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Detailing smectic SSFLC director profiles by half-leaky guided mode technique and genetic algorithm

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The genetic algorithm (GA), written to allow automatic analysis of optical reflectivity data obtained from liquid crystal cells using the half-leaky guided mode technique, has been developed to the point where liquid crystal cells can be analysed successfully giving greater detail of optical parameters and director profile than yielded by any other technique. The technique models the liquid crystal layer as a set of discrete, independent sub-layers which can map out the variation of the director through the thickness of the cell. Given sufficient high quality data, it is now possible automatically and accurately to fit the parameters of a complete liquid crystal cell. Using this highly adapted GA, half-leaky guided mode optical reflectivity data from the nematic, smectic A and smectic C* phases of SCE13 in a surface stabilized ferroelectric liquid crystal have been fitted to reveal director profiles and optical parameters of the cell in each phase.

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1. Introduction

The half-leaky guided mode (HLGM) technique was developed almost a decade ago [1, 2], but is still little used in the elucidation of the structures found within liquid crystal cells, a task for which it is ideally suited. The difficulty of the data fitting process and the lack of ability to prove the uniqueness of the results are the primary reasons for this. Were it not for these impediments, the technique could be widely used as a basic tool by LC workers.

HLGM was recently [3] combined with a genetic algorithm-based fitting routine with great success. This was a major step in making the HLGM technique viable as a uniquely powerful research tool to help answer questions over the details of director profiles within cells with complex mesophases and structures. However, since the LC layer was modelled as a single block with twist and tilt values linearly interpolated between pairs of values, the procedure as used was of limited utility.

The work presented here summarizes what has since been achieved by adding detail to the mapping of the director profile of the liquid crystal layer, from a starting point of modelling it as a single slab, to breaking it into a set of layers capable of following the variation of the director through the cell. This has allowed half-leaky guided mode optical reflectivity data from the nematic, smectic A and smectic C* phases of a typical surface stabilized ferroelectric liquid crystal (SSFLC) cell to be fitted.

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2. HLGM technique

Optical polarizing microscopy integrates the optical response through the entire thickness of the cell and so gives little detailed information about the structure within it. X-rays can only provide information about the layering within a cell. Even with their combined use, it is difficult to obtain any detailed information about the spatial variation of the director through the cell. Knowledge of this would give a much fuller picture of the structures assumed and the processes undergone inside the cell during switching. This information could then be used to predict cell behaviour. The half-leaky guided mode technique [1, 2] is a powerful probe that can give details of the way in which the director varies through the cell. The technique can be applied to any type of liquid crystal cell, or any material that can be contained within a waveguide structure.

Polarized laser light is used to probe the liquid crystal layer. As the angle of incidence is varied, there are a number of angles at which waveguide modes are excited.

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The reflected light is detected and each time a mode is excited, there is a dip in the reflectivity. The size, shape and position of the modes form a complex function related to the optical properties of the multilayer structure. By fitting the reflectivity trace to one generated theoretically by applying Fresnel's equations to multilayer optics, the parameters characterizing the multilayer structure can be estimated. Hitherto, this fitting process was primarily manual and extremely time consuming, with the need to find dozens of parameters simultaneously. Further, the final answer may be strongly prejudiced by the assumptions of the person fitting the data.

3. Genetic algorithms

Genetic algorithms (GAs) [3–8] are one of several general purpose stochastic search and optimization methods based on the principles of natural selection and natural genetics. Such algorithms navigate through the search space using a binary coded *population* of potential solutions. Population members, or solutions, which better describe the problem are given higher values of *fitness* and have a higher probability of proceeding to the next time step, or *generation*. Such methods are frequently superior to calculus-based 'hill-climber' type data fitting methods if the search space is large and highly complex. However, unlike many traditional methods, genetic algorithms require tailoring to the task at hand [9–12]. In order successfully to find fits to the reflectivity data from model tensor profiles of nematic cells much adaptation was made to a traditional GA as detailed in [3]. Due to the necessity to be able to prove that the answers found were the true solution, much of the initial development was undertaken on theoretically created data.

The adaptations included the use of multiple runs with *bound reduction*; approximate fitness evaluation; a variable mutation rate; pre-processing of the experimental data; the inclusion of a traditional direct fitting routine. These adaptations were made sequentially and serve to demonstrate the fact that such evolutionary approaches can rarely be successfully used in an off-the-shelf manner. The most important change was the inclusion of sequential bound reduction.

Usually in GAs the parameter bounds are decided upon and fixed for the duration of one long continuous optimization run. By contrast, an adapted GA, where the algorithm is run for only a few generations, but multiple times, is found to be far more efficient at approaching the solution. New bounds are then calculated from the statistical spread of values that each parameter settles upon in each short run. The algorithm is then re-initialized with these narrower bounds. This method takes advantage of the characteristic rapid optimization that occurs initially, without being slowed by the increasingly reduced rate of improvement as the number of generations increases. This method of multiple runs is found to be very robust (for this particular problem) in not excluding the actual parameter values from the bounds, which is found to be a problem when reducing bounds from the results of a single run.

4. Detailing the problem using theoretical smectic director profiles

In the work detailed in [3], modelling of a nematic phase was approximated by a single liquid crystal layer that had linearly interpolated twist and tilt values between the two pairs of fitted parameters (the values at the surfaces of the layer). Modelling of the smectic A phase is even simpler than the nematic phase if it is assumed that there is only a single value of twist and tilt through the cell (the rigid bookshelf structure). This can be easily implemented using the previous model for the nematic phase, by keeping the top and bottom surface twists and tilts equal.

