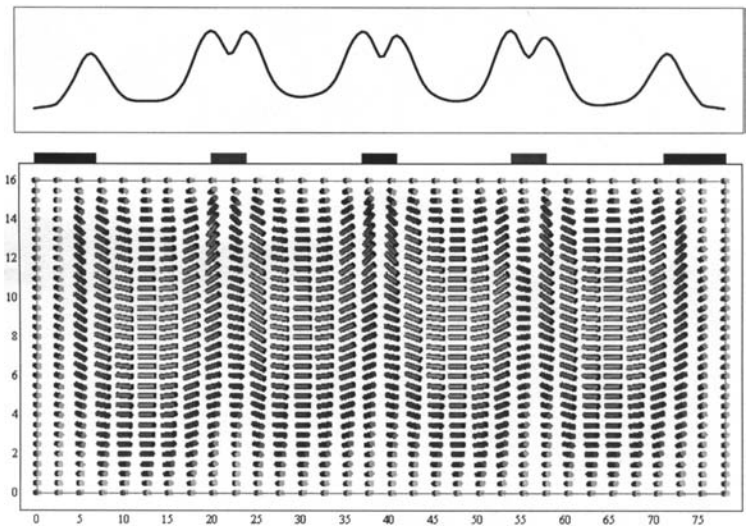

FIGURE 5 Director distribution over a vertical cross-section of the IPS structure. Calculated transmittance over the same section is plotted above.

Acknowledgements

This work is being performed with the support of the EC, under the Framework 5 programme, project GR1D-1999-10904.

References

[1] D.W. Berreman, *Philos. Trans. R. Soc. Lond.*, **vol. 309**, p. 203, (1983).

[2] F.Di Pasquale, H.F. Deng, F.A. Fernandez, S.E. Day, J.B. Davies, M.T. Johnson, A.A. van der Put, J.M.A. van de Eerenbeemd, J.A.M.M. van Haaren and J.A. Chapman, *IEEE Trans. Electron Devices*, **vol. 46**, No. 4, pp. 661-668, (1999).

Downloaded by [University of Haifa Library] at 09:08 14 August 2012

[3] P.G. de Gennes and J. Prost, The Physics of Liquid Crystals, Oxford Science Publications, Oxford, (1993).
[4] D.W. Berreman, *Appl. Phys. Lett.*, **vol. 25**, pp. 12-15, (1974).
[5] H. Woehler, M. Fritsch, G. Haas and D.A. Mlynski, *Proc. Intl. Display Research Conference*, Kyoto, Japan, pp. 376-379, (1989).
[6] M. Oh-e and K. Kondo, *Appl. Phys. Lett.*, **vol. 67**, No. 26, pp. 3895-3897, (1995).
[7] M. Oh-e and K. Kondo, *Appl. Phys. Lett.*, **vol. 69**, No. 5, pp. 623-625, (1996).

Downloaded by [University of Haifa Library] at 09:08 14 August 2012