Detailed numerical modeling of complex LCDs

Michael E. Becker

Display-Metrology & Systems, Marie-Alexandra-Str. 44, D-76135 Karlsruhe - Germany

Abstract

We present a family of elaborate numerical models for simulation and systematic optimization of complex LCDs for demanding applications (e.g. LCD-TV). These numerical models comprise modules for solving LCD-related problems in one, two and three dimensions. The three modules feature an intuitive graphical user surface for a jump-start into modeling, a common database for a range of materials and components as well as sophisticated and proven algorithms with more than 15 years of reliable performance in the LCD-industry. Methods for obtaining data required for the modeling of key components are presented.

1 Introduction

Analysis and research of liquid crystal display devices (LCDs) via numerical modeling has become indispensable in the research and development of new electro-optical effects in LCs and for the optimization of existing LC-display effects because it allows exact and individual control of all model parameters and provides fast results, thus being an ideal complement to the laboratory workbench.

Numerical modeling of LCDs was introduced by van Doorn [1] and Berreman [2] in 1975 to explain the origin of the "bounce" in the dynamical optical response of TN-cells. Even though the potential of the method was demonstrated by these papers it remained a tool for theoreticians and special research applications over many years. In 1987, when DIMOS was introduced as the first commercial multipurpose software tool for numerical modeling of LCDs [3], considerable efforts were undertaken both by the manufacturer of the software and the users in the LCD industry to compare the various results of modeling with experiments in order to check the validity of the numerical models which were mainly applied to TN and STN-cells in those days.

DIMOS for the first time combined computation of the field-induced alignment of the LC-director in the static and dynamic case (including elastic boundary coupling) with a 4x4-matrix method for evaluation of the optical properties of the display-system including light-source and filters.

In the meantime, the evolution of computers has made "number-crunching" several orders of magnitude faster, but at the same time the models became more refined and much more complex, just the same as the LCD-devices did. While in the late eighties computations were sometimes carried out over night and over the weekend, today most of time is consumed by definition and setup of the problem and evaluation and analysis of the result-data.

These days several software packages for numerical modeling of LCDs are commercially available (DIMOS, LCD-Master, TecWiz-LCD, Mouse/Pol-LCD [4]) and the numerical modeling of LCDs has become a standard procedure in the industry.

Numerical modeling of LCDs should be intuitive and easy to handle, because nobody wants to read manuals or even take courses before starting with modeling activities. A database for material and components must be available and accessible for all stages of modeling in one, two and three dimensions. Accurate and detailed definition of the problem to be solved consumes a considerable part of the time needed for numerical modeling and thus, the models shall be stored and made available for later use, i.e. the same model can be loaded and modified to save the biggest part of the time needed for definition of models from the beginning. This requires a well organized bookkeeping in order to keep track of all modifications that have been applied to the models, components and materials. The relations between the model and all of the data involved must never be lost or confused, otherwise the results are meaningless.

2 Numerical models

Numerical simulation of LC-displays is performed in two steps: first, the director distribution in the LC-layer is evaluated and then optical properties of the display-assembly are computed.

2.1 Foundations - Vector vs. tensor formalism

The orientation of the *director* (local *optic axis*) inside the LC-layer as a function of the position is described by the *director field*. Oseen, Frank, Leslie, Ericksen, and others developed the theory of LC-elasticity which can be used as a basis for calculation of the director orientation within the bulk of chiral-nematic LC-materials [5].