To model the smectic C* phase requires a minimum of two liquid crystal layers to enable a description of the chevron structure [13]. When hand-fitting, two layers were initially used. Once a close fit had been obtained, the number of liquid crystal layers was then increased to four to allow for thin surface layers, then to six to allow for features around the chevron interface. Often the chevron would be assumed symmetrical about the centre of the layer thereby halving the complexity of the fitting (see figure 1). If particular liquid crystal profiles were expected, the number of liquid crystal layers would be increased in appropriate regions to attempt to obtain greater local detail of the profile.

In order to allow for much more complex structures with the smectic C* phase, a large step was taken in the automatic routine by expanding the number of layers within the LC to ten—each with its own pairs of values for starting and finishing twist and tilt and individual thicknesses. The adapted GA with bound reduction was seen to home in on the region of the solution relatively rapidly, but then struggle as it attempted to find the solution to any degree of accuracy.

Four data sets were used in the fitting process, consisting of two polarization combinations at each of two azimuthal cell orientations [3]. This combination removed all the major forms of degeneracy when fitting nematic cell data, but appeared insufficient when attempting to fit theoretical smectic C* data. The use of more data sets was investigated, but this provided minimal improvement in the final answers, whilst significantly slowing the fitting process. Therefore a series of adaptations to the basic technique were begun.

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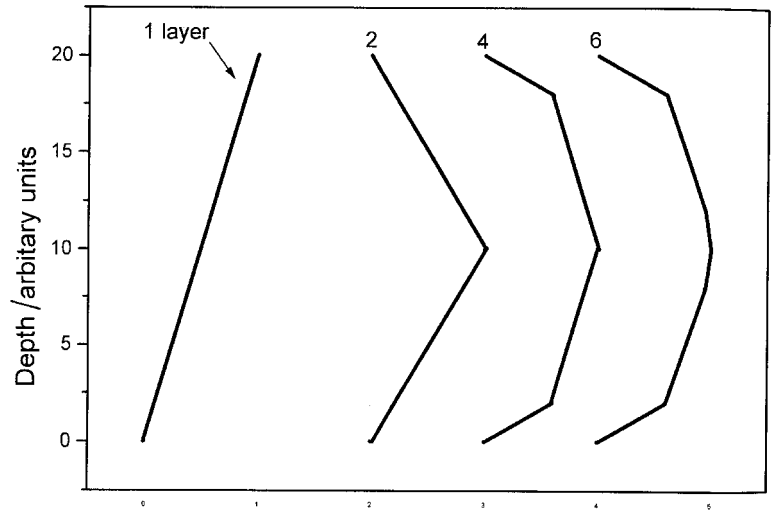

Figure 1. When hand-fitting a complex mesophase, the number of modelled layers into which the LC is broken is gradually increased to add more detail.

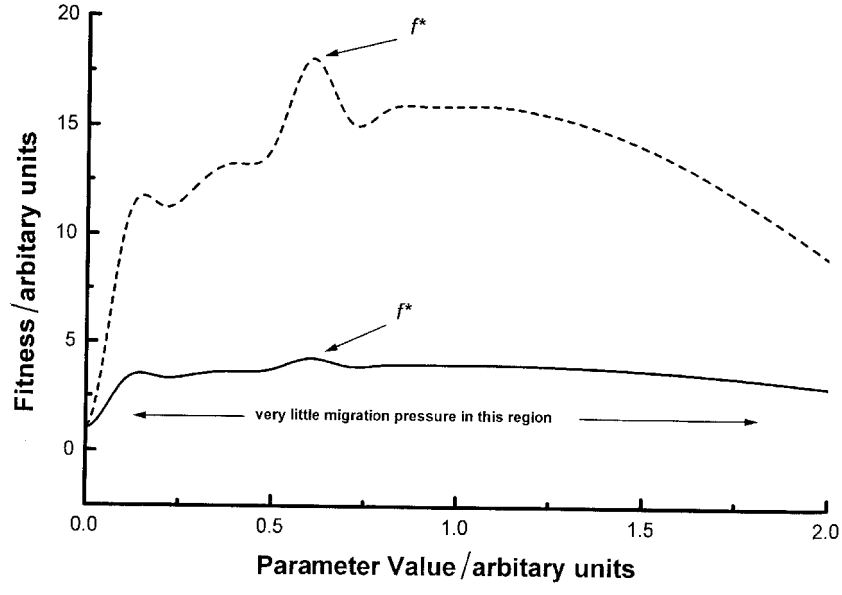

Figure 2. Representation of how the application of a scaling function to the hyperspace can help to overcome local optima. Here, scaling (applied to the solid line) has increased the ease of migration to the global optimum, f^* (by producing the dashed line).

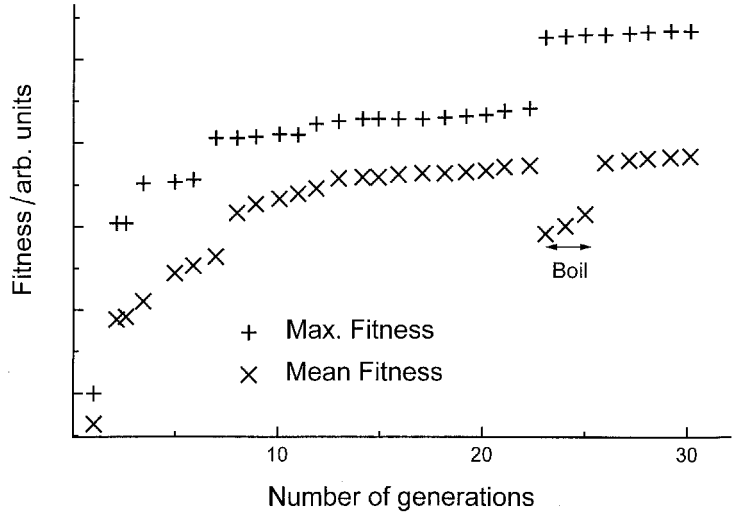

Figure 3. Typical effect of 'boiling' on the maximum and mean fitness of a population. The population is seen to progress via a series of discontinuities in fitness.

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4.1. *Approximate fitness function evaluation*

In order to increase the speed of generating a single estimate of the sum of squares (SOS) error between data and theory, a small sub-set of the data was used to reach an approximate answer quickly. A switch was then made to the full data set at the end of the routine to ensure final convergence. However, the fit tended to lock into a local minimum that was so deep that it never escaped even after the switch to the full data. Reducing the number of parameters, so that the ten liquid crystal layers all had an equal thickness, with separate block twist and tilt values for each layer, also had only a minimal effect on the final quality of the fit. On the assumption that there was still not enough information in the data to give unique solutions to the large number of parameters, the number of liquid crystal layers was reduced from ten to four. This on its own did little for the final quality of fit, suggesting that it may not be a simple problem of number of unknowns.

4.2. *Fitness function adaptation*

Since these approaches seemed to have little ability to improve the final fit, a different approach was adopted. The fitting to date had taken the SOS value created by the modelling program and used its reciprocal as the value of *fitness*. (The GA is usually presented as a maximization rather than a minimization routine; thus in our case $fitness = SOS^{-1}$.) Fits had suggested that the GA might be prematurely converging to the wrong answer and becoming stuck in a local optimum. This may have been due to the fact that SOS^{-1} rises extremely rapidly once SOS becomes less than 1. Instead, a linear function was used: $fitness = (A - SOS)$ if $SOS < A$, where A is a positive valued constant, or else $fitness = 0$. This should force slightly more rapid convergence near the start of the fitting process, but much slower convergence once the solution is approached. Analysis of plots of *fitness* against generation did indeed show a slower rate of convergence, and there was a visible difference between the final fitness and the quality of the fit to the director profile.

A qualitative picture of the hyperspace emerged as increasing amounts of model data were analysed. One possibility for the algorithm having difficulty in reaching the answer was that there was a broad local optimum near a dip adjacent to the true global optimum. In this case, the population would tend to converge onto the broad local feature (see figure 2). Despite being far better than calculus-based methods at overcoming local features, if they are extreme enough the GA will also suffer deception. It is possible to alter the former hyperspace by scaling the fitness function (figure 2). Raising the fitness function to a positive power (e.g. six) distorts the hyperspace such that the local optimum becomes less prominent compared with the global optimum to which the population now hopefully moves. Implementing this produced a slight improvement in the final quality of the fits obtained, but again these were still not perfect.

4.3. *Inclusion of a variable mutation rate*

Another way that potential premature convergence may be reduced is by 'boiling' the population for a few generations towards the end of each short GA run in order to increase temporarily the diversity of the population. This involves temporarily raising the mutation rate to a very high level. When this is done, the average fitness of the population is seen to drop sharply and then improve. In our implementation, each short GA run lasted for 30 generations and the population was 'boiled' for generations 23–25 inclusive, allowing five generations for things to settle down again (figure 3). Such an approach allows the solution vector to overcome local features in the landscape.

Figure 4 shows the percentage error for each parameter in the plot together with a comparison of the actual and fitted twist and tilt profiles. The list of

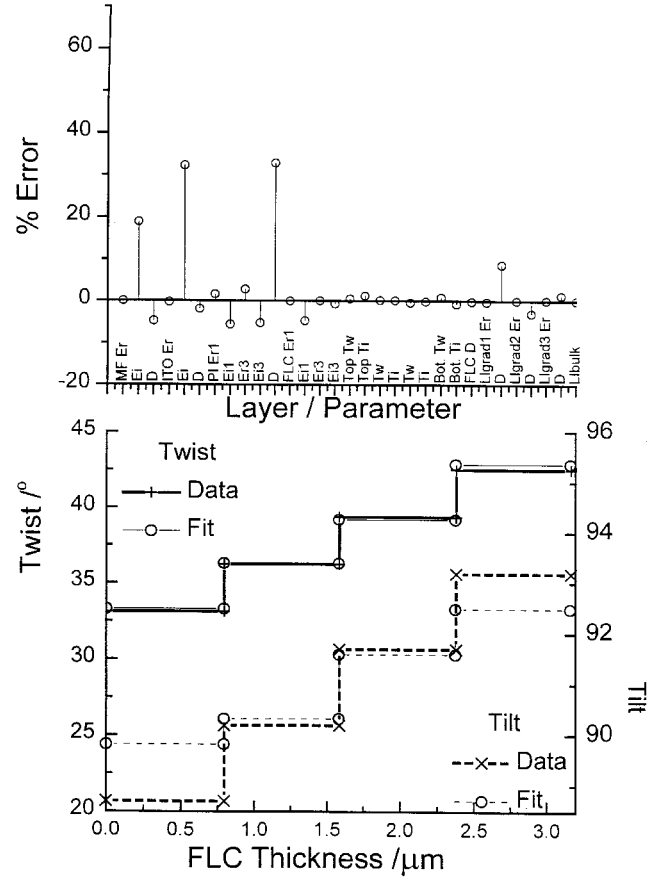

Figure 4. Parameter errors and director profile comparison for the very high quality fit obtained by chance (see the table for notation).

parameter values from the final fit is quoted together with estimated errors. A list of the actual parameters that were used to create the target experimental data is given in the table. However, the hyperspace is so complex that even then the final solution took considerable time (several hours) to locate on a fast PC.