Alternatively, the free energy of the liquid crystal can be written in terms of the *order parameter tensor Q*. This *tensor approach* maintains the physical equivalence of $\vec{n}$ and $-\vec{n}$ and thus is sometimes believed to be more „realistic" in the numerical modeling of LCDs. However, this approach can give rise to spontaneous transitions between topologically non-equivalent states without the generation of disclinations, which is unrealistic from the viewpoint of LC-physics.
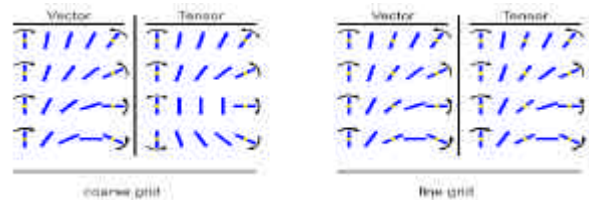

Figure 1*: Example demonstrating the effect of grid-spacing on spontaneous transitions into topologically non-equivalent states for vector and tensor formalism.*

The basic effect of the discretization (grid-spacing) on the director orientations for both approaches is illustrated in fig. 1. As soon as

the angular difference between the orientation at two adjacent grid-points (yellow dots, left diagram, bottom row) exceeds 90° the configuration obtained with the tensor formalism slips into a state with lower energy which is usually topologically different from the original one. Such spontaneous transitions do not take place in models based on the vector formalism. These transitions also involve the generation of disclinations in real LC-devices.

When the grid is refined (right diagram) with the same director field the angular difference between the orientation at two adjacent grid-points remains below 90° and thus even with the tensor formalism, no spontaneous transition into a new configuration takes place. With increasing density of the grid the configurations obtained with the tensor formalism approach those based on the vector formalism.

So where is the assumed advantage of the tensor formalism ? In addition, the mathematics involved in the vector approach are simpler, it requires fewer grid points for a given error, and as a consequence, the computing speed is higher. A detailed analysis of both approaches with practical examples and a comparison of the related features is published by [6].

2.2 Model Data

The more detailed the model becomes the more data is required for adequate description of the properties of the materials and components.

2.3 Solving the inverse problem

The optimistic user of numerical simulation however should never be discouraged by the lack of material parameters, but trusting on the quality of the model she/he tries to find out the values for the missing parameters by solving the "inverse problem", i.e. by iteratively adjusting the unknown parameter(s) until good agreement is reached with experimental results. Using this combination of experimental evaluation of external effects (e.g. transmission of light) together with iterative adaption of the key parameters in the numerical model a variety of parameters can be evaluated.

Shear viscosity coefficients

Based on a numerical model for the TN-cell that includes lateral flow effects, the shear-viscosities can be determined by iterative adaption of the parameters [7, 8].

Polar and azimuthal coupling elasticities

These parameters can be evaluated with approaches that compare the capacitance or the optical response of LC-layers in e.g. electric fields with predictions of the model [9, 10].

Polarizer refractive indices

A simple model for polarizers is limited to the layer with anisotropic absorption which is described by the imaginary parts of the refractive indices. They can be determined in DIMOS from the spectra of transmission of two parallel and a single polarizer.

Retarders

Detailed analysis of complex retarders (e.g. with splayed discotic layers) is based on either the measurement of the retardation as a function of the angle of light incidence or on the determination of the generalized ellipsometric parameters versus light incidence and numerical fitting to suitable optics models [11].

2.4 Sensitivity analysis

For the industrial manufacturing of LCDs it is often useful to know the sensitivity of a certain electro-optical effect with LCs with respect to variations of one specific parameter (e.g. cell-gap). Numerical modeling provides the means for such analyses by calculation of the partial derivatives (or difference quotients) of the output quantity with respect to all model parameters.

2.5 Stability considerations

Whenever a solution is obtained by numerical modeling the operator must be aware of the fact, that the model usually converges to the minimum of energy which is closest to the starting configuration. In order to decide if a solution is globally stable, similar configurations should be computed and their energies or configurations compared.

2.6 Multidimensional director field

First the energy or the corresponding Euler-equations must be discretized, this time however on a two (or three) dimensional) grid. Relaxation methods can be derived that are based on the elastic and electro-static energy of the model. A special problem of the more-dimensional case is the mutual dependence of the director orientation and the electrostatic potential distribution. An alternative to this Finite Difference Method (FDM) is the Finite Element Method (FEM) which uses a *mesh* rather than a *grid*. The mesh can be generated automatically and adapted to the geometry (LC-layer, electrodes, TFTs, etc.) more easily [12, 13]. Moreover, it can be refined locally to assure accuracy. A variety of shapes can be chosen for the elements (linear, nonlinear) and it is possible to mix different shapes if this may be suitable for the geometry.

After definition of all required parameters a suitable mesh is generated and locally refined. Then the initial director configuration is allowed to relax into a stable state of equilibrium before an electric field is applied to the electrodes and the director configuration relaxes into a new state of equilibrium. All resulting director fields should be checked with respect to their global stability (global minimum of energy).

2.7 Optics

DIMOS provides two methods for calculation of the optical properties of stratified media, the *Extended-Jones-2×2-Matrix-Method* and the *Characteristic-4×4-matrix-method* [14].

Multidimensional optics

Rapid lateral variations of the nematic director (e.g. in LCOS displays, high-resolution LCDs) resulting in rapid variations of the refractive index of the LC-material lead to diffraction effects which are not taken into account by *optics methods for stratified media*. Alternative optics approaches are:

- *Reduced-Order-Grating Methods*,
- *Finite Element and Finite Difference Time Domain Methods*,
- *Polarization Ray-Tracing Methods*,
- *Wide-Angle Vector Beam Propagation Methods*.

One-dimensional methods according to Berreman and Jones are fast and usually suited for most problems in the LCD-field unless lateral variations become too pronounced. This has to be decided separately for each resulting director field [15].

3   Realization and Implementation

The different numerical models of DIMOS use the same intuitive graphical user interface (GUI), the same database for material and component data and they have several basic features in common, e. g. application of the ***finite element method*** for computation of the director field in one, two and three dimensions [12]. Stepping towards stable solutions is achieved by suitable *relaxation methods* which also allow the simulation of the time dependent behavior in a natural way by use of dissipation functions which are based on the viscosities of the LC-material. Thus the director dynamics are computed on a *physical time-scale* [12, 13].

3.1 Graphical user interface

Since definition and editing of the models is the most demanding part for the user, DIMOS provides as much assistance in this step as possible with its unique graphical user interface.

After definition of all parameters of the layers included in the stack the *variations* have to be defined. The parameters describing materials, layers, electrical driving and illumination can be varied. *Variations* are sequences of parameter values replacing the current parameter value during the calculation. For example, a variation of the applied static voltage delivers the electro-distortional and electro-optical curve (EOC). Proper variation ranges of inclination and azimuth of the light source yield the viewing-direction dependence shown polar plots. Additional variation of the wavelength allows colorimetric evaluations, etc.

3.2 Number-crunching

The actual numerical work is performed by various *engines* in DIMOS. There are two basic classes of engines, those for computing the *director fields* (in one, two and three dimensions) and those for computing of the *optical properties*.
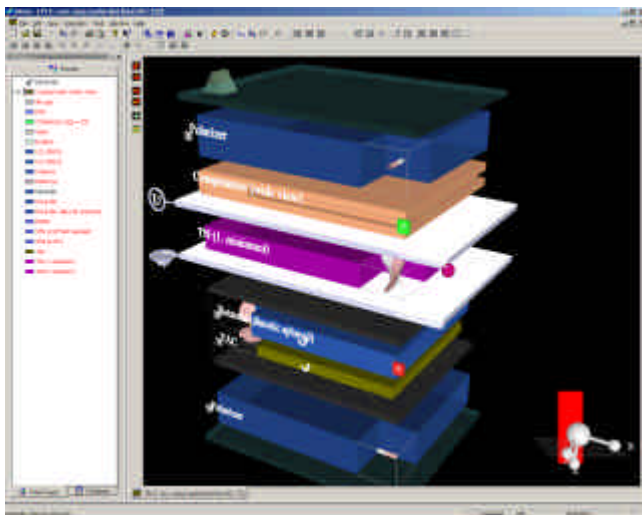