4.4. *Pre-processing of the experimental data*

One possibility for improving the effectiveness with which such an algorithm navigates through the search space is that of a direct transformation of the experimental data prior to the formation of the SOS function, in such a way that gives more weight to the more important aspects of the data. In the case of data sets at two azimuthal angles, we had used ***fitness*** defined as:

$$fitness = [100 - (SOS_{\phi_1} + SOS_{\phi_2})]^6;\ SOS_{\phi_1} + SOS_{\phi_2} < 100$$

$$fitness = 0;\ SOS_{\phi_1} + SOS_{\phi_2} > 100$$

with

$$SOS = \sum_{\text{angles}} (\Delta R_{\text{pp}} + \Delta R_{\text{ps}})$$

where ϕ_1 and ϕ_2 are the two azimuthal angles at which the two data sets data R_{pp}, R_{ps} are taken;

$$\Delta R_{\text{ps}} = (R_{\text{ps}}^{\text{theory}} - R_{\text{ps}}^{\text{data}})^2$$

and

$$\Delta R_{\text{pp}} = (R_{\text{pp}}^{\text{theory}} - R_{\text{pp}}^{\text{data}})^2.$$

At every model data point, in each of the four experimental data sets, ΔR_{pp} or ΔR_{ps} is calculated. Additional tests with varying numbers of points in the half-leaky region show, as expected, this region to be critical. Thus it was decided to apply a function to the reflectivity values to emphasize the deviations between theory and data in this area.

Table. Comparison of real and fitted values for four LC layer data.

Layer (thickness, d in metres)	Parameter	Real value	Fitted value	±Error
Matching fluid	ε_{r}	2·9949	2·9954	4·256E-04
	ε_{i}	3·0E-06	3·56E-06	1·226E-07
	d	7·00E-04	6·66E-04	3·390E-05
ITO	ε_{r}	3·85	3·84	7·415E-03
	ε_{i}	0·01	1·32E-02	1·105E-03
	d	6·800E-08	6·67E-08	9·189E-10
Polyimide alignment	ε_{r1}	2·693	2·735	2·826E-02
	ε_{i1}	0·799E-3	7·542E-04	6·328E-05
	ε_{r3}	2·752	2·829	6·346E-02
	ε_{i3}	0·825E-3	7·817E-04	4·894E-05
	d	2·300E-08	3·055E-08	3·894E-09
Liquid crystal	ε_{r1}	2·198	2·1979	7·469E-05
	ε_{i1}	7·7E-4	7·33E-04	3·257E-05
	ε_{r3}	2·591	2·592	3·576E-03
	ε_{i3}	6·8E-4	6·75E-04	7·432E-05
Director profile Euler angles/°	top layer twist	33·10	33·28	0·288
	top layer tilt	88·70	89·82	0·630
	2nd layer twist	26·23	36·29	0·206
	2nd layer tilt	90·19	90·32	0·408
	3rd layer twist	39·37	39·20	0·465
	3rd layer tilt	91·69	91·59	1·074
	bottom layer twist	42·50	42·85	0·579
	bottom layer tilt	93·18	92·49	0·849
	d	7·925E-07	7·910E-07	1·546E-09
3 Layer index grading on the low index plate	ε_{r}	2·1700	2·1641	2·289E-03
	d	2·5E-07	2·716E-07	4·131E-08
	ε_{r}	2·1600	2·1601	1·536E-04
	d	3·0E-06	2·909E-06	5·700E-08
	ε_{r}	2·1440	2·1461	2·148E-03
	d	0·50E-06	5·064E-07	2·755E-08
Bulk low index plate	ε_{r}	2·1403	2·1405	1·054E-04

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Various functions were tried to weight heavily the half-leaky modes by emphasizing the differences between theory and data, creating a new error estimator, SOS'. Since, for p-polarized reflectivity data, R_{pp}, most features are near a reflectivity of 1, raising the R_{pp} data to a power greater than 1 pulls all the features further towards 0, enlarging the mode depths. Thus, any difference between the R_{pp}^{data} and R_{pp}^{theory} values is effectively increased. The leaky modes for R_{pp} data are reduced in importance by the same mechanism, being near 0 reflectivity.

The opposite approach is needed for the polarization-conversion data, R_{ps}. Being near 0, the modes need to be pulled upwards towards 1. Thus the scaling power needs to be <1 and >0 (figure 5). The following were finally used:

$$SOS' = \sum_{\text{angles}} (\Delta R'_{pp} + \Delta R'_{ps})$$

where

$$\Delta R'_{pp} = [(R_{pp}^{theory})^3 - (R_{pp}^{data})^3]^2$$

and

$$\Delta R'_{ps} = [(R_{ps}^{theory})^{1/3} - (R_{ps}^{data})^{1/3}]^2.$$

This scaling function worked well (figure 6). A higher scaling power was found to reduce the quality of the fit once again.

4.5. *Use of a final direct search routine*

GAs are noted for how quickly they manage to find the hills (speaking of maximizing fitnesses), but can take a disproportionate length of time actually to climb to the top (the global optimum). It was felt that once the fit has progressed to the quality of that shown in figure 6, then possibly a final direct search might be able to reach the optimum more quickly.