Figure 2: *Editor for the stack of layers contained in the model of a TN-cell with retarders (lower retarder shown exploded with a TAC-layer and a splayed discotic layer). Layers that are available for this session are listed in the left window and accessible there for transfer to the stack via drag and drop and for editing down to the material level. The stack can be viewed from any direction.*
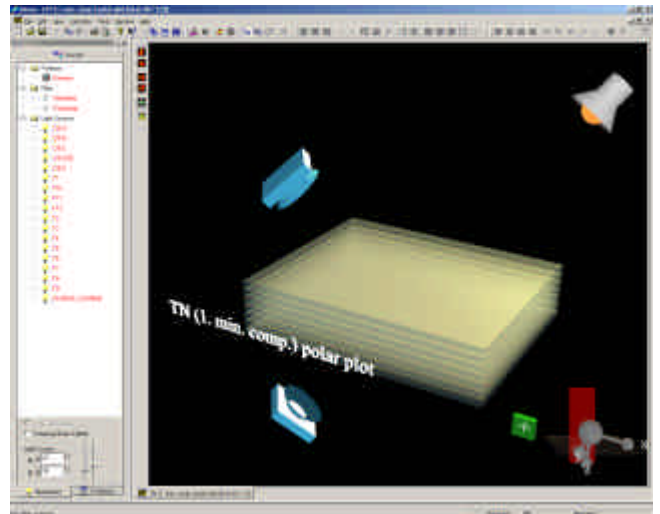

Figure 3: *Optical workbench with the collapsed stack of fig. 2 (TN-cell) together with a light source, a detector for light reflected from the stack of layers and a detector for the light transmitted trough the stack. The left window lists accessories available for the optical bench: polarizers and filters for the detectors and the source and standardized illuminants for the light source. Alternatively, a polarizing beamsplitter can be included in the optical workbench.*

3.3 Databases

All data related to simulation sessions (variations, settings), components (i.e. stacked layers) and materials are kept in databases. The same data is available for all DIMOS modules (i.e. 1, 2 and 3-dimensional version).

3.4 Assistants and helpers

For transformation of measured physical data into the target values for description of materials and layers in DIMOS (e.g. complex refractive indices for polarizers) *assistants* and *helper-*modules are provided as additional tools (e.g. polarizer assistant). The list of available assistants is currently being expanded.

3.5 Optimization

In many applications of DIMOS the task is to find optimum solutions for a special problem under a set of given restrictions. In order to evaluate the variation of the output quantity of interest with the selected parameter(s) the operator has to define appropriate variations of the parameters of the model. Evaluation of the *optimum condition* of the target quantity with *optimization loops* that can fit the results to predefined target functions and versatile parametric cost functions are in preparation.

3.6 2-dimensional modeling

2dimMOS is a module for calculating the electro-optical properties of LCDs in two spatial dimensions. Three elastic constants (k_{11}, k_{22}, k_{33}) and the natural pitch p_0 are taken into account for the sake of realistic modeling. The relaxation makes use of the rotational viscosity γ_1, so that the dynamics of the director configuration can be studied. Electrodes, dielectric layers and LC layers are defined by polygon lines of arbitrary shape. The coupling capacitance of all electrodes can be calculated at

arbitrary time levels. A voltage editor is included for the definition of various addressing schemes. Thus both static and stationary electro optical response as well as the dynamic behavior can be calculated. 2dimMOS provides access to the DIMOS-family database. Material data can be imported; samples of material properties along a vertical line through the model can be exported as a stack of layers (composite layer) for further processing (e.g. computation of the optical properties).

3.7 3-dimensional modeling

The introduction of an easy to handle module for 2-dimensional modeling triggered a demand for expansion of the modeling into 3 dimensions. The DIMOS family is currently being extended to include a 3dimMOS module based on a finite-element approach with relaxation into stable configurations of the LC-director.

The problems related to definition of the model geometry become more pronounced in the 3-dimensional case where a complex 3D geometry editor is required together with a postprocessor for definition of material properties, alignment parameters and initial director configurations. In 3-dimensional models the number of node variables describing elastic and electric energy of the system increases so much that computing power and storage capacities become severe issues.

When a equilibrium configuration is found it should be checked, if this is a globally stable solution before the respective optical properties are analyzed.

A numerical model in three dimensions alone does not solve any problem, it rather may cause problems when the model is too crude, e.g. geometry restricted to a shoe-box (brick)and when a finite difference method is used with coarse grid, because this is causing artifacts at the sharp edges of structures, especially however at the edges of electrodes.
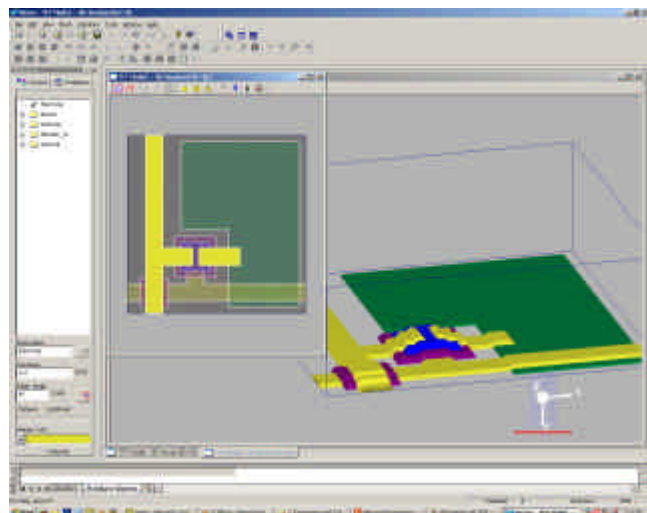

Figure 4: *Geometry editor of the 3dimMOS module. The small window shows the top-view on several layer-objects that are defined by polygone lines. These objects can be extruded and then positioned on top of each other according to the operators selection. A* morphing function *allows adaption of the shape of the layers as shown in the larger window and sharp edges can be beveled to make the geometry as realistic as possible.*
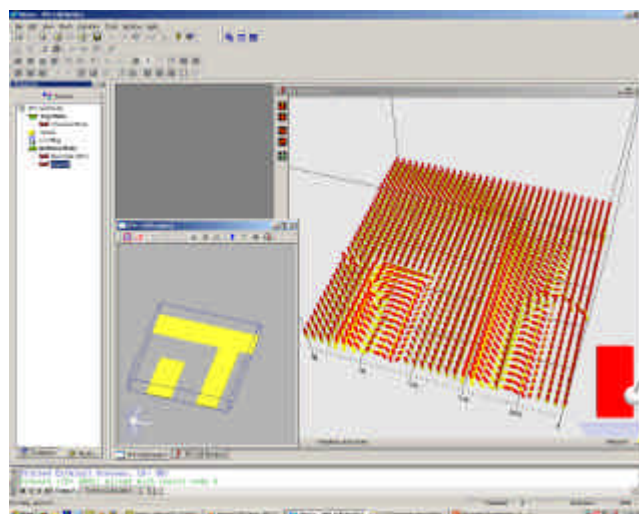

Figure 5: *Director field in a VA-cell. The small window in the lower left corner shows the shape of the electrodes and the large window shows the electric field induced director orientation.*

4 Conclusions

After 17 years of extensive application in the LCD-industry the numerical modules of DIMOS have recently been expanded to include realistic 3-dimensional modeling. DIMOS now provides all aspects required for fast and efficient analysis and optimization of LCDs: an intuitive graphical user interface, a database, assistants for data import and processing, the engines for computation of the director distribution and the optical properties.

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