A simple direct search (DS) routine was written based on the method proposed by Jeeves and Hooke [14]. The direct search was unbounded and the single elite (fittest) member from the high quality GA fit was used as the starting point for the search. Initial step size was taken to be 0·25% of each parameter's value. The routine fulfilled the condition of finding the solution (step size reduction) after approximately 40 000 iterations. The fit to the director profile was better than the starting fit—the twist overlaid perfectly and the tilt followed the real

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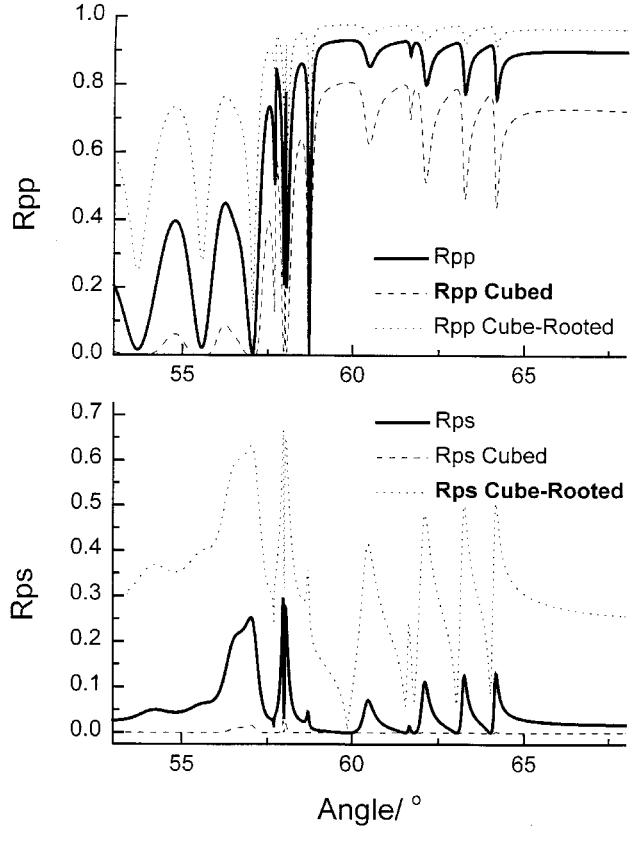

Figure 5. The effect of non-linear weighting on the reflectivity data.

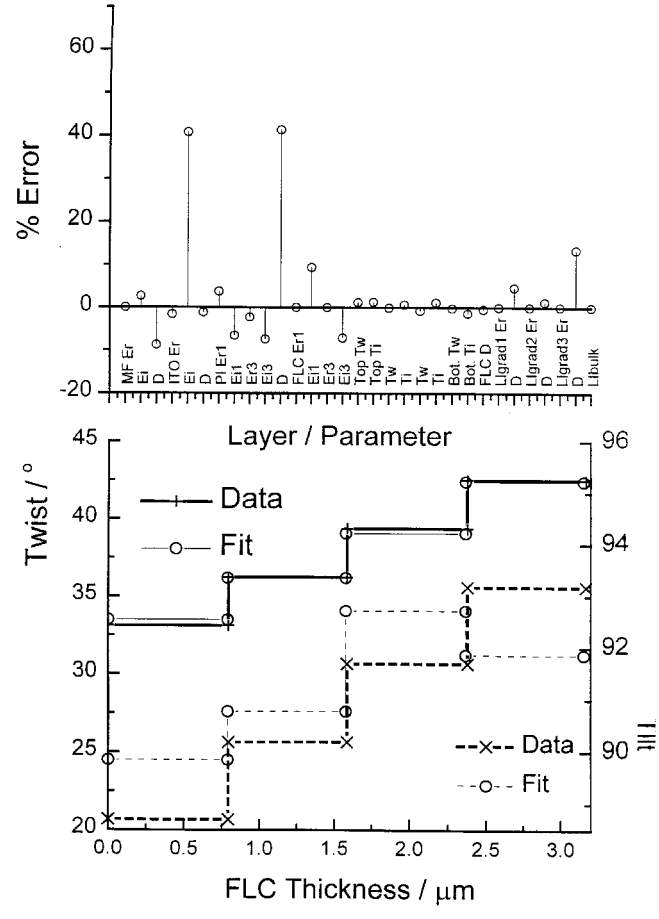

Figure 6. Parameter errors and director profile comparison for the fit obtained by using *fitness*[6] scaling and SOS'.

tilt very closely (figure 7). The complexity of the fitting model was then successfully increased from four to six block liquid crystal layers (see figure 8 for the fit and associated errors).

The final set of adaptations made to the GA to allow the fitting of theoretically produced smectic data can be summarized as:

(1) use of multiple, short runs;
(2) bound reduction based on result statistics;
(3) use of thinned data initially, then switching to the complete set;
(4) ensuring population diversity by making the mutation rate dynamic;
(5) functional changes to the least-squares error estimator;
(6) the inclusion of a simple direct search routine.

5. Results from fitting real smectic data

A cell was produced in a standard way apart from the use of glass plates of different refractive indices, required for the HLGM technique to work. The ITO coated plates had polymer spun coatings which were then rubbed and the cell was assembled using UV curing glue loaded with 3 μm spacer beads; the rubbing was parallel. It was filled with Merck liquid crystal SCE13. Under a microscope the cell at room temperature was found to consist of several large regions in the C1U and C2U states.

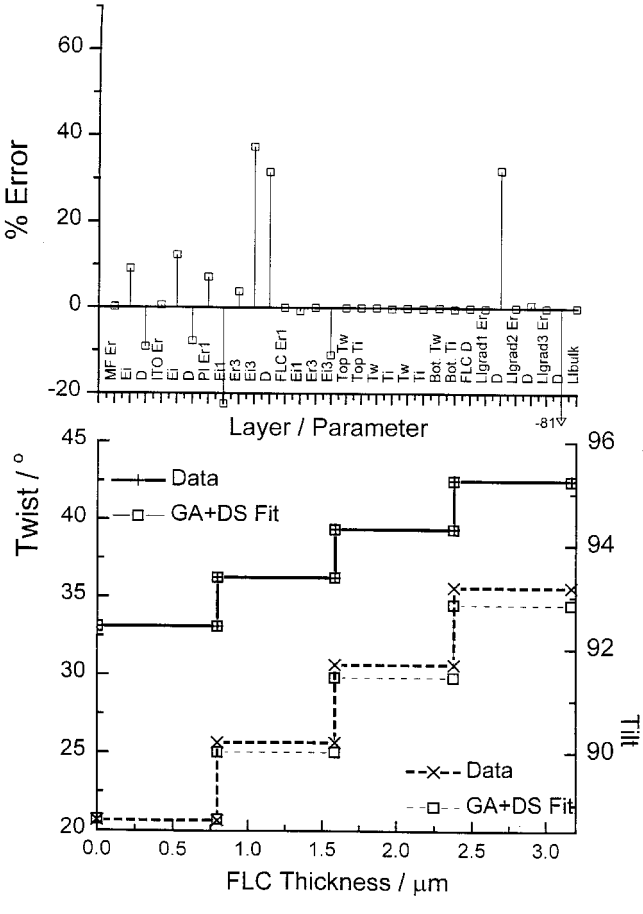

Figure 7. Parameter errors and director profile comparison for the fit obtained by using a direct search (DS) at the end of the genetic algorithm (GA) search.

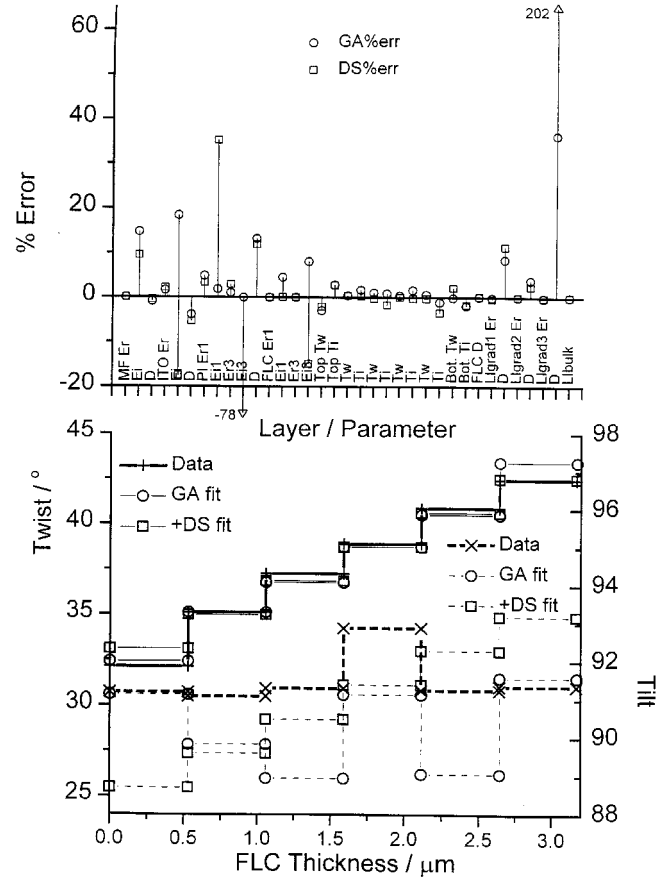

Figure 8. Parameter errors and director profile comparison for the fit obtained by repeating the use of a combination of genetic algorithm and direct search fitting six layer data with a six layer model.

Some nematic phase data had previously [3] been fitted using a single layer approximation to the liquid crystal with the earlier GA program. This approximation was now removed with the liquid crystal being represented by six layers; this is quite a severe test of the modelling. Fortunately, the twist profile compares very favourably with the previous GA fit to the data. As can be seen from figure 9, both the GA and GA + DS fits agree well with the earlier GA fit, with the GA + DS fit showing closest approximation to a smooth linear variation of twist between the two surfaces.

When previously fitting data from the smectic A phase, a perfect bookshelf had always been assumed. It proved interesting to allow a much higher degree of freedom to

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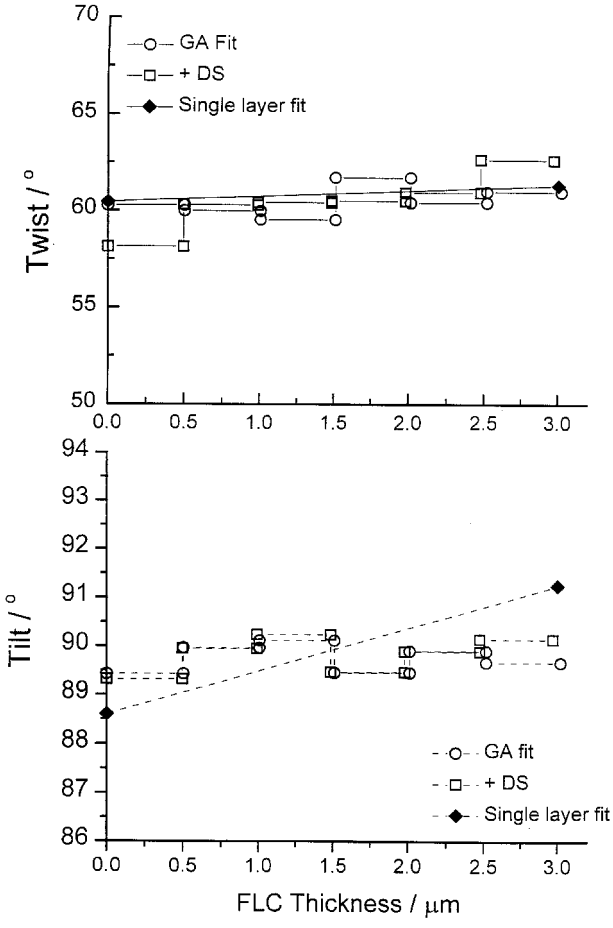

Figure 9. Genetic algorithm and subsequent direct search liquid crystal profiles found by fitting experimental data from the nematic phase data, with comparison with an earlier single layer fit to the same data.

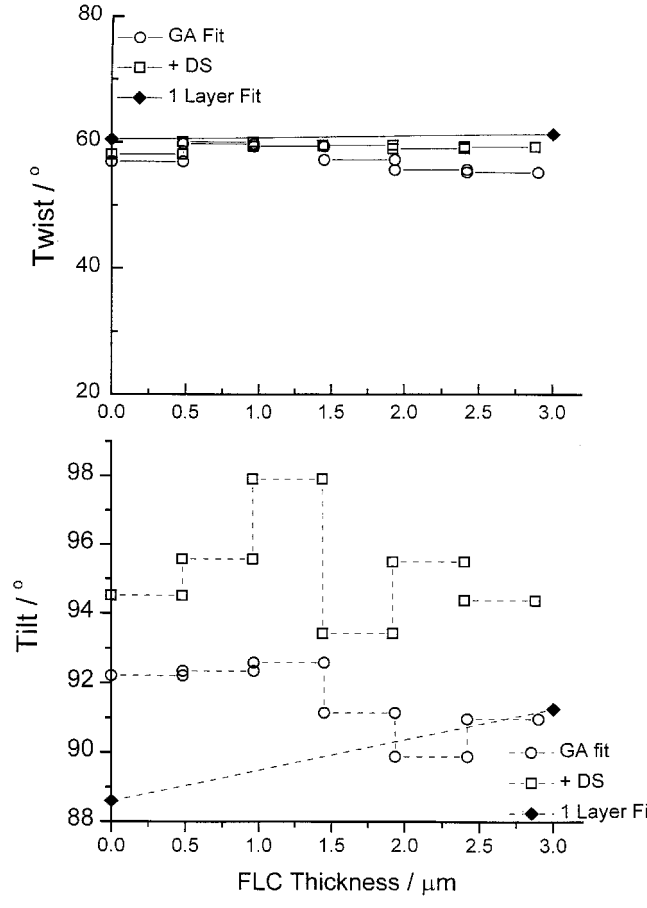

Figure 10. Parameters from fitting to real smectic A phase data, with comparison of single and multilayer approximations.

the fitting and explore what the fit suggests the structure to be. Figure 10 shows the results. Both the GA and the GA + DS produce twist profiles very close to straight lines, as predicted by theory. One might also anticipate that the tilt should also be a fixed value, but neither fit shows this. Either the cell does not behave according to simple theory or the fits are not close enough to the real solution to evaluate accurately any tilt values. The latter would appear to be the more likely answer, especially considering that the final SOS' value is four times that of the final nematic fit.

For the smectic C* phase data the director profiles from the final GA and GA + DS fits are shown in figure 11. The quality of the fit is very high, as shown in figure 12, with only a couple of minor deviations near some mode peaks. The values for all the surface layer parameters are again very similar to those obtained from the fits to the previous cell. The small change in director profile between the final GA and final DS answers suggests that the correct solution has been adapted. If the mid-point of the blocks are joined by a smooth curve, it is possible to visualize the smooth director profile of the cell (see figure 13). The high quality of the data taken at several azimuthal angles, the high quality fit and the fact that a chevron formed in the twist profile, together with associated smooth variation in tilt profile, all suggest that the final fit is very close to the actual liquid crystal director profile.

6. Conclusions

One of the most striking conclusions is the immense complexity and variability of the search space hyperspace for HLGM data. Whilst giving definite indications of correct values for some parameters, the hyperspace efficiently conceals the values of others. There is little information available to guide an automatic routine to the solution. In this situation, the only way to locate the optimum is by chance. This highly adapted GA, efficiently closes in on the solution giving approximate answers, then relies on mutation alone to perform the final random search. The accuracy to which parameters can be specified is high, being no worse than 50% for

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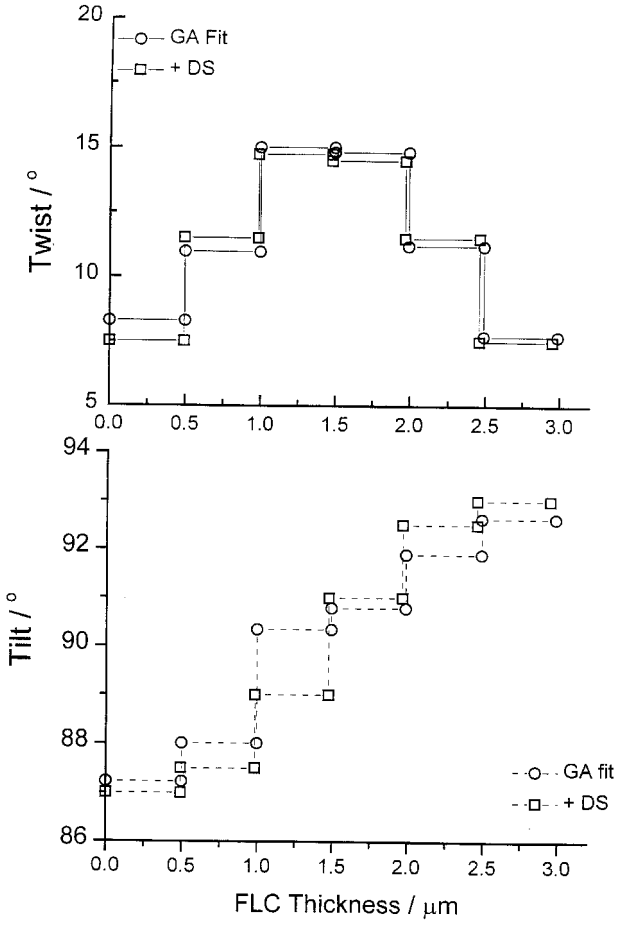

Figure 11. Fit to experimental smectic C* phase data.

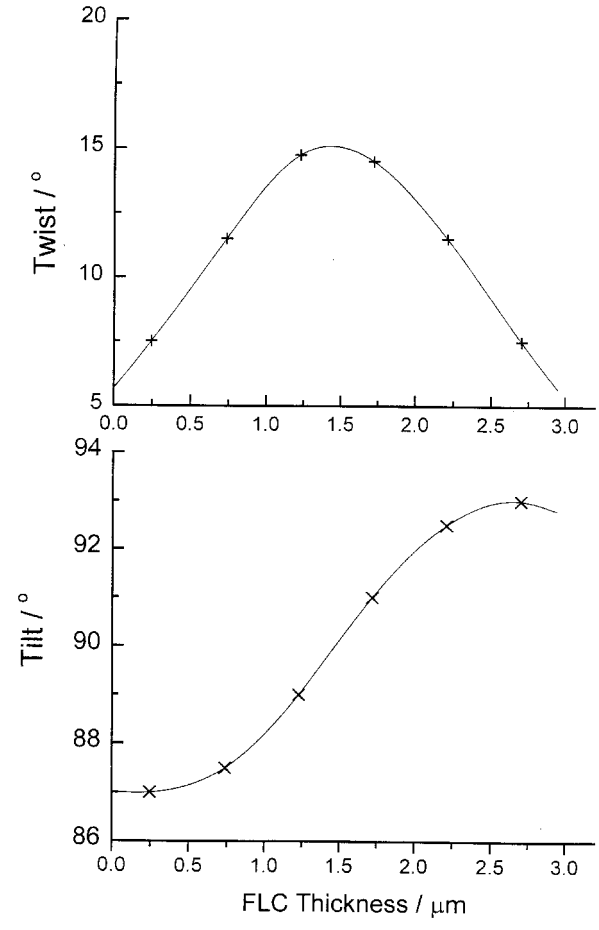

Figure 13. Smooth, spline interpolation of the six block layer fit to real smectic C* phase data.

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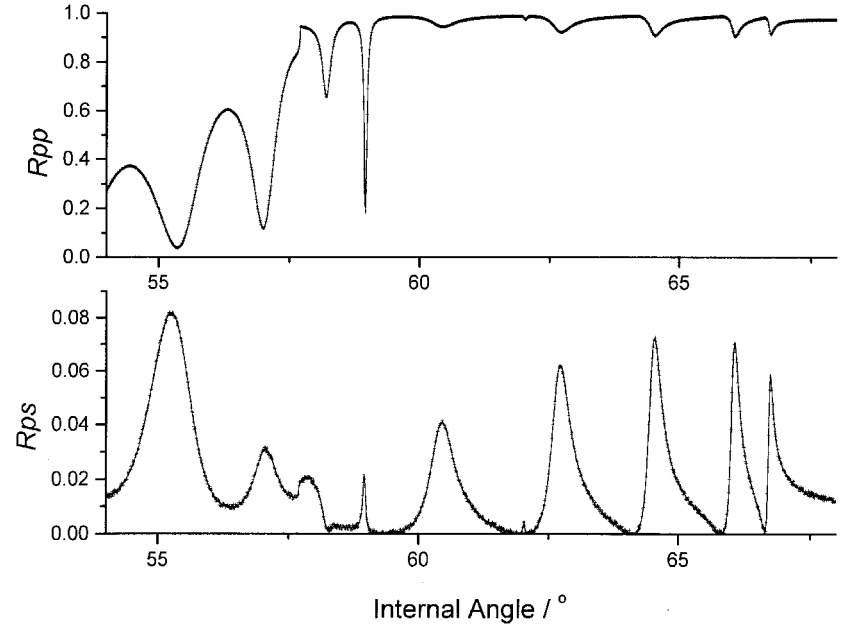

Figure 12. Fit (line) to experimental smectic C* data (at 21°C) (+).

even imaginary permittivities of thin surface layers and is typically within 1% for the liquid crystal parameters. This level of accuracy is surprising considering the small effect that some of the layers of the cell have on the reflected light.

Complete liquid crystal cells can be analysed successfully with HLGM to give greater detail of optical parameters and director profile than any other technique. It has continued to be apparent that the final quality of fit is intimately linked to both the quality of the data and features present (though not necessarily clearly visible) therein. Of course, here the investigation has almost exclusively been based on no-assumption fitting, which is the most difficult of procedures. Incorporating a simple theoretical model would help the routine lock into an answer; however it would only provide the closest solution that the model is able to predict about the true structure.

The modelling code could probably be extended to 10 layers with the advanced methods now in place in the GA and still produce high quality solutions for most of the parameters. Importantly, the twist would still be found to high accuracy, whilst the tilt may be rather poor. Theoretically linking the tilt to the twist in some manner might well solve this problem.

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7. Summary

For the first time the fitting of smectic C* phase HLGM data has been performed without the use of many assumptions, always previously necessary due to the number of parameters involved in a complete cell with the liquid crystal in such a phase.

The ability to obtain automatically high quality fits where all the parameters are found to relatively high accuracy, especially those of the liquid crystal, has been shown. However, automation is not complete in that the final fits and fit qualities (SOS') must still be analysed to permit deduction of the likely accuracy of some parameters. Given sufficient data of high enough quality, with an adequate number of features that are sufficiently influenced by the structure and optical parameters of the cell, it is now possible automatically to fit all the parameters for complete liquid crystal cells to a high accuracy.

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